



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:45 PM UTC

PDB ID : 4A51 / pdb_00004a51
Title : Crystal structure of human kinesin Eg5 in complex with 1-(3-(((2-Aminoethyl)thio)diphenylmethyl)phenyl)ethanone hydrochloride
Authors : Kaan, H.Y.K.; Kozielski, F.
Deposited on : 2011-10-24
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

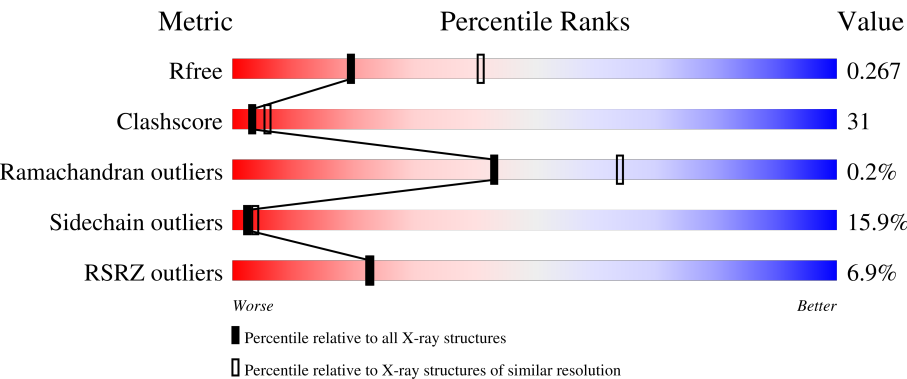
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	
1	C	368	
1	D	368	
1	E	368	

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Mol	Chain	Length	Quality of chain
1	F	368	
1	G	368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DQ8	E	801	-	-	X	-

2 Entry composition [i](#)

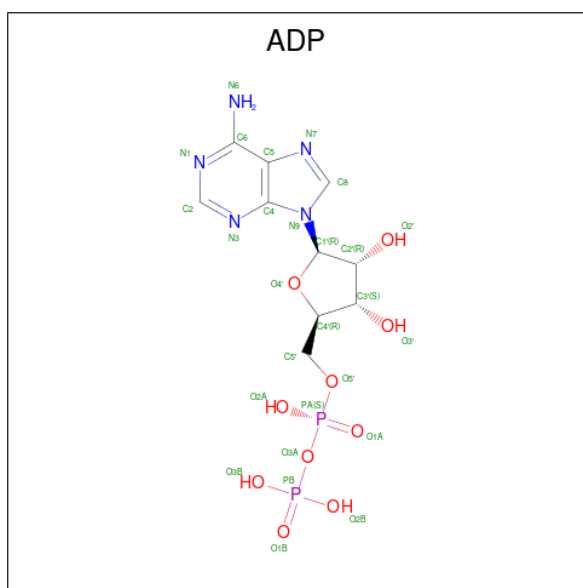
There are 7 unique types of molecules in this entry. The entry contains 18210 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2522	1586	438	488	10			
1	B	324	Total	C	N	O	S	0	1	0
			2552	1602	446	494	10			
1	C	325	Total	C	N	O	S	0	1	0
			2551	1599	445	497	10			
1	D	322	Total	C	N	O	S	0	1	0
			2526	1585	438	493	10			
1	E	321	Total	C	N	O	S	0	0	0
			2504	1573	435	486	10			
1	F	319	Total	C	N	O	S	0	1	0
			2487	1559	433	486	9			
1	G	318	Total	C	N	O	S	0	0	0
			2446	1537	428	472	9			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

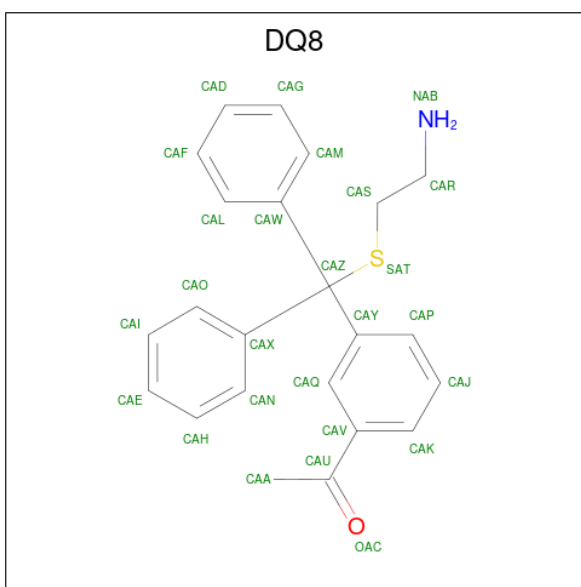


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1-(3-[[[(2-aminoethyl)sulfanyl](diphenyl)methyl]phenyl]ethanone (CCD ID: DQ8) (formula: C₂₃H₂₃NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	B	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	C	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	D	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	E	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	F	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	G	1	Total	C	N	O	S	0	0
			26	23	1	1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

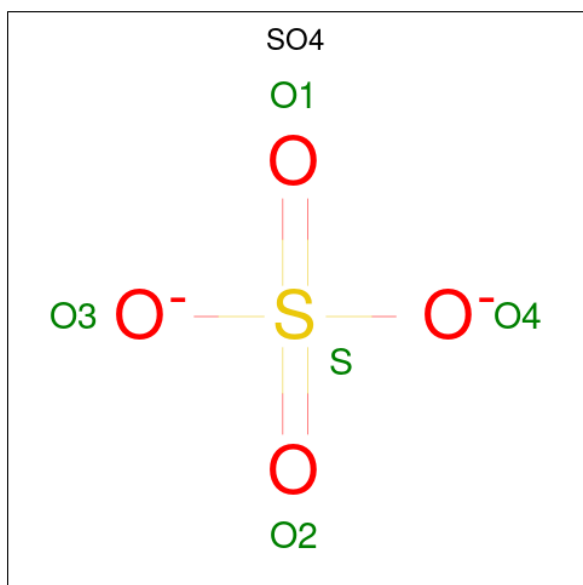
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	B	2	Total	Cl	0	0
			2	2		
5	C	3	Total	Cl	0	0
			3	3		
5	D	2	Total	Cl	0	0
			2	2		
5	E	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	34	Total	O	0	0
			34	34		
7	C	47	Total	O	0	0
			47	47		
7	D	46	Total	O	0	0
			46	46		
7	E	22	Total	O	0	0
			22	22		
7	F	25	Total	O	0	0
			25	25		

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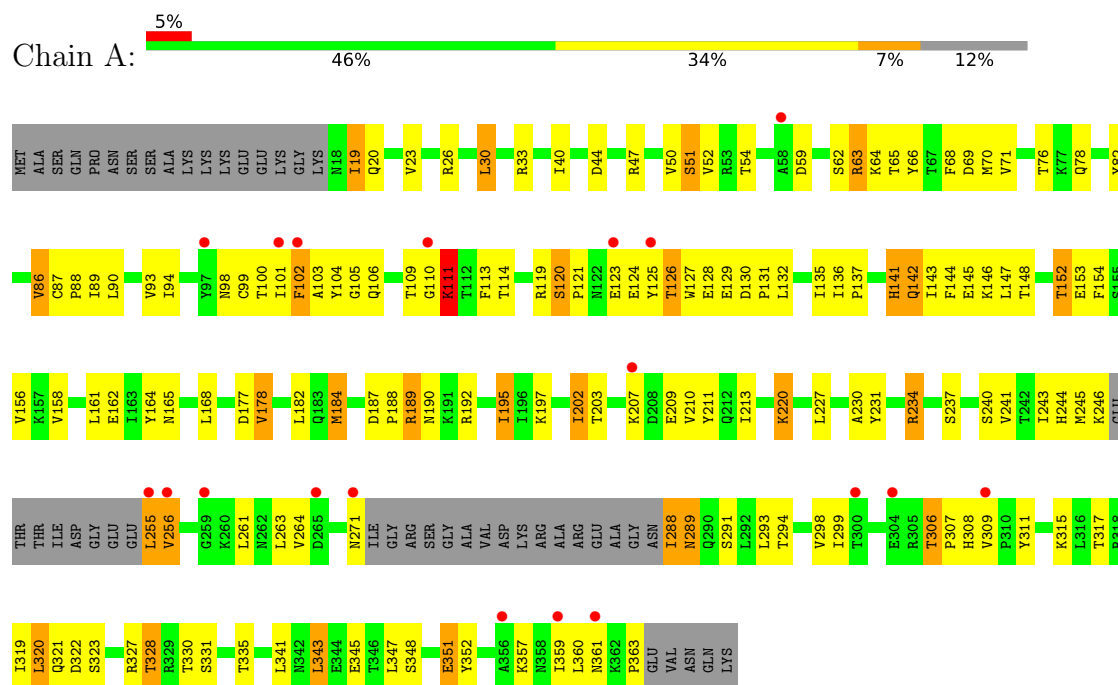
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	19	Total	O	0	0
			19	19		

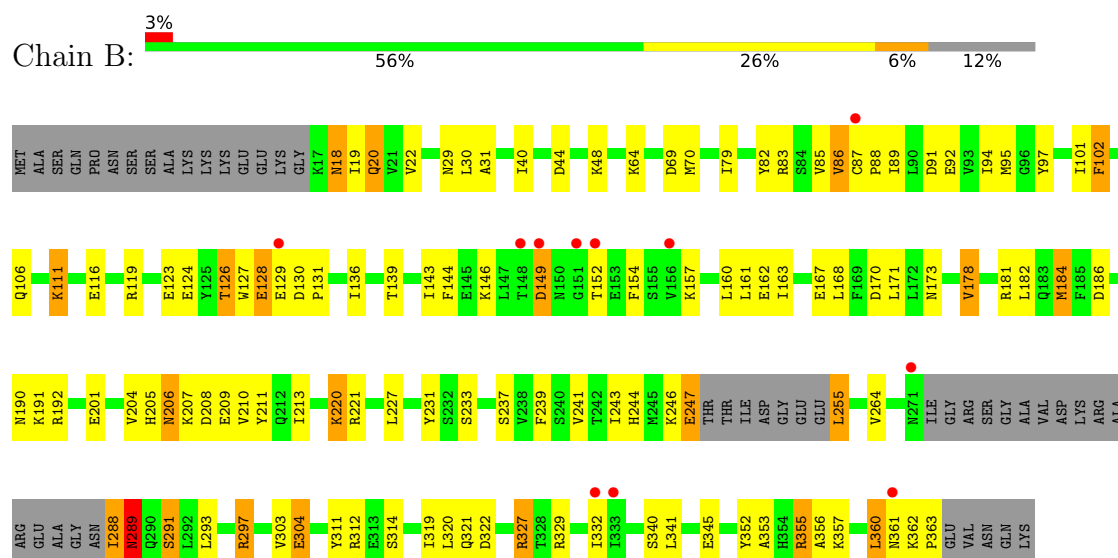
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11



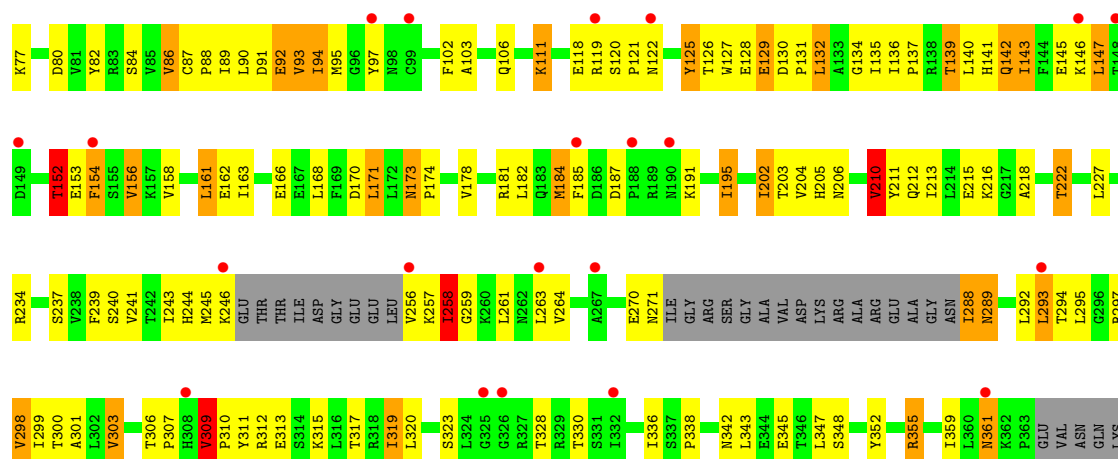
[illegible]

Chain D:

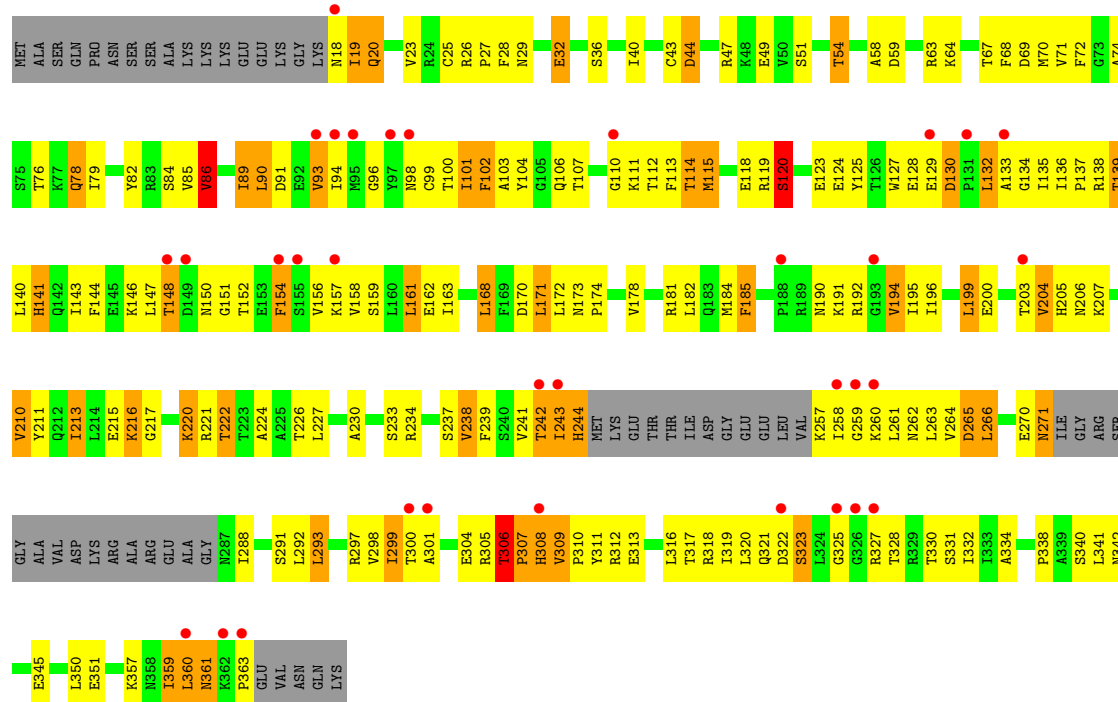
4% 52% 31% 12%

Residue	Type
K357	Polar
N358	Other
I359	Non-polar
L360	Non-polar
N361	Non-polar
LYS	Polar
PRO	Non-polar
PRO	Non-polar
GLU	Polar
GLU	Polar
VAL	Non-polar
ASN	Polar
GLN	Polar
LYS	Polar
K257	Polar
I258	Non-polar
L261	Non-polar
N262	Non-polar
L263	Non-polar
A267	Non-polar
N271	Non-polar
IIE	Other
GLY	Polar
ARG	Polar
SER	Polar
GLY	Polar
ALA	Non-polar
VAL	Non-polar
ASP	Charged
LYS	Polar
ARG	Polar
ALA	Non-polar
ARG	Polar
GLU	Polar
GLY	Polar
GLY	Polar
ASN	Polar
I288	Non-polar
S291	Non-polar
L292	Non-polar
L293	Non-polar
R297	Non-polar
V298	Non-polar
I299	Non-polar
V303	Non-polar
T306	Non-polar
P307	Non-polar
H308	Polar
V309	Non-polar
P310	Non-polar
Y311	Polar
R312	Non-polar
I319	Non-polar
L320	Non-polar
Q321	Polar
D322	Non-polar
G325	Polar
S337	Non-polar
L341	Non-polar
E351	Polar
H354	Polar
L161	Non-polar
E162	Non-polar
I163	Non-polar
E167	Non-polar
L168	Non-polar
L171	Non-polar
L182	Non-polar
Q183	Polar
M184	Non-polar
F185	Polar
D186	Non-polar
N190	Non-polar
K191	Polar
K192	Polar
I196	Non-polar
K197	Polar
N206	Non-polar
K207	Polar
V210	Non-polar
Y211	Polar
Q212	Polar
T213	Polar
L214	Non-polar
K220	Non-polar
R221	Non-polar
L227	Non-polar
H228	Polar
N229	Non-polar
A230	Non-polar
Y231	Polar
S232	Non-polar
H236	Polar
S237	Non-polar
S240	Non-polar
I243	Non-polar
H244	Polar
M245	Non-polar
K246	Polar
E247	Polar
THR	Other
THR	Other
IIE	Other
ASP	Charged
GLY	Polar
GLU	Polar
E254	Polar
L255	Non-polar
V256	Non-polar
H86	Polar
C87	Non-polar
P88	Non-polar
T89	Polar
L90	Non-polar
D91	Non-polar
E92	Polar
V93	Non-polar
I94	Non-polar
M95	Polar
G96	Non-polar
Y97	Polar
N98	Non-polar
C99	Non-polar
F102	Non-polar
G108	Polar
T109	Non-polar
G110	Polar
K111	Polar
M115	Non-polar
R119	Non-polar
S120	Non-polar
P121	Non-polar
N122	Polar
E123	Polar
E124	Polar
Y125	Polar
T126	Polar
W127	Non-polar
E128	Polar
E129	Polar
D130	Non-polar
P131	Non-polar
G134	Polar
T135	Polar
I136	Non-polar
P137	Non-polar
R138	Non-polar
T139	Non-polar
L140	Non-polar
H141	Polar
Q142	Polar
I143	Non-polar
K146	Polar
L147	Non-polar
T148	Non-polar
G151	Polar
T152	Polar
V158	Non-polar
S159	Non-polar
L160	Non-polar
MET	Other
ALA	Non-polar
SER	Polar
GLN	Polar
PRO	Non-polar
ASN	Polar
LYS	Polar
ALA	Non-polar
LYS	Polar
LYS	Polar
GLY	Polar
N18	Non-polar
I19	Non-polar
V22	Non-polar
C25	Non-polar
R26	Non-polar
P27	Non-polar
L30	Non-polar
A31	Non-polar
E32	Polar
R33	Polar
K34	Polar
A35	Non-polar
S36	Non-polar
I40	Non-polar
D44	Non-polar
S51	Polar
V52	Polar
R53	Polar
T54	Non-polar
G55	Non-polar
G56	Non-polar
K64	Polar
T65	Non-polar
V66	Non-polar
T67	Polar
M70	Non-polar
V71	Non-polar
A74	Non-polar
K77	Polar
Q78	Polar
L79	Non-polar
S82	Non-polar

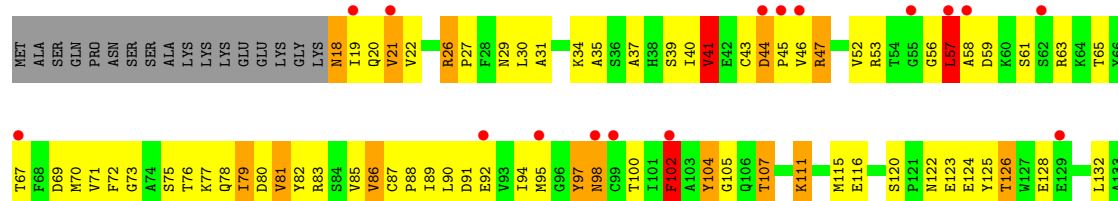
Chain E:

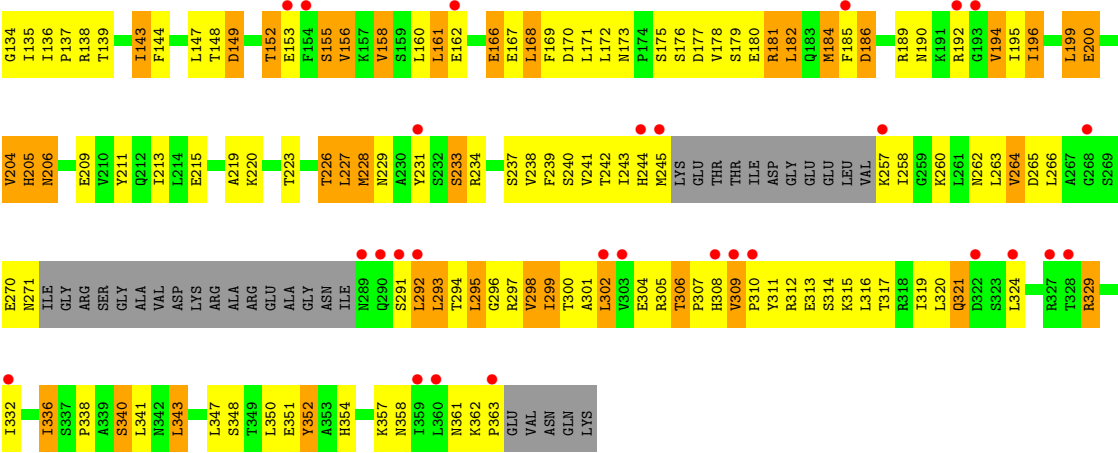


- Molecule 1: KINESIN-LIKE PROTEIN KIF11



- Molecule 1: KINESIN-LIKE PROTEIN KIF11





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.84Å 156.40Å 170.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.75 29.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.99-2.75) 97.3 (29.99-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.280 0.210 , 0.267	Depositor DCC
R_{free} test set	4939 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18210	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SO4, MG, CL, DQ8

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.85	0/2563	1.22	11/3467 (0.3%)
1	B	0.84	1/2593 (0.0%)	1.14	9/3505 (0.3%)
1	C	0.85	0/2589	1.21	23/3503 (0.7%)
1	D	0.84	0/2566	1.14	8/3471 (0.2%)
1	E	0.68	0/2542	1.09	17/3440 (0.5%)
1	F	0.72	0/2527	1.19	19/3421 (0.6%)
1	G	0.67	0/2483	1.13	17/3364 (0.5%)
All	All	0.78	1/17863 (0.0%)	1.16	104/24171 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	ILE	CA-CB	-6.24	1.50	1.54

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	210	VAL	N-CA-C	9.27	119.81	110.82
1	A	105	GLY	N-CA-C	8.89	121.54	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	N-CA-C	8.72	120.51	111.00
1	C	190	ASN	N-CA-C	-8.64	92.40	110.80
1	E	93	VAL	N-CA-C	-8.30	102.33	110.72
1	A	26	ARG	CA-C-N	8.07	128.10	119.78
1	A	26	ARG	C-N-CA	8.07	128.10	119.78
1	B	86	VAL	N-CA-C	7.88	119.59	111.00
1	C	86	VAL	N-CA-C	7.83	119.54	111.00
1	F	120	SER	CA-C-N	7.82	129.62	119.84
1	F	120	SER	C-N-CA	7.82	129.62	119.84
1	B	124	GLU	N-CA-C	7.64	120.58	111.33
1	B	241	VAL	CB-CA-C	-7.62	100.60	111.19
1	E	173	ASN	CA-C-N	7.61	127.26	119.19
1	E	173	ASN	C-N-CA	7.61	127.26	119.19
1	D	123	GLU	N-CA-C	7.50	122.14	112.92
1	F	86	VAL	N-CA-C	7.49	119.17	111.00
1	A	102	PHE	N-CA-C	7.30	121.38	109.85
1	E	152	THR	CB-CA-C	-7.25	106.19	116.34
1	F	306	THR	CA-C-N	7.15	128.78	119.84
1	F	306	THR	C-N-CA	7.15	128.78	119.84
1	G	156	VAL	N-CA-C	7.12	118.38	107.78
1	B	44	ASP	CA-C-N	7.11	126.63	119.24
1	B	44	ASP	C-N-CA	7.11	126.63	119.24
1	C	337	SER	CA-C-N	7.04	127.19	119.87
1	C	337	SER	C-N-CA	7.04	127.19	119.87
1	C	85	VAL	N-CA-C	7.02	117.63	110.82
1	C	26	ARG	CA-C-N	-7.02	113.47	120.98
1	C	26	ARG	C-N-CA	-7.02	113.47	120.98
1	C	102	PHE	N-CA-C	7.02	120.94	109.85
1	G	26	ARG	CA-C-N	-6.95	111.16	119.84
1	G	26	ARG	C-N-CA	-6.95	111.16	119.84
1	C	129	GLU	N-CA-C	6.83	121.33	112.92
1	C	306	THR	CA-C-N	6.80	126.04	118.97
1	C	306	THR	C-N-CA	6.80	126.04	118.97
1	B	206	ASN	CA-C-N	-6.71	112.83	122.77
1	B	206	ASN	C-N-CA	-6.71	112.83	122.77
1	A	110	GLY	N-CA-C	6.66	125.37	115.64
1	D	86	VAL	N-CA-C	6.64	117.43	110.72
1	E	258	ILE	CB-CA-C	-6.41	101.60	110.96
1	F	102	PHE	N-CA-C	6.32	119.88	108.69
1	C	54	THR	N-CA-C	6.30	121.12	113.38
1	G	102	PHE	N-CA-C	6.15	119.27	108.75
1	G	120	SER	CA-C-N	6.14	126.15	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	120	SER	C-N-CA	6.14	126.15	119.89
1	A	101	ILE	CB-CA-C	-6.12	103.44	110.73
1	C	117	GLY	N-CA-C	-6.12	103.86	111.70
1	F	360	LEU	N-CA-C	6.11	117.17	108.74
1	G	85	VAL	N-CA-C	6.08	117.63	111.00
1	E	156	VAL	N-CA-C	5.98	116.54	108.17
1	F	44	ASP	CA-C-N	5.95	125.66	119.05
1	F	44	ASP	C-N-CA	5.95	125.66	119.05
1	C	191	LYS	N-CA-C	5.93	121.25	113.30
1	E	289	ASN	N-CA-C	5.93	120.64	113.17
1	G	126	THR	N-CA-C	-5.92	103.12	110.41
1	G	57	LEU	N-CA-C	5.90	125.47	113.20
1	E	143	ILE	N-CA-C	-5.88	105.63	112.98
1	G	152	THR	N-CA-C	5.82	118.88	109.86
1	F	99	CYS	N-CA-C	5.77	118.86	109.06
1	G	97	TYR	N-CA-C	-5.72	98.61	110.80
1	B	289	ASN	N-CA-C	-5.67	106.03	113.17
1	G	41	VAL	N-CA-C	5.65	116.42	108.17
1	C	233	SER	N-CA-C	5.63	119.32	112.23
1	F	101	ILE	CB-CA-C	-5.62	102.46	110.83
1	G	95	MET	N-CA-C	-5.57	106.26	113.16
1	A	347	LEU	N-CA-C	-5.56	105.30	111.36
1	E	19	ILE	N-CA-C	5.54	116.20	108.89
1	E	309	VAL	CA-C-N	-5.53	116.06	121.65
1	E	309	VAL	C-N-CA	-5.53	116.06	121.65
1	D	126	THR	N-CA-C	-5.51	103.25	110.53
1	C	126	THR	N-CA-C	-5.50	102.77	110.35
1	F	54	THR	N-CA-C	5.47	120.11	113.38
1	F	185	PHE	N-CA-C	5.46	118.34	109.06
1	C	44	ASP	CA-C-N	5.46	125.54	119.32
1	C	44	ASP	C-N-CA	5.46	125.54	119.32
1	G	309	VAL	N-CA-C	5.45	120.64	108.88
1	E	135	ILE	N-CA-C	5.44	116.82	110.62
1	F	78	GLN	N-CA-C	5.44	117.29	111.36
1	E	152	THR	N-CA-C	5.42	116.02	108.00
1	G	65	THR	N-CA-C	5.40	117.98	108.75
1	G	295	LEU	N-CA-C	-5.38	105.45	112.23
1	F	84	SER	N-CA-C	5.32	116.76	110.97
1	A	202	ILE	CB-CA-C	-5.31	104.25	111.15
1	E	122	ASN	CB-CA-C	-5.31	108.91	116.34
1	C	40	ILE	N-CA-C	5.30	117.99	112.90
1	F	266	LEU	N-CA-C	5.26	117.61	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	129	GLU	N-CA-C	5.24	118.84	112.23
1	D	44	ASP	CA-C-N	5.24	124.86	119.05
1	D	44	ASP	C-N-CA	5.24	124.86	119.05
1	B	85	VAL	N-CA-C	5.22	115.89	110.82
1	D	210	VAL	N-CA-C	5.21	115.48	110.74
1	F	342	ASN	N-CA-C	5.19	119.31	112.92
1	F	233	SER	N-CA-C	5.18	117.83	111.82
1	A	111	LYS	N-CA-C	5.16	117.64	111.71
1	E	54	THR	N-CA-C	5.14	119.65	113.17
1	C	178	VAL	CB-CA-C	-5.14	104.55	112.05
1	C	344	GLU	N-CA-C	5.13	116.87	111.28
1	A	76	THR	CB-CA-C	-5.13	102.78	110.16
1	D	354	HIS	N-CA-C	5.12	117.53	111.33
1	G	63	ARG	N-CA-C	5.08	117.52	109.50
1	C	207	LYS	N-CA-C	-5.07	106.92	113.01
1	F	130	ASP	N-CA-C	-5.04	102.31	109.62
1	D	97	TYR	N-CA-C	5.02	117.62	109.79
1	C	289	ASN	N-CA-C	5.00	119.48	113.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLU	Peptide
1	C	189	ARG	Peptide
1	F	304	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2522	0	2550	146	0
1	B	2552	0	2584	87	0
1	C	2551	0	2563	127	0
1	D	2526	0	2539	95	0
1	E	2504	0	2520	146	0
1	F	2487	0	2494	233	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2446	0	2442	243	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	4	0
2	D	27	0	12	5	0
2	E	27	0	12	5	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	26	0	23	7	0
4	B	26	0	23	8	0
4	C	26	0	23	2	0
4	D	26	0	23	4	0
4	E	26	0	23	9	0
4	F	26	0	23	7	0
4	G	26	0	23	7	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	D	5	0	0	0	0
7	A	32	0	0	2	0
7	B	34	0	0	0	0
7	C	47	0	0	2	0
7	D	46	0	0	2	0
7	E	22	0	0	1	0
7	F	25	0	0	1	0
7	G	19	0	0	0	0
All	All	18210	0	17937	1104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:TYR:CE2	1:E:86:VAL:HG21	1.82	1.12
1:F:89:ILE:HD12	1:F:101:ILE:HD11	1.23	1.12
1:A:141:HIS:O	1:A:207:LYS:NZ	1.83	1.11
1:F:136:ILE:HD13	1:F:263:LEU:HD12	1.29	1.09
1:F:171:LEU:HD12	1:F:220:LYS:HB3	1.34	1.09
1:E:215:GLU:HA	4:E:801:DQ8:HAH	1.31	1.08
1:C:206:ASN:ND2	1:C:208:ASP:HB2	1.69	1.06
1:G:181:ARG:HG2	1:G:181:ARG:HH11	1.15	1.05
2:F:601:ADP:H5'1	2:F:601:ADP:H8	1.19	1.05
2:D:601:ADP:H5'1	2:D:601:ADP:H8	1.19	1.05
1:E:92:GLU:OE1	1:E:92:GLU:N	1.88	1.04
1:F:86:VAL:HA	1:F:89:ILE:HD13	1.42	1.02
1:F:89:ILE:CD1	1:F:101:ILE:HD11	1.92	1.00
1:A:144:PHE:CD2	1:A:207:LYS:HD2	1.97	1.00
1:D:31:ALA:O	1:D:34:LYS:HG3	1.62	0.98
1:A:192:ARG:NH1	1:A:322:ASP:OD1	1.96	0.98
1:G:82:TYR:CE1	1:G:86:VAL:HG21	1.98	0.98
1:D:255:LEU:HD12	1:D:256:VAL:H	1.26	0.97
1:A:144:PHE:HD2	1:A:207:LYS:HD2	1.28	0.97
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.46	0.96
1:E:306:THR:HG22	1:E:307:PRO:HD2	1.45	0.96
1:G:160:LEU:H	1:G:172:LEU:HD12	1.30	0.96
1:G:155:SER:OG	1:G:244:HIS:HB2	1.66	0.95
1:A:145:GLU:H	1:A:207:LYS:HZ3	1.02	0.94
1:F:306:THR:HG22	1:F:307:PRO:HD2	1.50	0.94
1:C:306:THR:HG23	1:C:307:PRO:HD2	1.47	0.93
1:G:40:ILE:CD1	1:G:340:SER:HA	1.98	0.92
1:A:51:SER:HB2	1:A:65:THR:OG1	1.68	0.92
1:G:56:GLY:C	1:G:58:ALA:HB3	1.92	0.92
2:D:601:ADP:H5'1	2:D:601:ADP:C8	2.03	0.92
2:F:601:ADP:H5'1	2:F:601:ADP:C8	2.04	0.92
1:A:306:THR:OG1	1:A:307:PRO:HD2	1.70	0.91
1:C:33:ARG:HD2	1:G:228:MET:HE1	1.51	0.91
1:G:196:ILE:HD11	1:G:199:LEU:HB2	1.51	0.90
1:G:205:HIS:O	1:G:206:ASN:ND2	2.04	0.89
1:F:172:LEU:HD23	1:F:216:LYS:HZ1	1.33	0.89
1:A:63:ARG:HH11	1:A:63:ARG:CG	1.86	0.89
1:A:264:VAL:HG21	1:A:320:LEU:HD11	1.56	0.87
1:D:102:PHE:CE1	1:D:320:LEU:HD13	2.09	0.87
1:G:181:ARG:HH11	1:G:181:ARG:CG	1.88	0.86
1:C:126:THR:HG23	1:C:129:GLU:HG2	1.57	0.86
1:B:162:GLU:OE1	1:B:231:TYR:OH	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ILE:HG22	1:F:263:LEU:HD13	1.56	0.86
1:F:136:ILE:HD12	1:F:239:PHE:CD2	2.11	0.85
1:G:262:ASN:HD22	1:G:320:LEU:HD22	1.42	0.84
1:D:152:THR:OG1	1:D:246:LYS:O	1.95	0.84
1:E:161:LEU:HD12	1:E:161:LEU:C	2.02	0.84
1:E:215:GLU:CA	4:E:801:DQ8:HAH	2.08	0.84
1:F:215:GLU:HA	4:F:801:DQ8:HAH	1.58	0.84
1:F:94:ILE:HD11	1:F:147:LEU:HD21	1.60	0.84
1:E:82:TYR:CZ	1:E:86:VAL:HG21	2.13	0.83
1:F:230:ALA:HB3	1:F:234:ARG:HD2	1.61	0.83
1:F:82:TYR:O	1:F:86:VAL:HG13	1.78	0.83
1:A:63:ARG:HH11	1:A:63:ARG:HG2	1.44	0.82
1:F:156:VAL:HG13	1:F:204:VAL:HG13	1.61	0.82
2:C:601:ADP:H5'1	2:C:601:ADP:H8	1.44	0.82
1:A:144:PHE:HE1	1:A:156:VAL:HG11	1.45	0.81
1:F:323:SER:O	1:F:330:THR:OG1	1.98	0.81
1:C:356:ALA:O	1:C:359:ILE:HG12	1.80	0.81
1:G:244:HIS:HA	1:G:258:ILE:HG23	1.61	0.81
1:A:102:PHE:HB3	1:A:264:VAL:HB	1.60	0.81
1:F:158:VAL:HG21	1:F:213:ILE:HD11	1.63	0.81
1:C:206:ASN:HD22	1:C:208:ASP:HB2	1.45	0.81
1:D:87:CYS:HB2	1:D:88:PRO:HD3	1.63	0.80
1:F:136:ILE:HD13	1:F:263:LEU:CD1	2.11	0.80
1:D:299:ILE:HG23	1:D:359:ILE:HD11	1.63	0.80
1:F:158:VAL:HB	1:F:239:PHE:HE1	1.46	0.80
1:E:102:PHE:HB3	1:E:264:VAL:HB	1.62	0.80
1:F:170:ASP:HB2	1:F:182:LEU:HD11	1.64	0.80
1:B:160:LEU:HD13	1:B:239:PHE:HD2	1.46	0.80
1:C:207:LYS:HZ1	1:G:123:GLU:HG2	1.47	0.79
1:E:300:THR:HG23	1:E:355:ARG:HH12	1.48	0.79
1:F:115:MET:O	1:F:136:ILE:HG12	1.81	0.79
1:F:322:ASP:O	1:F:328:THR:HG22	1.82	0.79
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.65	0.79
1:E:43:CYS:HB3	1:E:71:VAL:CG1	2.13	0.79
1:E:90:LEU:HD11	1:E:143:ILE:HD11	1.63	0.79
1:D:255:LEU:HD12	1:D:256:VAL:N	1.98	0.79
1:G:181:ARG:HG2	1:G:181:ARG:NH1	1.91	0.79
1:B:355:ARG:HB2	1:B:355:ARG:NH1	1.97	0.78
1:F:136:ILE:HB	1:F:137:PRO:HD3	1.63	0.78
1:G:228:MET:HA	1:G:228:MET:HE2	1.63	0.78
1:G:82:TYR:CD1	1:G:86:VAL:HG21	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:VAL:HA	1:F:89:ILE:CD1	2.13	0.77
1:F:98:ASN:O	1:F:328:THR:OG1	1.99	0.77
1:G:262:ASN:HD22	1:G:320:LEU:CD2	1.97	0.77
1:E:306:THR:CG2	1:E:307:PRO:HD2	2.14	0.77
1:G:40:ILE:HD11	1:G:340:SER:HA	1.66	0.77
1:G:347:LEU:HD12	1:G:348:SER:H	1.50	0.77
1:D:88:PRO:O	1:D:92:GLU:HG3	1.84	0.77
1:G:244:HIS:O	1:G:245:MET:HG3	1.85	0.77
1:E:86:VAL:CG2	1:E:87:CYS:N	2.48	0.77
1:G:156:VAL:HG12	1:G:204:VAL:O	1.85	0.76
1:G:312:ARG:O	1:G:313:GLU:HG2	1.84	0.76
1:C:119:ARG:HD3	1:C:211:TYR:OH	1.85	0.76
1:F:90:LEU:HD11	1:F:143:ILE:CD1	2.15	0.76
1:G:196:ILE:CD1	1:G:199:LEU:HB2	2.15	0.76
1:D:64:LYS:HE2	1:D:66:TYR:OH	1.86	0.76
1:A:162:GLU:OE1	1:A:231:TYR:OH	2.04	0.76
1:F:49:GLU:HG2	1:F:67:THR:HG22	1.68	0.76
1:D:190:ASN:OD1	1:D:192:ARG:N	2.19	0.75
1:E:156:VAL:HG23	1:E:204:VAL:HB	1.68	0.75
1:G:311:TYR:CG	1:G:321:GLN:HG3	2.21	0.75
1:F:100:THR:HG22	1:F:262:ASN:HB2	1.66	0.75
1:E:218:ALA:O	1:E:222:THR:HG23	1.87	0.75
2:C:601:ADP:H5'1	2:C:601:ADP:C8	2.20	0.75
1:B:247:GLU:N	1:B:247:GLU:OE1	2.20	0.75
1:D:102:PHE:CZ	1:D:320:LEU:HD13	2.20	0.75
1:D:120:SER:HB3	1:D:121:PRO:HD2	1.67	0.75
1:F:270:GLU:HG2	1:F:271:ASN:OD1	1.86	0.75
1:G:41:VAL:CG1	1:G:338:PRO:HA	2.15	0.75
1:G:184:MET:SD	1:G:194:VAL:HG11	2.27	0.75
1:F:43:CYS:HB3	1:F:71:VAL:CG1	2.18	0.74
1:G:177:ASP:H	1:G:180:GLU:HG3	1.50	0.74
1:F:306:THR:CG2	1:F:307:PRO:HD2	2.17	0.74
1:B:178:VAL:HG13	1:B:220:LYS:HG2	1.69	0.74
1:G:90:LEU:HD11	1:G:143:ILE:HD11	1.70	0.74
1:A:66:TYR:HE2	1:A:351:GLU:OE1	1.70	0.74
1:B:355:ARG:HB2	1:B:355:ARG:HH11	1.52	0.74
1:C:207:LYS:NZ	1:G:123:GLU:HG2	2.03	0.74
1:F:323:SER:HA	1:F:328:THR:CG2	2.17	0.74
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.70	0.74
5:D:1363:CL:CL	7:D:2037:HOH:O	2.43	0.74
1:B:92:GLU:OE2	1:B:329:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ASP:CG	1:E:173:ASN:HB2	2.13	0.73
1:G:56:GLY:O	1:G:58:ALA:HB3	1.88	0.73
1:G:312:ARG:HG2	1:G:313:GLU:H	1.52	0.73
1:A:255:LEU:HD12	1:A:256:VAL:N	2.04	0.73
1:G:170:ASP:OD2	1:G:200:GLU:HB2	1.88	0.73
1:F:19:ILE:HG23	1:F:359:ILE:O	1.89	0.73
1:G:162:GLU:HG3	1:G:171:LEU:HD13	1.70	0.73
1:A:59:ASP:C	1:A:59:ASP:OD1	2.30	0.73
1:G:347:LEU:HD12	1:G:348:SER:N	2.04	0.73
1:A:152:THR:HG22	1:A:153:GLU:H	1.54	0.72
1:B:157:LYS:NZ	1:B:201:GLU:OE1	2.18	0.72
1:D:26:ARG:HG3	1:D:26:ARG:HH11	1.55	0.72
1:G:104:TYR:HB2	1:G:266:LEU:HD12	1.71	0.72
1:G:26:ARG:NH1	1:G:29:ASN:HD22	1.87	0.72
1:F:141:HIS:C	1:F:141:HIS:HD1	1.97	0.72
1:A:294:THR:HG22	1:A:317:THR:HG21	1.71	0.72
1:A:142:GLN:OE1	1:A:146:LYS:NZ	2.22	0.72
1:G:161:LEU:C	1:G:161:LEU:HD12	2.15	0.72
1:A:99:CYS:O	1:A:261:LEU:HD12	1.90	0.72
1:D:247:GLU:HG3	1:D:255:LEU:O	1.90	0.72
1:E:299:ILE:O	1:E:303:VAL:HG23	1.89	0.72
1:F:148:THR:O	1:F:151:GLY:N	2.21	0.71
1:G:270:GLU:HG2	1:G:271:ASN:H	1.56	0.71
1:A:255:LEU:HD12	1:A:256:VAL:H	1.53	0.71
1:B:102:PHE:CE1	1:B:332:ILE:HG12	2.26	0.71
1:F:78:GLN:HG2	1:F:133:ALA:O	1.89	0.71
1:F:310:PRO:HB3	1:F:313:GLU:OE2	1.90	0.71
1:B:178:VAL:CG1	1:B:220:LYS:HG2	2.20	0.71
1:C:186:ASP:OD1	7:C:2030:HOH:O	2.08	0.71
1:G:270:GLU:OE1	1:G:270:GLU:N	2.22	0.71
1:C:186:ASP:OD2	1:C:312:ARG:NH2	2.23	0.71
1:A:144:PHE:CE1	1:A:156:VAL:HG11	2.25	0.71
1:D:54:THR:HG21	1:D:64:LYS:HG3	1.73	0.71
1:B:247:GLU:OE1	1:B:255:LEU:O	2.09	0.71
1:F:90:LEU:HD11	1:F:143:ILE:HD13	1.70	0.71
1:F:157:LYS:HG3	1:F:242:THR:HG23	1.73	0.71
1:C:126:THR:OG1	1:C:128:GLU:OE1	2.09	0.70
1:E:92:GLU:O	1:E:97:TYR:HB2	1.91	0.70
1:B:160:LEU:HD13	1:B:239:PHE:CD2	2.25	0.70
1:F:323:SER:HA	1:F:328:THR:HG23	1.72	0.70
2:D:601:ADP:H8	2:D:601:ADP:C5'	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ALA:HB1	1:F:111:LYS:HG2	1.74	0.70
1:B:192:ARG:HB2	1:B:321:GLN:CD	2.17	0.70
1:C:270:GLU:HG2	1:C:271:ASN:N	2.07	0.70
1:D:163:ILE:HG12	1:D:168:LEU:HD12	1.72	0.70
2:C:601:ADP:H8	2:C:601:ADP:C5'	2.04	0.70
1:A:145:GLU:N	1:A:207:LYS:HZ3	1.85	0.69
1:F:90:LEU:O	1:F:93:VAL:HG13	1.92	0.69
1:B:18:ASN:OD1	1:B:18:ASN:N	2.25	0.69
1:E:139:THR:O	1:E:143:ILE:HG12	1.92	0.69
1:F:136:ILE:CD1	1:F:263:LEU:HD12	2.17	0.69
1:G:362:LYS:HB3	1:G:363:PRO:HD2	1.73	0.69
1:G:152:THR:OG1	1:G:153:GLU:N	2.24	0.69
1:E:82:TYR:HA	1:E:86:VAL:HG13	1.74	0.69
1:F:90:LEU:O	1:F:90:LEU:HD12	1.92	0.69
1:A:141:HIS:O	1:A:207:LYS:CE	2.40	0.69
1:F:98:ASN:OD1	1:F:260:LYS:HB3	1.92	0.69
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.74	0.69
1:C:302:LEU:HB3	1:C:359:ILE:HG22	1.75	0.69
1:G:192:ARG:O	1:G:321:GLN:NE2	2.25	0.68
1:D:247:GLU:OE1	1:D:255:LEU:HB3	1.93	0.68
1:E:161:LEU:HD12	1:E:161:LEU:O	1.93	0.68
1:F:244:HIS:CD2	1:F:258:ILE:HG22	2.29	0.68
1:F:144:PHE:CE2	1:F:207:LYS:N	2.62	0.68
1:F:161:LEU:C	1:F:161:LEU:HD12	2.19	0.68
1:A:184:MET:HE1	1:A:319:ILE:HG13	1.75	0.68
1:C:361:ASN:O	1:C:363:PRO:HD3	1.93	0.68
1:F:82:TYR:HA	1:F:86:VAL:CG1	2.24	0.68
1:C:362:LYS:H	1:C:362:LYS:HD3	1.59	0.68
1:C:362:LYS:HD3	1:C:362:LYS:N	2.08	0.68
1:F:238:VAL:O	1:F:238:VAL:HG22	1.94	0.68
4:B:801:DQ8:HAO	4:B:801:DQ8:HAS2	1.75	0.67
1:E:86:VAL:HG22	1:E:87:CYS:N	2.09	0.67
2:E:601:ADP:C5'	2:E:601:ADP:H8	2.07	0.67
1:G:134:GLY:O	1:G:137:PRO:HD2	1.94	0.67
1:G:228:MET:O	1:G:229:ASN:CG	2.36	0.67
1:G:315:LYS:O	1:G:319:ILE:HD12	1.94	0.67
1:A:330:THR:HG22	1:A:331:SER:N	2.08	0.67
1:B:361:ASN:O	1:B:363:PRO:HD3	1.94	0.67
1:D:30:LEU:HD12	1:D:33:ARG:NH2	2.09	0.67
1:G:105:GLY:O	1:G:111:LYS:HE3	1.94	0.67
1:G:160:LEU:N	1:G:172:LEU:HD12	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:THR:CG2	1:C:307:PRO:HD2	2.20	0.67
1:G:111:LYS:NZ	2:G:601:ADP:O2B	2.28	0.67
1:G:295:LEU:O	1:G:298:VAL:HG12	1.95	0.67
1:E:82:TYR:CZ	1:E:86:VAL:CG2	2.78	0.67
1:E:147:LEU:HD21	1:E:245:MET:SD	2.34	0.67
1:G:111:LYS:NZ	1:G:111:LYS:HB2	2.10	0.67
1:A:62:SER:O	1:A:63:ARG:HG2	1.94	0.67
1:A:141:HIS:C	1:A:141:HIS:HD1	2.03	0.67
1:D:311:TYR:CD1	1:D:321:GLN:HG3	2.29	0.67
1:E:246:LYS:HA	1:E:256:VAL:HA	1.77	0.67
1:A:66:TYR:CE2	1:A:351:GLU:OE1	2.48	0.66
1:C:29:ASN:O	1:C:33:ARG:HG3	1.95	0.66
1:G:40:ILE:O	1:G:40:ILE:HG22	1.95	0.66
1:A:82:TYR:CD1	1:A:86:VAL:HB	2.30	0.66
1:C:54:THR:HG21	1:C:64:LYS:HG3	1.75	0.66
1:F:211:TYR:O	1:F:211:TYR:CD1	2.48	0.66
4:B:801:DQ8:HAS2	4:B:801:DQ8:CAO	2.26	0.66
1:G:170:ASP:CG	1:G:173:ASN:HB2	2.21	0.66
1:G:298:VAL:HG23	1:G:310:PRO:HB3	1.77	0.66
1:C:360:LEU:HD12	1:C:360:LEU:H	1.61	0.66
1:E:82:TYR:O	1:E:86:VAL:HG13	1.95	0.66
1:E:298:VAL:HG22	1:E:309:VAL:HG12	1.78	0.66
1:A:327:ARG:O	1:A:363:PRO:HA	1.95	0.66
1:E:106:GLN:OE1	1:E:345:GLU:HG2	1.96	0.66
1:A:154:PHE:HA	1:A:244:HIS:O	1.96	0.65
1:E:28:PHE:CE1	1:E:338:PRO:HG2	2.31	0.65
1:F:162:GLU:OE2	1:F:237:SER:HB3	1.97	0.65
1:G:57:LEU:N	1:G:58:ALA:O	2.30	0.65
1:C:62:SER:O	1:C:63:ARG:HD2	1.95	0.65
1:D:162:GLU:OE1	1:D:231:TYR:OH	2.13	0.65
1:F:102:PHE:HB3	1:F:264:VAL:CG1	2.26	0.65
1:C:19:ILE:CD1	1:C:359:ILE:HG13	2.25	0.65
1:F:124:GLU:HG2	1:F:125:TYR:CE1	2.31	0.65
1:B:102:PHE:HE1	1:B:332:ILE:CD1	2.09	0.65
1:G:209:GLU:O	1:G:213:ILE:HD13	1.97	0.65
1:A:98:ASN:O	1:A:328:THR:HG22	1.96	0.64
1:D:311:TYR:CG	1:D:321:GLN:HG3	2.32	0.64
2:E:601:ADP:C8	2:E:601:ADP:H5'1	2.32	0.64
1:D:196:ILE:HD11	1:D:319:ILE:HD11	1.80	0.64
1:C:245:MET:HE3	1:C:257:LYS:HG3	1.80	0.64
1:E:92:GLU:H	1:E:92:GLU:CD	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:601:ADP:H8	2:E:601:ADP:H5'1	1.62	0.64
1:F:86:VAL:O	1:F:89:ILE:HG12	1.97	0.64
1:G:317:THR:O	1:G:321:GLN:N	2.30	0.64
1:G:43:CYS:O	1:G:45:PRO:HD3	1.98	0.64
1:G:92:GLU:HG3	1:G:329:ARG:HD2	1.80	0.64
1:C:161:LEU:HD12	1:C:161:LEU:C	2.22	0.64
1:F:68:PHE:HA	1:F:357:LYS:NZ	2.13	0.64
1:F:136:ILE:HD12	1:F:239:PHE:HD2	1.62	0.64
1:A:141:HIS:C	1:A:141:HIS:ND1	2.55	0.64
1:E:43:CYS:HB3	1:E:71:VAL:HG11	1.80	0.64
1:A:306:THR:OG1	1:A:307:PRO:CD	2.46	0.64
1:B:69:ASP:O	1:B:70:MET:HG3	1.97	0.64
1:E:143:ILE:HD12	1:E:243:ILE:HD11	1.80	0.63
1:F:82:TYR:CD2	1:F:86:VAL:HG11	2.33	0.63
1:F:136:ILE:O	1:F:139:THR:HG22	1.97	0.63
1:F:162:GLU:HG3	1:F:171:LEU:CD2	2.28	0.63
1:G:161:LEU:HD12	1:G:162:GLU:N	2.13	0.63
1:G:270:GLU:HG2	1:G:271:ASN:N	2.11	0.63
1:B:87:CYS:HB2	1:B:88:PRO:HD3	1.80	0.63
1:F:102:PHE:HB3	1:F:264:VAL:HG12	1.79	0.63
1:E:86:VAL:HG22	1:E:87:CYS:H	1.61	0.63
4:E:801:DQ8:HAS1	4:E:801:DQ8:CAQ	2.28	0.63
1:C:178:VAL:HG13	1:C:220:LYS:HG3	1.81	0.63
1:F:82:TYR:CD2	1:F:138:ARG:HB2	2.34	0.63
1:F:141:HIS:C	1:F:141:HIS:ND1	2.56	0.63
1:D:306:THR:HG23	1:D:307:PRO:HD2	1.80	0.63
1:G:53:ARG:NH2	1:G:57:LEU:HA	2.13	0.63
1:G:102:PHE:CE1	1:G:332:ILE:HG12	2.34	0.63
1:F:28:PHE:CE1	1:F:338:PRO:HG2	2.34	0.63
4:F:801:DQ8:CAL	4:F:801:DQ8:HAP	2.28	0.63
1:A:178:VAL:CG1	1:A:220:LYS:HG2	2.29	0.63
1:E:143:ILE:HD12	1:E:243:ILE:CD1	2.29	0.62
1:E:184:MET:HE1	1:E:319:ILE:CD1	2.28	0.62
1:G:82:TYR:CE1	1:G:86:VAL:CG2	2.80	0.62
1:C:262:ASN:O	1:C:263:LEU:HD23	1.99	0.62
4:C:801:DQ8:CAQ	4:C:801:DQ8:HAS1	2.30	0.62
1:D:190:ASN:OD1	1:D:191:LYS:N	2.32	0.62
1:E:156:VAL:HG12	1:E:243:ILE:HG12	1.79	0.62
1:B:352:TYR:HA	1:B:355:ARG:NH1	2.15	0.62
1:E:168:LEU:HD21	1:E:315:LYS:HD2	1.81	0.62
1:F:20:GLN:NE2	1:F:85:VAL:HG23	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.33	0.62
1:C:365:VAL:O	1:C:366:ASN:HB2	1.98	0.62
1:D:306:THR:CG2	1:D:307:PRO:HD2	2.30	0.62
1:E:82:TYR:HA	1:E:86:VAL:CG1	2.29	0.62
1:E:120:SER:OG	1:E:132:LEU:HD23	1.99	0.62
1:E:154:PHE:O	1:E:154:PHE:CD1	2.52	0.62
1:G:306:THR:HG22	1:G:307:PRO:HD2	1.80	0.62
1:A:178:VAL:HG13	1:A:220:LYS:CG	2.30	0.62
1:G:175:SER:O	1:G:176:SER:HB2	2.00	0.62
1:A:209:GLU:O	1:A:213:ILE:HG13	2.00	0.61
1:F:306:THR:CB	1:F:307:PRO:HD2	2.28	0.61
1:C:206:ASN:N	1:C:206:ASN:OD1	2.33	0.61
1:F:18:ASN:OD1	1:F:360:LEU:HB3	1.99	0.61
1:F:158:VAL:HB	1:F:239:PHE:CE1	2.31	0.61
1:C:129:GLU:OE1	1:G:211:TYR:OH	2.16	0.61
1:E:54:THR:HG21	1:E:64:LYS:HD2	1.83	0.61
1:E:270:GLU:O	1:E:271:ASN:HB2	1.99	0.61
1:G:44:ASP:OD1	1:G:47:ARG:HB3	2.01	0.61
1:D:22:VAL:CG1	1:D:70:MET:HB2	2.30	0.61
1:G:21:VAL:CG1	1:G:357:LYS:HB3	2.30	0.61
1:C:27:PRO:HG2	1:G:227:LEU:HD21	1.81	0.61
1:D:143:ILE:HD13	1:D:243:ILE:HD11	1.81	0.61
1:E:309:VAL:HB	1:E:311:TYR:CE1	2.35	0.61
1:A:136:ILE:HG12	1:A:263:LEU:HD12	1.83	0.61
1:C:42:GLU:HA	1:C:42:GLU:OE1	2.00	0.61
1:F:184:MET:SD	1:F:318:ARG:HD3	2.41	0.61
2:D:601:ADP:C8	2:D:601:ADP:C5'	2.81	0.60
1:E:119:ARG:HD3	1:E:211:TYR:HE1	1.65	0.60
1:E:119:ARG:HG2	4:E:801:DQ8:HAO	1.82	0.60
1:F:204:VAL:HG21	1:F:210:VAL:HG23	1.83	0.60
1:G:170:ASP:C	1:G:170:ASP:OD1	2.43	0.60
4:A:801:DQ8:CAQ	4:A:801:DQ8:HAS1	2.31	0.60
4:B:801:DQ8:HAO	4:B:801:DQ8:CAS	2.29	0.60
1:D:22:VAL:HG12	1:D:70:MET:HB2	1.83	0.60
1:A:189:ARG:O	1:A:190:ASN:HB2	2.01	0.60
1:E:90:LEU:HD11	1:E:143:ILE:CD1	2.30	0.60
1:F:29:ASN:OD1	1:F:32:GLU:HB2	2.02	0.60
1:G:53:ARG:HH21	1:G:57:LEU:HA	1.67	0.60
1:G:139:THR:O	1:G:143:ILE:HG12	2.01	0.60
1:B:130:ASP:OD1	1:B:131:PRO:HD2	2.01	0.60
1:C:25:CYS:O	1:C:74:ALA:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:LEU:HD12	1:F:132:LEU:O	2.01	0.60
1:G:362:LYS:CB	1:G:363:PRO:HD2	2.31	0.60
2:E:601:ADP:C5'	2:E:601:ADP:C8	2.84	0.60
1:F:100:THR:HG22	1:F:262:ASN:CB	2.31	0.60
1:E:328:THR:O	1:E:361:ASN:ND2	2.35	0.60
1:F:100:THR:CG2	1:F:262:ASN:HB2	2.32	0.60
1:F:162:GLU:HG3	1:F:171:LEU:HD23	1.82	0.60
1:E:40:ILE:HD12	1:E:343:LEU:HD13	1.84	0.60
1:E:82:TYR:CD2	1:E:86:VAL:HG21	2.35	0.60
1:F:43:CYS:HB3	1:F:71:VAL:HG12	1.82	0.60
1:G:196:ILE:HD11	1:G:199:LEU:CB	2.29	0.60
1:E:136:ILE:HG12	1:E:263:LEU:HD12	1.84	0.60
1:E:161:LEU:C	1:E:161:LEU:CD1	2.72	0.60
1:F:18:ASN:HA	1:F:360:LEU:CB	2.31	0.60
1:G:196:ILE:CG1	1:G:199:LEU:HB2	2.32	0.60
1:C:293:LEU:HD21	1:C:297:ARG:NH2	2.17	0.59
1:G:26:ARG:NH1	1:G:29:ASN:ND2	2.49	0.59
1:E:309:VAL:HG12	1:E:310:PRO:HD2	1.85	0.59
1:A:202:ILE:HG21	1:A:213:ILE:HD13	1.85	0.59
1:G:78:GLN:O	1:G:81:VAL:HG23	2.02	0.59
1:G:147:LEU:HD21	1:G:245:MET:HE1	1.84	0.59
1:B:89:ILE:HD13	1:B:101:ILE:HD11	1.85	0.59
1:E:120:SER:HB3	1:E:121:PRO:HD2	1.84	0.59
1:F:140:LEU:O	1:F:143:ILE:HG22	2.02	0.59
1:B:129:GLU:HA	1:B:129:GLU:OE1	2.03	0.59
1:B:154:PHE:HA	1:B:244:HIS:O	2.03	0.59
1:F:311:TYR:CD1	1:F:321:GLN:HG3	2.38	0.59
1:G:233:SER:OG	1:G:234:ARG:HD2	2.03	0.59
1:C:238:VAL:HG22	1:C:264:VAL:HG22	1.83	0.59
1:B:126:THR:HG23	1:B:129:GLU:HB2	1.84	0.59
1:C:75:SER:O	1:C:77:LYS:HD2	2.03	0.59
1:E:244:HIS:ND1	1:E:258:ILE:HG23	2.18	0.59
1:F:150:ASN:O	1:F:152:THR:HG23	2.03	0.59
1:G:314:SER:OG	1:G:317:THR:OG1	2.13	0.59
1:B:168:LEU:HD12	1:B:168:LEU:N	2.17	0.58
1:C:72:PHE:CD1	1:C:76:THR:HG21	2.38	0.58
1:F:128:GLU:O	1:F:129:GLU:OE2	2.21	0.58
1:G:296:GLY:O	1:G:300:THR:HG23	2.03	0.58
1:G:311:TYR:CD1	1:G:321:GLN:HG3	2.38	0.58
1:F:18:ASN:HA	1:F:360:LEU:HB3	1.84	0.58
1:B:111:LYS:HB2	1:B:111:LYS:NZ	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:GLU:HG2	4:G:801:DQ8:CAK	2.34	0.58
1:D:102:PHE:CE1	1:D:320:LEU:CD1	2.86	0.58
1:E:187:ASP:HB2	1:E:195:ILE:HG23	1.85	0.58
1:G:312:ARG:HG2	1:G:313:GLU:N	2.17	0.58
1:C:118:GLU:OE1	1:G:226:THR:CG2	2.51	0.58
1:E:288:ILE:N	7:E:2015:HOH:O	2.36	0.58
1:G:47:ARG:O	1:G:47:ARG:HG3	2.00	0.58
1:A:63:ARG:HH11	1:A:63:ARG:HG3	1.68	0.58
1:A:145:GLU:H	1:A:207:LYS:NZ	1.88	0.58
1:B:184:MET:HE2	1:B:319:ILE:HG12	1.86	0.58
1:E:59:ASP:OD1	1:E:59:ASP:C	2.46	0.58
1:F:238:VAL:O	1:F:238:VAL:CG2	2.51	0.58
1:G:361:ASN:C	1:G:362:LYS:HD2	2.29	0.58
1:A:51:SER:HB2	1:A:65:THR:HG1	1.65	0.58
1:G:29:ASN:OD1	1:G:31:ALA:HB3	2.03	0.58
1:G:147:LEU:HD21	1:G:245:MET:CE	2.34	0.58
1:F:89:ILE:HG12	1:F:90:LEU:N	2.18	0.58
1:E:91:ASP:O	1:E:94:ILE:HB	2.04	0.57
1:F:102:PHE:CE1	1:F:332:ILE:HG12	2.39	0.57
1:G:144:PHE:CE2	1:G:206:ASN:C	2.82	0.57
1:E:154:PHE:HA	1:E:244:HIS:O	2.05	0.57
1:B:102:PHE:HE1	1:B:332:ILE:HD11	1.69	0.57
1:G:111:LYS:HB2	2:G:601:ADP:O2B	2.03	0.57
1:C:88:PRO:O	1:C:92:GLU:HG3	2.04	0.57
1:D:190:ASN:OD1	1:D:190:ASN:C	2.47	0.57
1:E:120:SER:OG	1:E:130:ASP:OD1	2.22	0.57
1:F:244:HIS:NE2	1:F:258:ILE:HG22	2.20	0.57
1:G:168:LEU:HD13	1:G:168:LEU:N	2.19	0.57
1:C:142:GLN:O	1:C:143:ILE:C	2.47	0.57
1:F:110:GLY:HA2	2:F:601:ADP:O2A	2.05	0.57
1:F:141:HIS:ND1	1:F:141:HIS:O	2.37	0.57
1:G:91:ASP:O	1:G:94:ILE:HG22	2.03	0.57
1:A:178:VAL:HG13	1:A:220:LYS:HG2	1.86	0.57
1:B:207:LYS:HD2	1:B:207:LYS:O	2.04	0.57
1:D:184:MET:HE2	1:D:319:ILE:HG13	1.86	0.57
1:E:143:ILE:HG22	1:E:143:ILE:O	2.03	0.57
1:E:210:VAL:O	1:E:213:ILE:HG22	2.04	0.57
1:A:82:TYR:CE1	1:A:86:VAL:HB	2.39	0.57
1:E:103:ALA:HB1	1:E:111:LYS:CG	2.34	0.57
1:F:361:ASN:OD1	1:F:361:ASN:N	2.38	0.57
1:G:40:ILE:HD12	1:G:340:SER:HA	1.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:CD1	1:B:146:LYS:HE3	2.35	0.57
1:A:137:PRO:HG3	4:A:801:DQ8:HAP	1.87	0.57
1:B:20:GLN:OE1	1:B:70:MET:CE	2.53	0.57
1:B:288:ILE:HG13	1:B:289:ASN:N	2.20	0.57
1:C:327:ARG:HG2	1:C:362:LYS:O	2.05	0.57
1:F:158:VAL:HG21	1:F:213:ILE:CD1	2.35	0.57
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.04	0.56
1:D:130:ASP:OD1	1:D:131:PRO:HD2	2.05	0.56
4:F:801:DQ8:CAL	4:F:801:DQ8:CAP	2.78	0.56
1:C:126:THR:HG23	1:C:129:GLU:CG	2.30	0.56
1:G:82:TYR:CD1	1:G:86:VAL:CG2	2.88	0.56
1:G:107:THR:HB	1:G:270:GLU:OE2	2.05	0.56
1:A:230:ALA:HB3	1:A:234:ARG:NE	2.20	0.56
1:F:101:ILE:HG22	1:F:115:MET:HE1	1.86	0.56
1:E:152:THR:HG22	1:E:153:GLU:H	1.70	0.56
1:F:190:ASN:OD1	1:F:191:LYS:N	2.38	0.56
1:G:44:ASP:OD1	1:G:46:VAL:HG23	2.06	0.56
1:G:155:SER:CB	1:G:244:HIS:HB2	2.35	0.56
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.71	0.56
1:A:330:THR:CG2	1:A:331:SER:N	2.69	0.56
1:D:92:GLU:O	1:D:97:TYR:HB2	2.06	0.56
1:D:247:GLU:OE2	1:D:257:LYS:HE3	2.05	0.56
1:F:19:ILE:HG21	1:F:359:ILE:HG22	1.87	0.56
1:G:21:VAL:HG11	1:G:357:LYS:HB3	1.87	0.56
1:E:299:ILE:HG23	1:E:359:ILE:HD11	1.87	0.56
1:G:244:HIS:C	1:G:245:MET:HG3	2.30	0.56
1:D:26:ARG:NH2	1:D:32:GLU:OE2	2.36	0.56
1:F:139:THR:O	1:F:143:ILE:HB	2.05	0.56
1:G:136:ILE:HG12	1:G:263:LEU:HD13	1.88	0.56
1:G:186:ASP:OD1	1:G:186:ASP:N	2.39	0.56
1:A:127:TRP:CE2	1:A:128:GLU:HG3	2.40	0.56
1:C:288:ILE:HD12	1:C:288:ILE:H	1.72	0.56
1:F:144:PHE:HE2	1:F:207:LYS:N	2.02	0.56
1:A:69:ASP:O	1:A:70:MET:HG3	2.07	0.55
1:B:91:ASP:O	1:B:95:MET:HG2	2.07	0.55
1:D:18:ASN:N	1:D:361:ASN:H	2.04	0.55
1:D:186:ASP:OD2	1:D:312:ARG:NH2	2.39	0.55
1:G:295:LEU:O	1:G:299:ILE:HG12	2.06	0.55
1:E:87:CYS:SG	1:E:88:PRO:HD3	2.47	0.55
1:E:323:SER:HA	1:E:328:THR:HB	1.88	0.55
1:A:210:VAL:O	1:A:211:TYR:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:GLU:OE1	1:G:226:THR:HG21	2.07	0.55
4:D:801:DQ8:CAQ	4:D:801:DQ8:HAS1	2.36	0.55
1:G:158:VAL:HA	1:G:240:SER:O	2.07	0.55
1:A:289:ASN:O	1:A:293:LEU:HD13	2.07	0.55
1:D:34:LYS:HD2	1:D:35:ALA:N	2.22	0.55
1:G:98:ASN:HD22	1:G:98:ASN:H	1.53	0.55
1:G:312:ARG:CG	1:G:313:GLU:H	2.18	0.55
1:E:343:LEU:HD11	1:E:347:LEU:HD11	1.88	0.55
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.07	0.55
4:B:801:DQ8:HAS1	4:B:801:DQ8:CAQ	2.36	0.55
1:G:20:GLN:O	1:G:20:GLN:HG3	2.05	0.55
1:G:69:ASP:O	1:G:70:MET:HG2	2.07	0.55
1:E:310:PRO:HB2	1:E:313:GLU:HG3	1.87	0.55
1:F:230:ALA:CB	1:F:234:ARG:HD2	2.34	0.55
1:G:19:ILE:O	1:G:19:ILE:HG13	2.06	0.55
1:G:104:TYR:CD1	1:G:104:TYR:C	2.84	0.55
1:D:293:LEU:HD12	1:D:297:ARG:CZ	2.37	0.54
1:E:323:SER:O	1:E:330:THR:HG21	2.07	0.54
1:F:82:TYR:CE2	1:F:138:ARG:HB2	2.42	0.54
1:G:41:VAL:HG11	1:G:338:PRO:HA	1.86	0.54
1:C:89:ILE:O	1:C:93:VAL:HG23	2.07	0.54
1:D:26:ARG:NE	1:D:108:GLY:O	2.41	0.54
1:A:141:HIS:O	1:A:141:HIS:ND1	2.39	0.54
1:F:19:ILE:HG22	1:F:360:LEU:HA	1.88	0.54
1:F:135:ILE:O	1:F:139:THR:HB	2.08	0.54
1:F:265:ASP:OD1	1:F:265:ASP:C	2.50	0.54
1:B:178:VAL:HG13	1:B:220:LYS:CG	2.37	0.54
1:C:265:ASP:OD1	1:C:265:ASP:C	2.50	0.54
1:D:212:GLN:CD	1:D:212:GLN:H	2.15	0.54
1:F:325:GLY:HA2	1:F:360:LEU:O	2.07	0.54
1:A:132:LEU:HD23	1:A:132:LEU:N	2.21	0.54
1:A:288:ILE:HG23	1:A:289:ASN:H	1.71	0.54
1:D:90:LEU:HD22	1:D:139:THR:HG23	1.88	0.54
1:F:120:SER:OG	1:F:130:ASP:OD1	2.25	0.54
1:F:134:GLY:O	1:F:137:PRO:HD2	2.07	0.54
1:F:44:ASP:OD1	1:F:47:ARG:HG3	2.08	0.54
1:F:157:LYS:HB3	1:F:203:THR:HG22	1.89	0.54
1:G:136:ILE:HG12	1:G:263:LEU:CD1	2.37	0.54
1:G:362:LYS:HB3	1:G:363:PRO:CD	2.38	0.54
1:D:115:MET:O	1:D:136:ILE:HG13	2.07	0.54
1:F:114:THR:O	1:F:134:GLY:HA3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:GLU:C	1:G:125:TYR:H	2.13	0.54
1:C:186:ASP:OD1	1:C:186:ASP:N	2.36	0.54
1:E:168:LEU:HB2	1:E:182:LEU:HB2	1.90	0.54
1:F:172:LEU:HD23	1:F:216:LYS:NZ	2.14	0.54
1:G:137:PRO:HB3	4:G:801:DQ8:CAF	2.38	0.54
1:G:177:ASP:O	1:G:179:SER:N	2.41	0.54
1:A:103:ALA:HB1	1:A:111:LYS:HB3	1.88	0.54
1:D:126:THR:HG23	1:D:129:GLU:HB2	1.90	0.54
1:F:91:ASP:O	1:F:94:ILE:HG22	2.08	0.54
1:F:143:ILE:HG12	1:F:243:ILE:HD11	1.88	0.54
1:F:185:PHE:O	1:F:194:VAL:HG12	2.08	0.54
1:E:170:ASP:HB2	1:E:182:LEU:HD11	1.90	0.53
1:G:215:GLU:HB2	4:G:801:DQ8:HAH	1.90	0.53
1:B:204:VAL:HG22	1:B:213:ILE:CD1	2.39	0.53
1:F:123:GLU:C	1:F:123:GLU:CD	2.75	0.53
1:D:161:LEU:C	1:D:161:LEU:HD12	2.34	0.53
1:E:137:PRO:HD3	4:E:801:DQ8:HAJ	1.90	0.53
1:D:67:THR:O	1:D:357:LYS:HE2	2.08	0.53
1:F:54:THR:HG21	1:F:64:LYS:HG3	1.90	0.53
1:G:102:PHE:HB2	1:G:264:VAL:HG22	1.89	0.53
1:A:120:SER:OG	1:A:130:ASP:OD1	2.27	0.53
1:C:262:ASN:C	1:C:263:LEU:HD23	2.32	0.53
2:C:601:ADP:C8	2:C:601:ADP:C5'	2.85	0.53
1:F:100:THR:OG1	1:F:323:SER:OG	2.09	0.53
1:G:82:TYR:O	1:G:86:VAL:HG22	2.09	0.53
1:A:63:ARG:HG2	1:A:63:ARG:NH1	2.20	0.53
1:C:121:PRO:HG2	7:C:2023:HOH:O	2.07	0.53
1:D:26:ARG:HG3	1:D:26:ARG:NH1	2.22	0.53
1:E:352:TYR:O	1:E:355:ARG:HB2	2.09	0.53
1:G:156:VAL:CG1	1:G:204:VAL:O	2.56	0.53
1:A:130:ASP:OD1	1:A:131:PRO:HD2	2.08	0.53
1:B:206:ASN:OD1	1:B:208:ASP:HB2	2.09	0.53
1:C:23:VAL:HG11	1:C:50:VAL:HG21	1.89	0.53
1:C:150:ASN:OD1	1:C:152:THR:HG22	2.09	0.53
1:F:82:TYR:O	1:F:86:VAL:CG1	2.56	0.53
1:E:301:ALA:HB3	1:E:309:VAL:HG13	1.90	0.53
1:F:327:ARG:O	1:F:363:PRO:HA	2.09	0.52
1:F:163:ILE:HG12	1:F:168:LEU:HD23	1.91	0.52
1:G:56:GLY:O	1:G:57:LEU:HD13	2.09	0.52
1:D:102:PHE:HE1	1:D:320:LEU:HD13	1.70	0.52
1:E:125:TYR:CD1	1:E:125:TYR:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:ILE:HG22	1:G:52:VAL:HG13	1.91	0.52
1:A:144:PHE:HB2	1:A:207:LYS:NZ	2.25	0.52
1:B:144:PHE:HZ	1:B:204:VAL:HG12	1.74	0.52
1:E:28:PHE:CD1	1:E:338:PRO:HG2	2.44	0.52
1:E:51:SER:OG	1:E:63:ARG:HD2	2.10	0.52
1:G:30:LEU:O	1:G:34:LYS:HE2	2.10	0.52
1:G:90:LEU:O	1:G:94:ILE:HB	2.09	0.52
1:A:63:ARG:CG	1:A:63:ARG:NH1	2.55	0.52
1:B:190:ASN:OD1	1:B:191:LYS:N	2.42	0.52
1:F:154:PHE:N	1:F:154:PHE:HD1	2.07	0.52
1:F:270:GLU:CG	1:F:271:ASN:OD1	2.57	0.52
1:B:94:ILE:HD12	1:B:146:LYS:HE3	1.91	0.52
1:F:221:ARG:O	1:F:224:ALA:N	2.42	0.52
1:B:20:GLN:OE1	1:B:70:MET:HE2	2.10	0.52
1:C:365:VAL:O	1:C:366:ASN:CB	2.58	0.52
1:F:90:LEU:O	1:F:93:VAL:CG1	2.57	0.52
1:F:154:PHE:N	1:F:154:PHE:CD1	2.77	0.52
1:G:83:ARG:HA	1:G:87:CYS:SG	2.50	0.52
1:G:123:GLU:O	1:G:125:TYR:N	2.41	0.52
1:A:98:ASN:CB	1:A:328:THR:HG23	2.39	0.52
1:F:196:ILE:HB	1:F:199:LEU:HB2	1.91	0.52
1:F:239:PHE:CD1	1:F:239:PHE:C	2.86	0.52
1:G:166:GLU:HG3	1:G:315:LYS:CG	2.40	0.52
1:D:64:LYS:CE	1:D:66:TYR:OH	2.57	0.52
1:A:141:HIS:O	1:A:207:LYS:HE3	2.10	0.51
1:C:159:SER:HB2	1:C:199:LEU:HD11	1.92	0.51
1:A:123:GLU:C	1:A:125:TYR:H	2.19	0.51
4:B:801:DQ8:CAO	4:B:801:DQ8:CAS	2.86	0.51
1:G:40:ILE:CD1	1:G:343:LEU:HB2	2.40	0.51
1:G:354:HIS:CE1	1:G:358:ASN:HA	2.46	0.51
1:C:341:LEU:O	1:C:341:LEU:HD22	2.10	0.51
1:D:30:LEU:CD1	1:D:33:ARG:HH21	2.24	0.51
1:A:188:PRO:HD3	1:A:195:ILE:HD12	1.93	0.51
1:C:137:PRO:HD3	4:C:801:DQ8:HAJ	1.92	0.51
1:E:173:ASN:CG	1:E:174:PRO:HD2	2.35	0.51
1:F:82:TYR:HA	1:F:86:VAL:HG12	1.93	0.51
1:A:109:THR:O	1:A:335:THR:CG2	2.59	0.51
1:E:86:VAL:HG23	1:E:87:CYS:N	2.24	0.51
1:D:25:CYS:O	1:D:74:ALA:HA	2.10	0.51
1:F:89:ILE:HD12	1:F:101:ILE:CD1	2.16	0.51
1:A:23:VAL:HG21	1:A:68:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:ALA:CB	1:E:111:LYS:HG2	2.41	0.51
1:E:234:ARG:HD3	1:E:288:ILE:CG2	2.41	0.51
1:F:59:ASP:C	1:F:59:ASP:OD1	2.53	0.51
1:G:98:ASN:HD22	1:G:98:ASN:N	2.09	0.51
1:A:289:ASN:OD1	1:A:289:ASN:N	2.38	0.51
1:E:264:VAL:HG21	1:E:320:LEU:HD21	1.92	0.51
1:G:238:VAL:HG22	1:G:264:VAL:HB	1.92	0.51
1:E:29:ASN:ND2	1:E:32:GLU:OE1	2.42	0.51
4:A:801:DQ8:CAQ	4:A:801:DQ8:CAS	2.89	0.51
1:D:143:ILE:CD1	1:D:243:ILE:HD11	2.40	0.51
1:E:306:THR:HG22	1:E:307:PRO:CD	2.30	0.51
1:F:310:PRO:HB3	1:F:313:GLU:HG3	1.92	0.51
1:G:98:ASN:CB	1:G:260:LYS:HB3	2.41	0.50
1:E:154:PHE:CD1	1:E:154:PHE:C	2.89	0.50
1:G:41:VAL:HG13	1:G:338:PRO:HA	1.90	0.50
1:F:211:TYR:O	1:F:215:GLU:HB2	2.11	0.50
1:G:72:PHE:HB3	1:G:76:THR:OG1	2.12	0.50
1:B:22:VAL:HG11	1:B:70:MET:HE3	1.94	0.50
1:G:124:GLU:HG2	1:G:125:TYR:CD2	2.46	0.50
1:C:365:VAL:HG12	1:C:366:ASN:N	2.24	0.50
1:D:26:ARG:HG3	1:D:27:PRO:O	2.11	0.50
1:D:236:HIS:HD1	1:D:267:ALA:H	1.58	0.50
1:E:127:TRP:CD1	1:E:211:TYR:HB2	2.46	0.50
1:A:100:THR:OG1	1:A:323:SER:OG	2.10	0.50
1:E:126:THR:HG22	1:E:129:GLU:OE1	2.11	0.50
1:E:261:LEU:HD21	1:E:263:LEU:HD21	1.92	0.50
1:F:59:ASP:OD1	1:F:59:ASP:O	2.30	0.50
1:F:190:ASN:OD1	1:F:192:ARG:N	2.45	0.50
1:F:216:LYS:HZ3	1:F:217:GLY:N	2.09	0.50
1:G:56:GLY:O	1:G:57:LEU:CD1	2.60	0.50
1:G:228:MET:HE2	1:G:228:MET:CA	2.37	0.50
1:F:102:PHE:CB	1:F:264:VAL:HG13	2.42	0.50
1:F:119:ARG:HG2	4:F:801:DQ8:CAM	2.42	0.50
1:E:184:MET:HE1	1:E:319:ILE:HD12	1.94	0.50
1:G:181:ARG:CG	1:G:181:ARG:NH1	2.57	0.50
1:A:144:PHE:HD2	1:A:207:LYS:CD	2.12	0.50
1:C:102:PHE:HB3	1:C:264:VAL:HB	1.93	0.50
1:E:82:TYR:CA	1:E:86:VAL:HG13	2.42	0.50
1:F:320:LEU:O	1:F:323:SER:N	2.43	0.50
4:G:801:DQ8:CAO	4:G:801:DQ8:HAS2	2.42	0.50
1:E:234:ARG:HD3	1:E:288:ILE:HG21	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:HIS:C	1:G:310:PRO:HD2	2.37	0.49
1:C:19:ILE:HD13	1:C:359:ILE:HG13	1.91	0.49
1:E:102:PHE:CB	1:E:264:VAL:HB	2.39	0.49
1:B:162:GLU:CD	1:B:171:LEU:HD11	2.36	0.49
1:E:140:LEU:HD21	1:E:241:VAL:HG22	1.94	0.49
1:E:294:THR:O	1:E:295:LEU:C	2.54	0.49
1:F:90:LEU:HD12	1:F:90:LEU:C	2.37	0.49
1:G:37:ALA:HB1	1:G:340:SER:OG	2.11	0.49
1:A:98:ASN:C	1:A:328:THR:HG22	2.36	0.49
1:C:353:ALA:O	1:C:356:ALA:HB3	2.12	0.49
1:G:86:VAL:HG11	1:G:135:ILE:HG23	1.93	0.49
1:A:178:VAL:HG13	1:A:220:LYS:HG3	1.93	0.49
1:B:186:ASP:OD2	1:B:312:ARG:NH2	2.45	0.49
1:G:170:ASP:OD2	1:G:173:ASN:HB2	2.11	0.49
1:B:167:GLU:OE1	1:B:181:ARG:NE	2.43	0.49
1:F:154:PHE:HD1	1:F:154:PHE:H	1.61	0.49
1:A:187:ASP:OD1	1:A:188:PRO:HD2	2.12	0.49
1:B:205:HIS:N	1:B:209:GLU:OE1	2.32	0.49
1:E:29:ASN:ND2	1:E:32:GLU:HB2	2.28	0.49
1:G:111:LYS:HB2	1:G:111:LYS:HZ3	1.77	0.49
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.95	0.49
1:E:239:PHE:CD1	1:E:239:PHE:C	2.91	0.49
1:F:215:GLU:CA	4:F:801:DQ8:HAH	2.36	0.49
1:G:196:ILE:C	1:G:196:ILE:HD12	2.37	0.49
1:C:190:ASN:OD1	1:C:190:ASN:C	2.55	0.49
1:G:111:LYS:HB2	1:G:111:LYS:HZ2	1.78	0.49
1:G:231:TYR:O	1:G:234:ARG:N	2.31	0.49
1:A:271:ASN:O	7:A:2025:HOH:O	2.20	0.49
1:C:309:VAL:HB	1:C:311:TYR:CE2	2.48	0.49
1:G:295:LEU:O	1:G:295:LEU:HD12	2.12	0.49
1:G:354:HIS:CE1	1:G:358:ASN:OD1	2.66	0.49
1:A:40:ILE:HD13	1:A:343:LEU:HB2	1.95	0.48
1:F:173:ASN:OD1	1:F:174:PRO:HD2	2.13	0.48
1:G:26:ARG:HD2	1:G:27:PRO:O	2.12	0.48
1:G:160:LEU:H	1:G:172:LEU:CD1	2.13	0.48
1:G:311:TYR:CB	1:G:321:GLN:HG3	2.43	0.48
1:D:119:ARG:HA	1:D:130:ASP:OD2	2.12	0.48
1:G:295:LEU:HD12	1:G:298:VAL:HG12	1.95	0.48
1:E:170:ASP:OD2	1:E:173:ASN:HB2	2.13	0.48
1:F:40:ILE:HD13	1:F:340:SER:HA	1.94	0.48
1:F:309:VAL:HG13	1:F:311:TYR:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:GLU:HB2	1:G:169:PHE:CE1	2.48	0.48
1:B:291:SER:HA	1:B:314:SER:HB2	1.95	0.48
1:C:143:ILE:HD13	1:C:243:ILE:HD11	1.94	0.48
1:E:82:TYR:CD2	1:E:86:VAL:HG11	2.48	0.48
1:E:134:GLY:O	1:E:137:PRO:HD2	2.13	0.48
1:F:264:VAL:HG11	1:F:320:LEU:HD21	1.95	0.48
1:F:311:TYR:CE1	1:F:321:GLN:HG3	2.48	0.48
1:G:137:PRO:HB3	4:G:801:DQ8:HAF	1.94	0.48
1:D:139:THR:HG21	1:D:261:LEU:HD23	1.94	0.48
1:F:136:ILE:HG23	1:F:239:PHE:CE2	2.49	0.48
1:G:361:ASN:O	1:G:362:LYS:HD2	2.13	0.48
1:A:119:ARG:HD3	4:A:801:DQ8:CAG	2.44	0.48
1:A:123:GLU:O	1:A:125:TYR:N	2.46	0.48
1:E:163:ILE:HG12	1:E:168:LEU:CD1	2.43	0.48
1:A:178:VAL:CG1	1:A:220:LYS:CG	2.90	0.48
1:C:77:LYS:HG2	1:G:219:ALA:HB1	1.94	0.48
1:C:308:HIS:O	1:C:308:HIS:ND1	2.46	0.48
1:F:144:PHE:CE2	1:F:206:ASN:C	2.92	0.48
1:G:102:PHE:CB	1:G:264:VAL:HG22	2.43	0.48
1:D:171:LEU:HD13	1:D:221:ARG:HB2	1.96	0.48
1:E:25:CYS:HB2	1:E:336:ILE:CG1	2.43	0.48
1:G:94:ILE:HD11	1:G:245:MET:HE1	1.96	0.48
1:G:311:TYR:HB2	1:G:321:GLN:HG3	1.96	0.48
1:E:90:LEU:HD12	1:E:90:LEU:O	2.14	0.48
1:F:49:GLU:HG2	1:F:67:THR:CG2	2.42	0.48
1:F:68:PHE:HA	1:F:357:LYS:HZ1	1.78	0.48
1:G:40:ILE:O	1:G:40:ILE:CG2	2.61	0.48
1:B:29:ASN:OD1	1:B:31:ALA:HB3	2.14	0.48
1:C:293:LEU:HD21	1:C:297:ARG:HH22	1.78	0.48
1:G:147:LEU:HD11	1:G:245:MET:CE	2.44	0.48
1:G:298:VAL:O	1:G:302:LEU:HD12	2.14	0.48
1:A:158:VAL:HG12	1:A:241:VAL:HG22	1.96	0.47
1:C:360:LEU:HD12	1:C:360:LEU:N	2.27	0.47
1:E:94:ILE:O	1:E:245:MET:HE1	2.13	0.47
1:F:140:LEU:O	1:F:143:ILE:N	2.41	0.47
1:G:158:VAL:HG22	1:G:239:PHE:CE1	2.48	0.47
1:G:170:ASP:OD1	1:G:172:LEU:N	2.47	0.47
1:A:288:ILE:HG23	1:A:289:ASN:OD1	2.14	0.47
1:B:102:PHE:CD1	1:B:332:ILE:HG12	2.49	0.47
1:C:144:PHE:O	1:C:146:LYS:N	2.48	0.47
1:E:49:GLU:HG2	1:E:67:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:ARG:HH12	1:G:29:ASN:ND2	2.11	0.47
1:G:35:ALA:CB	1:G:341:LEU:HD11	2.45	0.47
1:G:102:PHE:HB2	1:G:264:VAL:O	2.14	0.47
1:C:320:LEU:O	1:C:323:SER:HB2	2.14	0.47
1:E:323:SER:HB3	1:E:330:THR:HG21	1.94	0.47
1:C:135:ILE:HG22	1:C:263:LEU:HD13	1.95	0.47
1:E:170:ASP:C	1:E:170:ASP:OD1	2.57	0.47
1:E:245:MET:O	1:E:257:LYS:N	2.44	0.47
1:E:300:THR:CG2	1:E:355:ARG:HH12	2.21	0.47
1:F:307:PRO:O	1:F:308:HIS:C	2.57	0.47
1:F:19:ILE:CG2	1:F:359:ILE:O	2.62	0.47
1:F:113:PHE:CD1	1:F:113:PHE:C	2.91	0.47
1:F:161:LEU:HD12	1:F:161:LEU:O	2.14	0.47
1:F:221:ARG:O	1:F:222:THR:C	2.56	0.47
1:F:345:GLU:OE1	1:F:345:GLU:HA	2.14	0.47
1:B:162:GLU:OE2	1:B:221:ARG:NE	2.46	0.47
1:D:196:ILE:CD1	1:D:319:ILE:HD11	2.44	0.47
1:E:103:ALA:HB1	1:E:111:LYS:HG2	1.97	0.47
1:G:77:LYS:O	1:G:80:ASP:HB2	2.14	0.47
1:A:98:ASN:HB2	1:A:328:THR:HG23	1.96	0.47
1:A:126:THR:O	1:A:127:TRP:C	2.57	0.47
1:B:192:ARG:HD2	1:B:322:ASP:OD1	2.15	0.47
1:C:178:VAL:CG1	1:C:220:LYS:HG3	2.43	0.47
1:D:90:LEU:O	1:D:90:LEU:HD12	2.14	0.47
1:D:142:GLN:O	1:D:146:LYS:HB2	2.15	0.47
1:D:163:ILE:HG12	1:D:168:LEU:CD1	2.42	0.47
2:E:601:ADP:H8	2:E:601:ADP:H5'2	1.79	0.47
1:F:128:GLU:OE1	1:F:128:GLU:HA	2.13	0.47
1:F:135:ILE:CG2	1:F:263:LEU:HD13	2.38	0.47
1:F:156:VAL:CG1	1:F:204:VAL:HG13	2.38	0.47
1:F:301:ALA:O	1:F:305:ARG:HA	2.14	0.47
1:G:98:ASN:HB3	1:G:260:LYS:HB3	1.95	0.47
1:G:311:TYR:CG	1:G:321:GLN:CG	2.97	0.47
1:B:144:PHE:CZ	1:B:204:VAL:HG12	2.50	0.47
1:F:271:ASN:O	7:F:2020:HOH:O	2.20	0.47
1:G:166:GLU:HG3	1:G:315:LYS:HG2	1.95	0.47
1:G:262:ASN:ND2	1:G:320:LEU:CD2	2.74	0.47
1:C:309:VAL:O	1:C:311:TYR:N	2.45	0.47
1:E:128:GLU:HG2	1:E:141:HIS:ND1	2.30	0.47
1:E:152:THR:CG2	1:E:153:GLU:H	2.26	0.47
1:B:40:ILE:HD13	1:B:340:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:HD12	1:C:161:LEU:O	2.13	0.47
1:C:264:VAL:HG21	1:C:320:LEU:HD21	1.97	0.47
1:E:86:VAL:O	1:E:90:LEU:N	2.46	0.47
1:G:53:ARG:NH2	1:G:57:LEU:CA	2.78	0.47
1:G:308:HIS:O	1:G:310:PRO:O	2.32	0.47
1:G:343:LEU:O	1:G:347:LEU:HG	2.14	0.47
1:D:162:GLU:OE1	1:D:231:TYR:CE2	2.68	0.46
1:D:197:LYS:NZ	1:F:58:ALA:O	2.45	0.46
1:E:89:ILE:O	1:E:93:VAL:HG23	2.15	0.46
1:F:68:PHE:HA	1:F:357:LYS:CE	2.44	0.46
1:F:101:ILE:HA	1:F:331:SER:O	2.14	0.46
1:G:20:GLN:HB2	1:G:69:ASP:OD2	2.15	0.46
1:C:72:PHE:HB3	1:C:76:THR:HG21	1.97	0.46
1:F:317:THR:O	1:F:321:GLN:N	2.48	0.46
1:G:293:LEU:HA	1:G:352:TYR:HE2	1.80	0.46
4:G:801:DQ8:HAA1	4:G:801:DQ8:HAK	1.61	0.46
1:C:128:GLU:OE2	1:C:207:LYS:HE3	2.15	0.46
1:E:178:VAL:O	1:E:178:VAL:HG22	2.16	0.46
1:G:123:GLU:HA	1:G:123:GLU:OE1	2.15	0.46
1:A:156:VAL:HG13	1:A:156:VAL:O	2.15	0.46
1:C:59:ASP:C	1:C:59:ASP:OD1	2.58	0.46
1:E:152:THR:HG22	1:E:153:GLU:N	2.29	0.46
1:E:158:VAL:HA	1:E:240:SER:O	2.15	0.46
1:F:89:ILE:HG12	1:F:90:LEU:H	1.80	0.46
1:F:102:PHE:HD1	1:F:102:PHE:O	1.97	0.46
1:A:30:LEU:CD2	1:A:33:ARG:HD2	2.46	0.46
1:F:161:LEU:C	1:F:161:LEU:CD1	2.88	0.46
1:F:293:LEU:CD2	1:F:297:ARG:HH21	2.29	0.46
1:G:136:ILE:CG1	1:G:263:LEU:HD13	2.46	0.46
1:G:177:ASP:N	1:G:180:GLU:HG3	2.26	0.46
1:G:347:LEU:O	1:G:351:GLU:N	2.44	0.46
1:A:293:LEU:H	1:A:293:LEU:CD1	2.29	0.46
1:B:139:THR:O	1:B:143:ILE:HG13	2.15	0.46
1:E:103:ALA:HB1	1:E:111:LYS:HG3	1.97	0.46
1:F:91:ASP:OD1	1:F:146:LYS:NZ	2.48	0.46
1:B:247:GLU:CD	1:B:255:LEU:O	2.59	0.46
1:A:19:ILE:HG22	1:A:361:ASN:OD1	2.15	0.46
1:E:142:GLN:O	1:E:146:LYS:HB2	2.15	0.46
1:A:104:TYR:CE2	1:A:352:TYR:CE1	3.04	0.46
1:C:306:THR:CG2	1:C:307:PRO:CD	2.93	0.46
4:D:801:DQ8:CAL	4:D:801:DQ8:CAP	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ILE:HD11	1:F:147:LEU:CD2	2.38	0.46
1:F:299:ILE:HA	1:F:359:ILE:HD11	1.98	0.46
1:A:144:PHE:HB2	1:A:207:LYS:HZ2	1.80	0.45
1:C:308:HIS:O	1:C:308:HIS:CG	2.68	0.45
1:C:327:ARG:HB3	1:C:363:PRO:HA	1.98	0.45
1:D:30:LEU:CD1	1:D:33:ARG:NH2	2.76	0.45
1:D:212:GLN:CD	1:D:212:GLN:N	2.74	0.45
1:G:40:ILE:HD12	1:G:343:LEU:HB2	1.99	0.45
1:D:40:ILE:O	1:D:52:VAL:HA	2.15	0.45
4:E:801:DQ8:CAQ	4:E:801:DQ8:HAN	2.46	0.45
1:F:28:PHE:CD1	1:F:338:PRO:HG2	2.50	0.45
1:G:26:ARG:CZ	1:G:29:ASN:HD22	2.28	0.45
1:G:293:LEU:CD2	1:G:297:ARG:HE	2.30	0.45
1:B:79:ILE:O	1:B:83:ARG:HB2	2.17	0.45
1:E:289:ASN:O	1:E:293:LEU:HB2	2.17	0.45
1:F:49:GLU:CG	1:F:67:THR:HG22	2.44	0.45
1:G:40:ILE:HD11	1:G:340:SER:CA	2.42	0.45
1:A:40:ILE:HD12	1:A:52:VAL:CG1	2.47	0.45
1:A:184:MET:HE1	1:A:319:ILE:CG1	2.45	0.45
1:C:92:GLU:O	1:C:97:TYR:HB2	2.17	0.45
1:D:120:SER:HB3	1:D:121:PRO:CD	2.40	0.45
1:F:293:LEU:HD22	1:F:297:ARG:HH21	1.79	0.45
4:A:801:DQ8:HAP	4:A:801:DQ8:CAL	2.46	0.45
1:B:106:GLN:NE2	1:B:345:GLU:HG3	2.32	0.45
1:B:130:ASP:OD1	1:B:131:PRO:CD	2.64	0.45
1:C:163:ILE:HG12	1:C:168:LEU:HD23	1.97	0.45
1:D:18:ASN:HB2	1:D:360:LEU:HD23	1.98	0.45
1:G:73:GLY:O	1:G:75:SER:N	2.49	0.45
1:G:190:ASN:O	1:G:192:ARG:N	2.50	0.45
1:C:146:LYS:HB2	1:C:146:LYS:HE2	1.70	0.45
1:C:173:ASN:ND2	1:E:57:LEU:HD22	2.32	0.45
1:C:187:ASP:HA	1:C:188:PRO:HD3	1.88	0.45
1:G:132:LEU:HD23	1:G:132:LEU:HA	1.87	0.45
1:G:309:VAL:N	1:G:310:PRO:HD2	2.32	0.45
1:D:322:ASP:OD1	1:D:322:ASP:N	2.47	0.45
1:B:355:ARG:O	1:B:356:ALA:C	2.60	0.45
1:F:25:CYS:O	1:F:74:ALA:HA	2.17	0.45
1:F:82:TYR:CE2	1:F:86:VAL:HG21	2.51	0.45
1:G:87:CYS:HB2	1:G:88:PRO:HD3	1.98	0.45
1:G:310:PRO:HB2	1:G:311:TYR:CD1	2.52	0.45
1:A:78:GLN:NE2	1:A:113:PHE:CE1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TYR:CD1	1:B:86:VAL:HB	2.51	0.45
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.75	0.45
1:F:144:PHE:O	1:F:147:LEU:N	2.50	0.45
1:A:106:GLN:NE2	1:A:345:GLU:HG2	2.32	0.45
1:A:136:ILE:HG13	1:A:263:LEU:HD13	1.99	0.45
1:B:92:GLU:O	1:B:97:TYR:HB2	2.17	0.45
1:C:33:ARG:CD	1:G:228:MET:HE1	2.34	0.45
1:C:142:GLN:C	1:C:144:PHE:N	2.72	0.45
1:D:18:ASN:HA	1:D:360:LEU:HA	1.98	0.45
1:G:302:LEU:CD1	1:G:324:LEU:HD23	2.47	0.45
1:B:149:ASP:OD1	1:B:149:ASP:N	2.50	0.44
1:D:115:MET:HE3	1:D:263:LEU:HB3	1.97	0.44
4:E:801:DQ8:CAL	4:E:801:DQ8:CAP	2.92	0.44
1:F:82:TYR:CD1	1:F:82:TYR:C	2.95	0.44
1:A:202:ILE:HG21	1:A:213:ILE:CD1	2.46	0.44
1:B:152:THR:HA	1:B:246:LYS:O	2.17	0.44
1:F:118:GLU:O	4:F:801:DQ8:HAG	2.17	0.44
1:G:245:MET:C	1:G:257:LYS:O	2.61	0.44
1:A:123:GLU:HB2	1:A:124:GLU:H	1.44	0.44
1:A:288:ILE:HG13	1:A:289:ASN:N	2.32	0.44
4:A:801:DQ8:CAS	4:A:801:DQ8:HAQ	2.48	0.44
1:C:39:SER:HA	1:C:338:PRO:O	2.17	0.44
1:F:23:VAL:HA	1:F:334:ALA:O	2.18	0.44
1:G:299:ILE:HG12	1:G:299:ILE:H	1.61	0.44
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.32	0.44
1:A:152:THR:HG22	1:A:153:GLU:N	2.29	0.44
1:C:266:LEU:HD22	1:C:316:LEU:HD21	1.99	0.44
1:F:124:GLU:C	1:F:125:TYR:CD1	2.96	0.44
1:F:184:MET:HE1	1:F:319:ILE:HG13	1.99	0.44
1:F:241:VAL:HG12	1:F:261:LEU:HB3	1.99	0.44
1:G:20:GLN:O	1:G:20:GLN:CG	2.64	0.44
1:A:90:LEU:O	1:A:93:VAL:HG22	2.18	0.44
1:A:192:ARG:HH21	1:A:327:ARG:NH1	2.15	0.44
1:F:72:PHE:HB3	1:F:76:THR:HG21	1.99	0.44
1:F:134:GLY:O	1:F:135:ILE:C	2.59	0.44
1:F:144:PHE:CE1	1:F:156:VAL:HG11	2.52	0.44
1:G:18:ASN:N	1:G:18:ASN:OD1	2.50	0.44
1:G:205:HIS:O	1:G:206:ASN:CB	2.66	0.44
1:G:293:LEU:O	1:G:297:ARG:HG3	2.18	0.44
1:B:327:ARG:O	1:B:363:PRO:HA	2.18	0.44
1:D:245:MET:HE3	1:D:245:MET:HB2	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LYS:O	1:E:80:ASP:HB2	2.18	0.44
1:F:27:PRO:HB3	1:F:74:ALA:HB1	2.00	0.44
1:F:63:ARG:HH11	1:F:63:ARG:HG3	1.82	0.44
1:G:59:ASP:OD1	1:G:61:SER:O	2.36	0.44
1:B:157:LYS:HB2	1:B:157:LYS:HE3	1.77	0.44
1:D:55:GLY:O	1:D:56:GLY:C	2.61	0.44
1:F:132:LEU:H	1:F:132:LEU:HG	1.63	0.44
1:F:135:ILE:HD12	1:F:135:ILE:N	2.33	0.44
1:F:309:VAL:HG13	1:F:311:TYR:CD2	2.53	0.44
1:G:57:LEU:HD22	1:G:57:LEU:O	2.17	0.44
1:A:168:LEU:HD21	1:A:315:LYS:HD2	1.99	0.43
1:A:293:LEU:O	1:A:294:THR:C	2.60	0.43
1:C:100:THR:HG22	1:C:101:ILE:N	2.32	0.43
1:E:55:GLY:O	1:E:56:GLY:C	2.60	0.43
1:G:53:ARG:HH21	1:G:57:LEU:CA	2.30	0.43
1:G:199:LEU:HD13	1:G:200:GLU:N	2.33	0.43
1:G:295:LEU:HD12	1:G:298:VAL:CG1	2.48	0.43
1:A:153:GLU:HG3	1:A:246:LYS:HE2	2.00	0.43
1:C:302:LEU:CB	1:C:359:ILE:HG22	2.45	0.43
1:E:205:HIS:O	1:E:206:ASN:HB3	2.18	0.43
1:F:19:ILE:CG2	1:F:360:LEU:HA	2.47	0.43
1:F:104:TYR:CD1	1:F:104:TYR:C	2.95	0.43
1:F:168:LEU:HB2	1:F:182:LEU:HB2	1.99	0.43
1:F:178:VAL:HG22	1:F:178:VAL:O	2.18	0.43
1:F:309:VAL:O	1:F:311:TYR:N	2.51	0.43
1:A:63:ARG:HG3	1:A:63:ARG:NH1	2.29	0.43
1:A:311:TYR:CE1	1:A:321:GLN:HG3	2.53	0.43
1:C:86:VAL:O	1:C:87:CYS:C	2.61	0.43
1:C:149:ASP:N	1:C:149:ASP:OD1	2.50	0.43
1:A:87:CYS:O	1:A:88:PRO:C	2.60	0.43
1:A:98:ASN:HB3	1:A:328:THR:HG23	2.00	0.43
1:A:245:MET:HE3	1:A:245:MET:HB2	1.69	0.43
1:B:264:VAL:HG21	1:B:320:LEU:HD11	1.99	0.43
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.53	0.43
1:B:327:ARG:HG3	1:B:362:LYS:O	2.18	0.43
1:C:270:GLU:HG2	1:C:271:ASN:H	1.83	0.43
1:C:322:ASP:O	1:C:328:THR:HB	2.19	0.43
1:E:158:VAL:HG13	1:E:204:VAL:HG21	2.00	0.43
1:F:128:GLU:OE2	1:F:141:HIS:NE2	2.51	0.43
1:G:70:MET:HE2	1:G:70:MET:HB3	1.93	0.43
1:A:109:THR:OG1	1:A:335:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:HG2	4:B:801:DQ8:CAK	2.48	0.43
1:F:146:LYS:HE3	1:F:146:LYS:HB3	1.66	0.43
1:A:308:HIS:ND1	7:A:2026:HOH:O	2.32	0.43
1:C:23:VAL:HG21	1:C:68:PHE:CE2	2.53	0.43
1:C:306:THR:HG23	1:C:307:PRO:CD	2.33	0.43
1:E:106:GLN:HE22	1:E:342:ASN:HB3	1.84	0.43
1:E:156:VAL:CG2	1:E:204:VAL:O	2.67	0.43
1:F:205:HIS:O	1:F:206:ASN:HB3	2.17	0.43
1:F:309:VAL:HA	1:F:310:PRO:HD3	1.80	0.43
1:G:177:ASP:C	1:G:179:SER:N	2.76	0.43
1:E:86:VAL:O	1:E:89:ILE:N	2.51	0.43
1:G:196:ILE:O	1:G:196:ILE:HG13	2.18	0.43
1:A:202:ILE:HD12	1:A:202:ILE:N	2.34	0.43
4:A:801:DQ8:CAL	4:A:801:DQ8:CAP	2.95	0.43
1:B:293:LEU:HD11	1:B:297:ARG:NH1	2.34	0.43
1:B:352:TYR:O	1:B:353:ALA:C	2.62	0.43
1:C:19:ILE:HD11	1:C:359:ILE:HG13	1.98	0.43
1:G:124:GLU:HG2	1:G:125:TYR:CE2	2.54	0.43
1:G:293:LEU:HD21	1:G:297:ARG:HH21	1.84	0.43
4:E:801:DQ8:HAK	4:E:801:DQ8:HAA1	1.83	0.43
1:F:91:ASP:O	1:F:94:ILE:N	2.52	0.43
1:A:99:CYS:O	1:A:261:LEU:CD1	2.65	0.43
1:A:230:ALA:O	1:A:234:ARG:HB2	2.19	0.43
1:B:167:GLU:CD	1:B:181:ARG:HE	2.27	0.43
1:D:26:ARG:NH1	1:D:26:ARG:CG	2.81	0.43
1:E:202:ILE:HG13	1:E:213:ILE:HD11	2.00	0.43
1:F:102:PHE:HB3	1:F:264:VAL:HG13	1.98	0.43
1:A:168:LEU:HD22	1:A:168:LEU:N	2.34	0.42
1:C:210:VAL:HG12	1:C:211:TYR:N	2.34	0.42
1:E:49:GLU:HG2	1:E:67:THR:HG22	2.01	0.42
1:F:216:LYS:NZ	1:F:217:GLY:N	2.66	0.42
1:G:79:ILE:HG12	1:G:83:ARG:CZ	2.49	0.42
1:G:102:PHE:CZ	1:G:295:LEU:HD21	2.54	0.42
1:G:115:MET:HE3	1:G:263:LEU:HB3	2.01	0.42
1:C:115:MET:HE3	1:C:263:LEU:HB3	2.01	0.42
1:E:91:ASP:HB3	1:E:95:MET:HE3	2.00	0.42
1:E:156:VAL:CG2	1:E:204:VAL:HB	2.46	0.42
1:F:190:ASN:OD1	1:F:190:ASN:C	2.62	0.42
1:G:231:TYR:H	1:G:231:TYR:HD1	1.63	0.42
1:A:47:ARG:HG3	1:A:47:ARG:HH11	1.84	0.42
1:A:144:PHE:O	1:A:145:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:O	1:B:211:TYR:C	2.60	0.42
1:D:26:ARG:HD3	1:D:109:THR:HA	2.00	0.42
1:F:170:ASP:CG	1:F:173:ASN:HB2	2.44	0.42
1:G:43:CYS:HB3	1:G:71:VAL:CG1	2.49	0.42
1:G:196:ILE:HG12	1:G:199:LEU:HD23	2.00	0.42
1:B:357:LYS:HE2	1:B:357:LYS:HB3	1.77	0.42
1:C:165:ASN:O	1:C:166:GLU:HB2	2.19	0.42
1:C:342:ASN:O	1:C:343:LEU:C	2.63	0.42
1:E:162:GLU:HG3	1:E:171:LEU:HD21	2.02	0.42
1:F:172:LEU:CD2	1:F:216:LYS:HZ1	2.18	0.42
1:G:78:GLN:O	1:G:81:VAL:CG2	2.68	0.42
1:A:164:TYR:O	1:A:165:ASN:C	2.60	0.42
1:F:123:GLU:OE1	1:F:124:GLU:N	2.52	0.42
1:G:91:ASP:HA	1:G:94:ILE:HG22	2.01	0.42
1:G:169:PHE:CD1	1:G:169:PHE:N	2.87	0.42
1:G:336:ILE:HA	1:G:336:ILE:HD13	1.61	0.42
1:A:144:PHE:HE1	1:A:156:VAL:CG1	2.23	0.42
1:C:143:ILE:CD1	1:C:243:ILE:HD11	2.49	0.42
1:C:245:MET:HE3	1:C:245:MET:HB2	1.90	0.42
1:E:82:TYR:CD1	1:E:82:TYR:C	2.97	0.42
1:G:44:ASP:CG	1:G:47:ARG:HB3	2.45	0.42
1:B:303:VAL:CG2	1:B:304:GLU:HG3	2.50	0.42
1:D:64:LYS:HE2	1:D:66:TYR:CZ	2.53	0.42
1:F:102:PHE:O	1:F:102:PHE:CD1	2.72	0.42
1:F:262:ASN:C	1:F:263:LEU:HD23	2.45	0.42
1:B:102:PHE:CE1	1:B:332:ILE:CG1	2.98	0.42
1:B:362:LYS:HA	1:B:363:PRO:HD3	1.82	0.42
1:C:170:ASP:OD2	1:C:199:LEU:HA	2.20	0.42
1:C:212:GLN:HE21	1:C:212:GLN:HB2	1.68	0.42
1:E:93:VAL:O	1:E:259:GLY:HA3	2.20	0.42
1:F:306:THR:CB	1:F:307:PRO:CD	2.96	0.42
4:F:801:DQ8:HAK	4:F:801:DQ8:HAA1	1.77	0.42
1:G:78:GLN:HB2	1:G:138:ARG:NH2	2.35	0.42
1:A:33:ARG:HG2	1:A:33:ARG:NH1	2.34	0.42
1:G:167:GLU:CD	1:G:181:ARG:HD3	2.45	0.42
1:G:270:GLU:O	1:G:271:ASN:C	2.63	0.42
1:A:309:VAL:HB	1:A:311:TYR:CE2	2.55	0.42
1:C:144:PHE:C	1:C:146:LYS:N	2.76	0.42
1:E:26:ARG:H	1:E:26:ARG:HG3	1.65	0.42
1:E:72:PHE:CD2	1:E:76:THR:HG21	2.55	0.42
1:E:195:ILE:HG13	1:E:195:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:LEU:HD12	1:E:292:LEU:HA	1.77	0.42
1:G:149:ASP:OD1	1:G:149:ASP:N	2.44	0.42
1:G:155:SER:HB2	1:G:244:HIS:ND1	2.35	0.42
1:G:352:TYR:CD1	1:G:352:TYR:C	2.98	0.42
1:D:134:GLY:O	1:D:138:ARG:HG3	2.20	0.41
1:D:158:VAL:HA	1:D:240:SER:O	2.19	0.41
1:D:214:LEU:HD13	4:D:801:DQ8:CAJ	2.50	0.41
1:F:23:VAL:HG21	1:F:68:PHE:CE2	2.54	0.41
1:F:106:GLN:O	1:F:107:THR:C	2.61	0.41
1:F:159:SER:HA	1:F:172:LEU:HD12	2.02	0.41
1:A:136:ILE:HB	1:A:137:PRO:HD3	2.02	0.41
1:C:33:ARG:NH1	1:G:179:SER:OG	2.54	0.41
1:C:354:HIS:C	1:C:356:ALA:N	2.78	0.41
1:C:357:LYS:H	1:C:357:LYS:HG3	1.66	0.41
1:C:362:LYS:N	1:C:362:LYS:CD	2.79	0.41
1:D:98:ASN:C	1:D:99:CYS:SG	3.03	0.41
1:F:143:ILE:HD12	1:F:143:ILE:HA	1.87	0.41
1:F:350:LEU:HD23	1:F:350:LEU:HA	1.82	0.41
1:G:160:LEU:HD22	4:G:801:DQ8:HAA2	2.02	0.41
1:G:182:LEU:HD12	1:G:182:LEU:HA	1.58	0.41
1:A:144:PHE:O	1:A:147:LEU:N	2.53	0.41
1:A:322:ASP:O	1:A:328:THR:OG1	2.37	0.41
1:D:162:GLU:HG2	1:D:237:SER:HB3	2.03	0.41
1:E:293:LEU:HD23	1:E:297:ARG:NH1	2.35	0.41
1:E:294:THR:HG22	1:E:317:THR:HG21	2.01	0.41
1:F:128:GLU:CD	1:F:141:HIS:CD2	2.98	0.41
1:A:144:PHE:HB2	1:A:207:LYS:CD	2.51	0.41
1:A:177:ASP:OD1	1:A:177:ASP:C	2.64	0.41
1:A:320:LEU:HA	1:A:320:LEU:HD23	1.66	0.41
1:C:104:TYR:CD1	1:C:104:TYR:C	2.99	0.41
1:C:261:LEU:HG	1:C:263:LEU:HD21	2.03	0.41
1:F:144:PHE:HE1	1:F:156:VAL:HG11	1.84	0.41
1:G:136:ILE:O	1:G:137:PRO:C	2.60	0.41
1:G:161:LEU:CD1	1:G:162:GLU:N	2.82	0.41
1:A:94:ILE:O	1:A:94:ILE:HG22	2.21	0.41
4:B:801:DQ8:HAK	4:B:801:DQ8:HAA1	1.87	0.41
1:D:77:LYS:HD2	1:D:77:LYS:HA	1.82	0.41
1:D:210:VAL:O	1:D:211:TYR:C	2.64	0.41
1:G:161:LEU:C	1:G:161:LEU:CD1	2.87	0.41
1:G:167:GLU:C	1:G:168:LEU:HD13	2.45	0.41
1:G:177:ASP:O	1:G:178:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:ASN:OD1	1:G:271:ASN:O	2.38	0.41
1:G:305:ARG:HD3	1:G:306:THR:N	2.36	0.41
1:A:64:LYS:HE2	1:A:64:LYS:HB3	1.88	0.41
1:A:330:THR:CG2	1:A:331:SER:H	2.33	0.41
1:B:92:GLU:OE2	1:B:329:ARG:CZ	2.68	0.41
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.77	0.41
1:D:51:SER:HB2	1:D:65:THR:OG1	2.21	0.41
1:D:64:LYS:HE3	1:D:64:LYS:HB3	1.63	0.41
1:E:61:SER:O	1:F:64:LYS:HA	2.21	0.41
1:F:124:GLU:O	1:F:125:TYR:CD1	2.73	0.41
1:A:120:SER:HA	1:A:121:PRO:HD3	1.94	0.41
4:B:801:DQ8:HAS1	4:B:801:DQ8:HAQ	2.01	0.41
1:C:119:ARG:HA	1:C:130:ASP:OD2	2.21	0.41
1:C:164:TYR:CD1	1:C:164:TYR:C	2.98	0.41
1:C:206:ASN:HD21	1:C:208:ASP:HB2	1.75	0.41
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.76	0.41
4:E:801:DQ8:HAS1	4:E:801:DQ8:HAQ	2.00	0.41
1:F:93:VAL:O	1:F:96:GLY:N	2.40	0.41
1:F:127:TRP:O	1:F:127:TRP:CE3	2.74	0.41
1:F:222:THR:O	1:F:226:THR:HG23	2.20	0.41
1:B:102:PHE:CE1	1:B:332:ILE:CD1	2.97	0.41
1:B:143:ILE:HD13	1:B:243:ILE:HD11	2.01	0.41
1:C:309:VAL:HG11	1:C:311:TYR:CZ	2.56	0.41
1:D:136:ILE:O	1:D:137:PRO:C	2.61	0.41
1:F:171:LEU:HA	1:F:171:LEU:HD13	1.77	0.41
1:F:263:LEU:HD23	1:F:263:LEU:N	2.36	0.41
1:F:266:LEU:HD22	1:F:316:LEU:HD21	2.03	0.41
1:F:291:SER:HB3	1:F:316:LEU:HB3	2.03	0.41
1:F:298:VAL:O	1:F:299:ILE:C	2.63	0.41
1:A:126:THR:O	1:A:129:GLU:N	2.54	0.41
1:C:82:TYR:CD1	1:C:86:VAL:HB	2.56	0.41
1:D:83:ARG:HA	1:D:87:CYS:SG	2.61	0.41
1:D:123:GLU:O	1:D:125:TYR:N	2.54	0.41
1:D:168:LEU:HB2	1:D:182:LEU:HB2	2.03	0.41
1:G:144:PHE:HE2	1:G:206:ASN:O	2.03	0.41
1:G:162:GLU:OE2	1:G:231:TYR:OH	2.37	0.41
1:A:20:GLN:O	1:A:331:SER:HA	2.21	0.40
1:B:170:ASP:CG	1:B:173:ASN:HB2	2.46	0.40
1:B:288:ILE:HD12	1:B:288:ILE:O	2.20	0.40
1:C:70:MET:C	1:C:71:VAL:HG23	2.46	0.40
1:D:120:SER:N	1:D:130:ASP:OD2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:ASP:O	1:F:70:MET:HG3	2.21	0.40
1:F:146:LYS:C	1:F:147:LEU:HD23	2.46	0.40
1:G:237:SER:HB3	1:G:265:ASP:HB3	2.03	0.40
1:A:144:PHE:H	1:A:207:LYS:HZ2	1.69	0.40
1:B:184:MET:HE2	1:B:319:ILE:CG1	2.51	0.40
1:D:127:TRP:CE2	1:D:128:GLU:HG3	2.56	0.40
1:E:59:ASP:OD2	1:F:64:LYS:NZ	2.55	0.40
1:E:345:GLU:H	1:E:345:GLU:CD	2.29	0.40
1:F:234:ARG:HD3	1:F:288:ILE:HD11	2.02	0.40
1:G:292:LEU:HD12	1:G:292:LEU:HA	1.73	0.40
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.80	0.40
1:C:266:LEU:CD2	1:C:316:LEU:HD21	2.52	0.40
1:D:229:ASN:O	1:D:230:ALA:HB3	2.21	0.40
1:F:242:THR:HB	1:F:260:LYS:HG3	2.03	0.40
1:A:86:VAL:O	1:A:89:ILE:N	2.54	0.40
1:A:93:VAL:HG11	1:A:261:LEU:HB2	2.02	0.40
1:A:103:ALA:HB1	1:A:111:LYS:CB	2.51	0.40
1:A:192:ARG:NH2	1:A:327:ARG:HG3	2.37	0.40
1:B:127:TRP:O	1:B:128:GLU:C	2.63	0.40
1:B:312:ARG:HA	1:B:312:ARG:HD3	1.86	0.40
1:D:111:LYS:HB2	2:D:601:ADP:O2B	2.20	0.40
1:E:143:ILE:HG23	1:E:243:ILE:HD13	2.04	0.40
1:F:199:LEU:HD12	1:F:200:GLU:N	2.37	0.40
1:G:168:LEU:C	1:G:169:PHE:CD1	2.99	0.40
1:A:114:THR:O	1:A:135:ILE:HG13	2.22	0.40
1:B:18:ASN:HA	1:B:360:LEU:HA	2.03	0.40
1:C:162:GLU:OE1	1:C:231:TYR:OH	2.29	0.40
1:C:293:LEU:CD2	1:C:297:ARG:NH2	2.85	0.40
1:C:308:HIS:HB3	7:D:2024:HOH:O	2.21	0.40
1:D:137:PRO:HD3	4:D:801:DQ8:HAJ	2.02	0.40
1:E:130:ASP:OD1	1:E:131:PRO:HD2	2.22	0.40
1:F:136:ILE:CG2	1:F:239:PHE:CE2	3.05	0.40
1:F:184:MET:CE	1:F:319:ILE:HG13	2.52	0.40
1:F:243:ILE:N	1:F:259:GLY:O	2.44	0.40
1:G:301:ALA:HA	1:G:304:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/368 (86%)	300 (95%)	17 (5%)	0	100	100
1	B	319/368 (87%)	308 (97%)	11 (3%)	0	100	100
1	C	320/368 (87%)	302 (94%)	17 (5%)	1 (0%)	36	56
1	D	317/368 (86%)	303 (96%)	14 (4%)	0	100	100
1	E	315/368 (86%)	300 (95%)	15 (5%)	0	100	100
1	F	314/368 (85%)	286 (91%)	27 (9%)	1 (0%)	36	56
1	G	312/368 (85%)	277 (89%)	33 (11%)	2 (1%)	21	38
All	All	2214/2576 (86%)	2076 (94%)	134 (6%)	4 (0%)	43	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	206	ASN
1	G	97	TYR
1	C	190	ASN
1	F	307	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/322 (88%)	243 (86%)	41 (14%)	3	5
1	B	288/322 (89%)	257 (89%)	31 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/322 (89%)	249 (87%)	38 (13%)	4	7
1	D	284/322 (88%)	251 (88%)	33 (12%)	5	10
1	E	281/322 (87%)	233 (83%)	48 (17%)	2	3
1	F	279/322 (87%)	225 (81%)	54 (19%)	1	2
1	G	269/322 (84%)	200 (74%)	69 (26%)	0	1
All	All	1972/2254 (88%)	1658 (84%)	314 (16%)	2	4

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	30	LEU
1	A	50	VAL
1	A	51	SER
1	A	63	ARG
1	A	71	VAL
1	A	111	LYS
1	A	120	SER
1	A	126	THR
1	A	141	HIS
1	A	142	GLN
1	A	148	THR
1	A	152	THR
1	A	161	LEU
1	A	178	VAL
1	A	182	LEU
1	A	184	MET
1	A	189	ARG
1	A	195	ILE
1	A	197	LYS
1	A	203	THR
1	A	220	LYS
1	A	227	LEU
1	A	234	ARG
1	A	237	SER
1	A	240	SER
1	A	255	LEU
1	A	256	VAL
1	A	288	ILE
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	291	SER
1	A	298	VAL
1	A	306	THR
1	A	320	LEU
1	A	328	THR
1	A	341	LEU
1	A	343	LEU
1	A	348	SER
1	A	351	GLU
1	A	357	LYS
1	A	360	LEU
1	B	18	ASN
1	B	19	ILE
1	B	20	GLN
1	B	30	LEU
1	B	64	LYS
1	B	102	PHE
1	B	111	LYS
1	B	119	ARG
1	B	123	GLU
1	B	126	THR
1	B	128	GLU
1	B	149	ASP
1	B	161	LEU
1	B	163	ILE
1	B	178	VAL
1	B	182	LEU
1	B	184	MET
1	B	220	LYS
1	B	227	LEU
1	B	233	SER
1	B	237	SER
1	B	247	GLU
1	B	255	LEU
1	B	288	ILE
1	B	289	ASN
1	B	291	SER
1	B	297	ARG
1	B	327	ARG
1	B	341	LEU
1	B	355	ARG
1	B	360	LEU

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Mol	Chain	Res	Type
1	C	22	VAL
1	C	30	LEU
1	C	34	LYS
1	C	67	THR
1	C	94	ILE
1	C	119	ARG
1	C	126	THR
1	C	129	GLU
1	C	145[A]	GLU
1	C	145[B]	GLU
1	C	149	ASP
1	C	161	LEU
1	C	162	GLU
1	C	168	LEU
1	C	178	VAL
1	C	186	ASP
1	C	189	ARG
1	C	190	ASN
1	C	203	THR
1	C	206	ASN
1	C	207	LYS
1	C	212	GLN
1	C	216	LYS
1	C	227	LEU
1	C	234	ARG
1	C	258	ILE
1	C	298	VAL
1	C	300	THR
1	C	308	HIS
1	C	320	LEU
1	C	324	LEU
1	C	337	SER
1	C	340	SER
1	C	341	LEU
1	C	351	GLU
1	C	359	ILE
1	C	360	LEU
1	C	362	LYS
1	D	19	ILE
1	D	34	LYS
1	D	36	SER
1	D	64	LYS

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Mol	Chain	Res	Type
1	D	67	THR
1	D	71	VAL
1	D	79	ILE
1	D	86	VAL
1	D	90	LEU
1	D	93	VAL
1	D	123	GLU
1	D	126	THR
1	D	128	GLU
1	D	148	THR
1	D	160	LEU
1	D	167	GLU
1	D	168	LEU
1	D	184	MET
1	D	206	ASN
1	D	207	LYS
1	D	220	LYS
1	D	227	LEU
1	D	229	ASN
1	D	232	SER
1	D	237	SER
1	D	291	SER
1	D	293	LEU
1	D	303	VAL
1	D	309	VAL
1	D	337	SER
1	D	341	LEU
1	D	351	GLU
1	D	357	LYS
1	E	19	ILE
1	E	20	GLN
1	E	26	ARG
1	E	33	ARG
1	E	36	SER
1	E	59	ASP
1	E	65	THR
1	E	84	SER
1	E	86	VAL
1	E	92	GLU
1	E	94	ILE
1	E	111	LYS
1	E	118	GLU

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Mol	Chain	Res	Type
1	E	125	TYR
1	E	132	LEU
1	E	139	THR
1	E	142	GLN
1	E	145	GLU
1	E	147	LEU
1	E	152	THR
1	E	154	PHE
1	E	161	LEU
1	E	166	GLU
1	E	171	LEU
1	E	181	ARG
1	E	184	MET
1	E	185	PHE
1	E	191	LYS
1	E	195	ILE
1	E	202	ILE
1	E	203	THR
1	E	210	VAL
1	E	212	GLN
1	E	216	LYS
1	E	222	THR
1	E	227	LEU
1	E	237	SER
1	E	258	ILE
1	E	288	ILE
1	E	293	LEU
1	E	298	VAL
1	E	303	VAL
1	E	309	VAL
1	E	312	ARG
1	E	319	ILE
1	E	348	SER
1	E	355	ARG
1	E	361	ASN
1	F	19	ILE
1	F	20	GLN
1	F	26	ARG
1	F	32	GLU
1	F	36	SER
1	F	51	SER
1	F	79	ILE

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Mol	Chain	Res	Type
1	F	86	VAL
1	F	89	ILE
1	F	90	LEU
1	F	93	VAL
1	F	112	THR
1	F	114	THR
1	F	115	MET
1	F	120	SER
1	F	132	LEU
1	F	139	THR
1	F	141	HIS
1	F	148	THR
1	F	154	PHE
1	F	161	LEU
1	F	168	LEU
1	F	171	LEU
1	F	181	ARG
1	F	194	VAL
1	F	195	ILE
1	F	199	LEU
1	F	204	VAL
1	F	210	VAL
1	F	213	ILE
1	F	216	LYS
1	F	220	LYS
1	F	222	THR
1	F	227	LEU
1	F	238	VAL
1	F	242	THR
1	F	243	ILE
1	F	244	HIS
1	F	257	LYS
1	F	265	ASP
1	F	271	ASN
1	F	292	LEU
1	F	293	LEU
1	F	299	ILE
1	F	300	THR
1	F	306	THR
1	F	308	HIS
1	F	309	VAL
1	F	312	ARG

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Mol	Chain	Res	Type
1	F	323	SER
1	F	341	LEU
1	F	351	GLU
1	F	359	ILE
1	F	361	ASN
1	G	18	ASN
1	G	21	VAL
1	G	22	VAL
1	G	39	SER
1	G	41	VAL
1	G	44	ASP
1	G	47	ARG
1	G	57	LEU
1	G	67	THR
1	G	79	ILE
1	G	81	VAL
1	G	86	VAL
1	G	89	ILE
1	G	98	ASN
1	G	100	THR
1	G	102	PHE
1	G	104	TYR
1	G	107	THR
1	G	111	LYS
1	G	122	ASN
1	G	126	THR
1	G	128	GLU
1	G	143	ILE
1	G	148	THR
1	G	149	ASP
1	G	155	SER
1	G	158	VAL
1	G	161	LEU
1	G	166	GLU
1	G	168	LEU
1	G	181	ARG
1	G	182	LEU
1	G	184	MET
1	G	185	PHE
1	G	186	ASP
1	G	189	ARG
1	G	194	VAL

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Mol	Chain	Res	Type
1	G	195	ILE
1	G	196	ILE
1	G	199	LEU
1	G	200	GLU
1	G	204	VAL
1	G	205	HIS
1	G	220	LYS
1	G	223	THR
1	G	226	THR
1	G	227	LEU
1	G	228	MET
1	G	233	SER
1	G	241	VAL
1	G	242	THR
1	G	243	ILE
1	G	264	VAL
1	G	291	SER
1	G	292	LEU
1	G	293	LEU
1	G	294	THR
1	G	298	VAL
1	G	299	ILE
1	G	302	LEU
1	G	306	THR
1	G	316	LEU
1	G	321	GLN
1	G	329	ARG
1	G	336	ILE
1	G	340	SER
1	G	343	LEU
1	G	350	LEU
1	G	352	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	262	ASN
1	B	106	GLN
1	B	205	HIS
1	B	212	GLN
1	B	290	GLN

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Mol	Chain	Res	Type
1	B	308	HIS
1	C	141	HIS
1	D	18	ASN
1	D	106	GLN
1	D	183	GLN
1	D	321	GLN
1	D	361	ASN
1	E	262	ASN
1	E	290	GLN
1	E	342	ASN
1	F	78	GLN
1	F	290	GLN
1	G	142	GLN
1	G	212	GLN
1	G	262	ASN
1	G	354	HIS
1	G	361	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 21 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DQ8	B	801	-	28,28,28	0.67	0	38,38,38	1.05	2 (5%)
4	DQ8	F	801	-	28,28,28	0.76	1 (3%)	38,38,38	1.09	3 (7%)
6	SO4	D	1362	-	4,4,4	0.33	0	6,6,6	0.38	0
2	ADP	A	601	3	28,29,29	1.47	6 (21%)	43,45,45	1.99	13 (30%)
4	DQ8	E	801	-	28,28,28	0.71	1 (3%)	38,38,38	1.08	4 (10%)
2	ADP	G	601	3	28,29,29	1.47	3 (10%)	43,45,45	2.06	10 (23%)
4	DQ8	A	801	-	28,28,28	0.85	1 (3%)	38,38,38	1.12	1 (2%)
4	DQ8	G	801	-	28,28,28	0.91	2 (7%)	38,38,38	1.26	5 (13%)
4	DQ8	D	801	-	28,28,28	0.97	1 (3%)	38,38,38	1.37	5 (13%)
4	DQ8	C	801	-	28,28,28	0.77	0	38,38,38	1.32	6 (15%)
2	ADP	F	601	3	28,29,29	1.60	6 (21%)	43,45,45	1.66	8 (18%)
2	ADP	E	601	3	28,29,29	1.49	6 (21%)	43,45,45	1.79	10 (23%)
2	ADP	C	601	3	28,29,29	1.56	5 (17%)	43,45,45	1.84	12 (27%)
2	ADP	B	601	3	28,29,29	1.34	4 (14%)	43,45,45	2.12	14 (32%)
2	ADP	D	601	3	28,29,29	1.38	4 (14%)	43,45,45	1.97	13 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DQ8	B	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	F	801	-	-	0/27/27/27	0/3/3/3
2	ADP	A	601	3	-	2/16/32/32	0/3/3/3
4	DQ8	E	801	-	-	2/27/27/27	0/3/3/3
2	ADP	G	601	3	-	1/16/32/32	0/3/3/3
4	DQ8	A	801	-	-	0/27/27/27	0/3/3/3
4	DQ8	G	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	D	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	C	801	-	-	2/27/27/27	0/3/3/3
2	ADP	F	601	3	-	2/16/32/32	0/3/3/3
2	ADP	E	601	3	-	5/16/32/32	0/3/3/3
2	ADP	C	601	3	-	3/16/32/32	0/3/3/3
2	ADP	B	601	3	-	2/16/32/32	0/3/3/3
2	ADP	D	601	3	-	1/16/32/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	ADP	C5-C4	5.11	1.48	1.39
2	F	601	ADP	C5-C4	5.06	1.48	1.39
2	C	601	ADP	C5-C4	4.83	1.47	1.39
2	E	601	ADP	C5-C4	4.67	1.47	1.39
2	A	601	ADP	C5-C4	4.52	1.47	1.39
2	B	601	ADP	C5-C4	3.97	1.46	1.39
2	D	601	ADP	C5-C4	3.65	1.45	1.39
2	D	601	ADP	C5-N7	-3.47	1.32	1.39
2	A	601	ADP	C5-C6	2.94	1.49	1.41
2	C	601	ADP	C8-N7	2.93	1.37	1.31
2	F	601	ADP	C5-N7	-2.81	1.33	1.39
2	C	601	ADP	C4-N9	-2.62	1.32	1.37
2	F	601	ADP	PA-O3A	2.59	1.62	1.59
2	C	601	ADP	C5-C6	2.57	1.48	1.41
2	B	601	ADP	C5-N7	-2.57	1.34	1.39
4	A	801	DQ8	CAS-SAT	2.56	1.86	1.81
2	F	601	ADP	C5-C6	2.53	1.48	1.41
2	F	601	ADP	C8-N7	2.52	1.36	1.31
2	G	601	ADP	C5-C6	2.50	1.48	1.41
2	E	601	ADP	C8-N7	2.50	1.36	1.31
2	E	601	ADP	C4-N9	-2.43	1.32	1.37
2	B	601	ADP	C5-C6	2.39	1.47	1.41
4	D	801	DQ8	CAS-SAT	2.36	1.86	1.81
4	F	801	DQ8	CAS-SAT	2.35	1.86	1.81
2	C	601	ADP	C5-N7	-2.34	1.34	1.39
2	D	601	ADP	C8-N9	-2.33	1.33	1.37
2	E	601	ADP	C5-C6	2.31	1.47	1.41
2	G	601	ADP	C5-N7	-2.30	1.34	1.39
2	D	601	ADP	C4-N9	-2.27	1.33	1.37
4	G	801	DQ8	CAZ-CAW	-2.26	1.50	1.54
2	A	601	ADP	PA-O3A	2.18	1.61	1.59
4	E	801	DQ8	CAS-SAT	2.18	1.86	1.81
2	A	601	ADP	C8-N7	2.14	1.35	1.31
2	E	601	ADP	PA-O3A	2.10	1.61	1.59
4	G	801	DQ8	CAS-SAT	2.09	1.85	1.81
2	A	601	ADP	C4-N9	-2.07	1.33	1.37
2	F	601	ADP	C4-N9	-2.06	1.33	1.37
2	B	601	ADP	C8-N7	2.06	1.35	1.31
2	E	601	ADP	C5-N7	-2.01	1.35	1.39
2	A	601	ADP	C5-N7	-2.01	1.35	1.39

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-6.63	117.59	126.72
2	G	601	ADP	C5-C4-N3	-6.26	118.10	126.72
2	A	601	ADP	C5-C4-N3	-5.80	118.74	126.72
2	G	601	ADP	N3-C4-N9	5.60	136.69	127.17
2	D	601	ADP	C5-C4-N3	-5.41	119.26	126.72
2	D	601	ADP	N3-C4-N9	5.34	136.25	127.17
2	F	601	ADP	C5-C4-N3	-5.32	119.40	126.72
2	B	601	ADP	N3-C4-N9	5.04	135.74	127.17
2	G	601	ADP	C5'-C4'-C3'	-4.71	98.25	115.21
2	E	601	ADP	C5-C4-N3	-4.66	120.30	126.72
2	A	601	ADP	N3-C4-N9	4.52	134.86	127.17
2	C	601	ADP	C5-C4-N3	-4.38	120.69	126.72
2	A	601	ADP	C4-C5-N7	-4.14	105.85	110.58
2	B	601	ADP	C2-N3-C4	3.92	121.41	111.83
2	F	601	ADP	N3-C4-N9	3.90	133.81	127.17
2	E	601	ADP	N3-C4-N9	3.80	133.63	127.17
2	E	601	ADP	N3-C2-N1	-3.73	122.94	128.58
2	G	601	ADP	C2-N3-C4	3.66	120.77	111.83
2	D	601	ADP	C2'-C1'-N9	-3.64	104.26	113.30
2	D	601	ADP	C4-N9-C8	3.50	109.41	105.74
2	C	601	ADP	N3-C4-N9	3.48	133.09	127.17
2	B	601	ADP	C4-C5-N7	-3.48	106.60	110.58
2	F	601	ADP	C4-C5-N7	-3.47	106.61	110.58
2	A	601	ADP	C2-N3-C4	3.37	120.07	111.83
2	A	601	ADP	C4-N9-C8	3.31	109.21	105.74
2	C	601	ADP	N3-C2-N1	-3.30	123.58	128.58
2	E	601	ADP	C2-N3-C4	3.27	119.82	111.83
2	C	601	ADP	C4-N9-C8	3.25	109.16	105.74
2	C	601	ADP	C2-N1-C6	3.17	123.94	118.73
2	C	601	ADP	O2'-C2'-C1'	-3.14	99.29	110.10
2	D	601	ADP	N6-C6-N1	3.03	125.13	118.38
2	B	601	ADP	O3B-PB-O1B	3.02	122.58	110.83
2	G	601	ADP	N3-C2-N1	-3.01	124.02	128.58
4	C	801	DQ8	CAJ-CAK-CAV	-3.01	117.41	120.36
2	A	601	ADP	C5-N7-C8	3.01	108.17	103.45
2	C	601	ADP	C4-C5-N7	-2.99	107.16	110.58
4	D	801	DQ8	CAH-CAN-CAX	-2.97	117.73	120.75
2	D	601	ADP	C5'-C4'-C3'	-2.96	104.55	115.21
2	C	601	ADP	C2-N3-C4	2.96	119.05	111.83
2	E	601	ADP	C4-N9-C8	2.95	108.84	105.74
4	G	801	DQ8	CAR-CAS-SAT	2.94	118.05	109.95
2	F	601	ADP	O3B-PB-O2B	2.93	118.80	107.80
2	B	601	ADP	N3-C2-N1	-2.88	124.22	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ADP	O3B-PB-O2B	2.88	118.59	107.80
2	B	601	ADP	O3A-PA-O1A	-2.86	102.09	110.70
2	E	601	ADP	C2-N1-C6	2.83	123.38	118.73
2	F	601	ADP	C2-N3-C4	2.79	118.66	111.83
2	B	601	ADP	C5-N7-C8	2.76	107.78	103.45
4	C	801	DQ8	CAG-CAM-CAW	-2.74	117.96	120.75
2	E	601	ADP	C4-C5-N7	-2.74	107.45	110.58
4	D	801	DQ8	CAK-CAV-CAQ	2.73	122.41	119.25
4	G	801	DQ8	CAP-CAY-CAZ	-2.70	115.75	121.02
2	D	601	ADP	C2-N3-C4	2.66	118.32	111.83
2	A	601	ADP	O2A-PA-O1A	2.65	124.78	112.44
2	A	601	ADP	N3-C2-N1	-2.59	124.67	128.58
2	A	601	ADP	O3B-PB-O1B	2.56	120.83	110.83
4	E	801	DQ8	CAX-CAZ-CAY	2.54	118.08	111.04
2	A	601	ADP	N9-C8-N7	-2.53	110.35	113.94
2	C	601	ADP	C5'-C4'-C3'	-2.51	106.16	115.21
4	B	801	DQ8	CAX-CAZ-CAY	2.44	117.82	111.04
4	G	801	DQ8	CAK-CAV-CAU	-2.44	115.28	120.83
2	G	601	ADP	O3B-PB-O2B	2.43	116.90	107.80
4	D	801	DQ8	CAE-CAI-CAO	-2.42	117.25	120.24
4	C	801	DQ8	CAW-CAZ-CAX	-2.40	104.39	111.04
2	G	601	ADP	N6-C6-N1	2.39	123.71	118.38
2	G	601	ADP	C4-N9-C8	2.39	108.25	105.74
2	G	601	ADP	C1'-N9-C8	-2.36	121.86	127.09
4	E	801	DQ8	CAW-CAZ-CAY	-2.34	104.55	111.04
2	F	601	ADP	N3-C2-N1	-2.30	125.10	128.58
2	D	601	ADP	C5-N7-C8	2.30	107.07	103.45
2	B	601	ADP	O3B-PB-O3A	-2.30	96.92	104.64
4	F	801	DQ8	CAO-CAX-CAZ	-2.29	116.55	121.02
4	C	801	DQ8	CAX-CAZ-CAY	2.27	117.33	111.04
4	F	801	DQ8	CAR-CAS-SAT	2.26	116.18	109.95
4	E	801	DQ8	CAK-CAV-CAQ	2.26	121.87	119.25
2	C	601	ADP	N9-C8-N7	-2.25	110.74	113.94
2	G	601	ADP	C4-C5-N7	-2.25	108.02	110.58
2	F	601	ADP	C5-N7-C8	2.24	106.97	103.45
4	G	801	DQ8	CAQ-CAY-CAZ	2.23	124.40	120.71
4	F	801	DQ8	CAH-CAN-CAX	-2.22	118.50	120.75
4	G	801	DQ8	CAX-CAZ-CAY	2.22	117.19	111.04
4	E	801	DQ8	CAR-CAS-SAT	2.20	116.01	109.95
2	F	601	ADP	C2-N1-C6	2.19	122.32	118.73
4	D	801	DQ8	CAJ-CAK-CAV	-2.18	118.22	120.36
4	B	801	DQ8	CAK-CAV-CAQ	2.18	121.77	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	ADP	C6-C5-N7	2.17	136.28	132.09
2	B	601	ADP	C4-N9-C8	2.16	108.01	105.74
4	D	801	DQ8	CAX-CAZ-CAY	2.16	117.04	111.04
2	D	601	ADP	C1'-N9-C8	-2.16	122.30	127.09
2	D	601	ADP	C4-C5-N7	-2.16	108.11	110.58
2	D	601	ADP	N3-C2-N1	-2.14	125.34	128.58
4	C	801	DQ8	CAQ-CAV-CAU	-2.13	115.06	120.01
2	D	601	ADP	N9-C8-N7	-2.13	110.91	113.94
2	B	601	ADP	C3'-C2'-C1'	2.13	105.49	101.46
2	D	601	ADP	C5-C6-N6	-2.13	118.02	123.29
2	E	601	ADP	O3B-PB-O2B	2.12	115.75	107.80
2	B	601	ADP	N9-C8-N7	-2.12	110.93	113.94
4	C	801	DQ8	CAM-CAW-CAL	2.12	121.19	118.03
2	B	601	ADP	O4'-C1'-N9	2.09	112.11	108.09
2	B	601	ADP	O2A-PA-O1A	2.09	122.18	112.44
2	C	601	ADP	C5-N7-C8	2.09	106.73	103.45
2	A	601	ADP	C6-C5-N7	2.08	136.09	132.09
4	A	801	DQ8	CAX-CAZ-CAY	2.07	116.79	111.04
2	E	601	ADP	O4'-C4'-C5'	-2.02	102.87	109.33
2	A	601	ADP	O2B-PB-O3A	2.01	111.38	104.64
2	A	601	ADP	C2'-C1'-N9	-2.00	108.32	113.30

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	C5'-O5'-PA-O2A
2	E	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	PA-O3A-PB-O1B
2	C	601	ADP	PA-O3A-PB-O2B
2	G	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	C5'-O5'-PA-O1A
2	F	601	ADP	O4'-C4'-C5'-O5'
4	G	801	DQ8	CAQ-CAY-CAZ-SAT
2	E	601	ADP	O4'-C4'-C5'-O5'
4	C	801	DQ8	CAQ-CAY-CAZ-SAT
4	D	801	DQ8	CAQ-CAY-CAZ-SAT
2	C	601	ADP	C3'-C4'-C5'-O5'
4	B	801	DQ8	CAQ-CAY-CAZ-SAT
4	B	801	DQ8	CAP-CAY-CAZ-SAT
4	C	801	DQ8	CAP-CAY-CAZ-SAT

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Mol	Chain	Res	Type	Atoms
4	D	801	DQ8	CAP-CAY-CAZ-SAT
4	E	801	DQ8	CAQ-CAY-CAZ-SAT
4	G	801	DQ8	CAP-CAY-CAZ-SAT
2	A	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	PA-O3A-PB-O3B
2	C	601	ADP	O4'-C4'-C5'-O5'
4	E	801	DQ8	CAP-CAY-CAZ-SAT
2	E	601	ADP	PB-O3A-PA-O2A
2	F	601	ADP	PB-O3A-PA-O2A

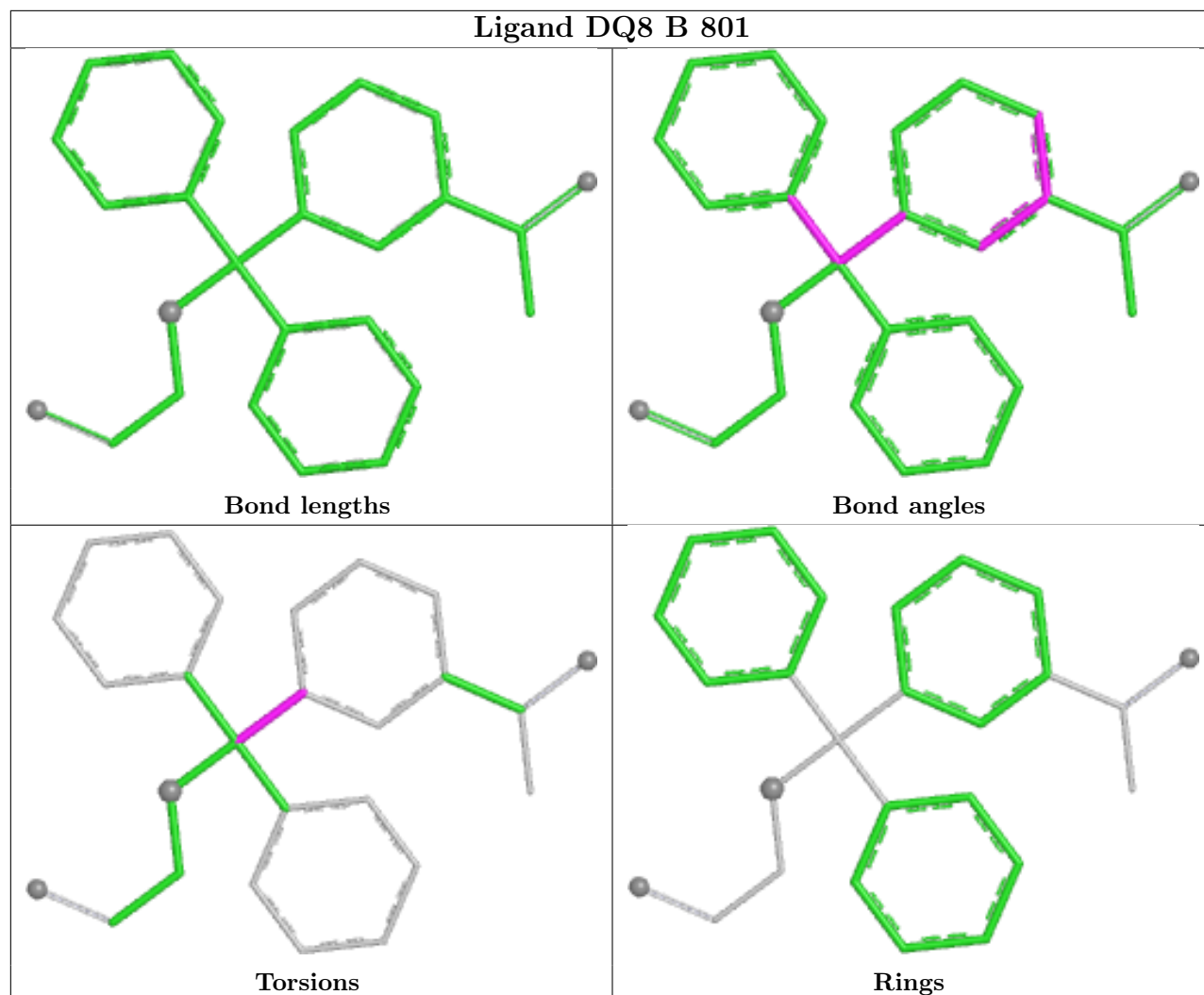
There are no ring outliers.

12 monomers are involved in 63 short contacts:

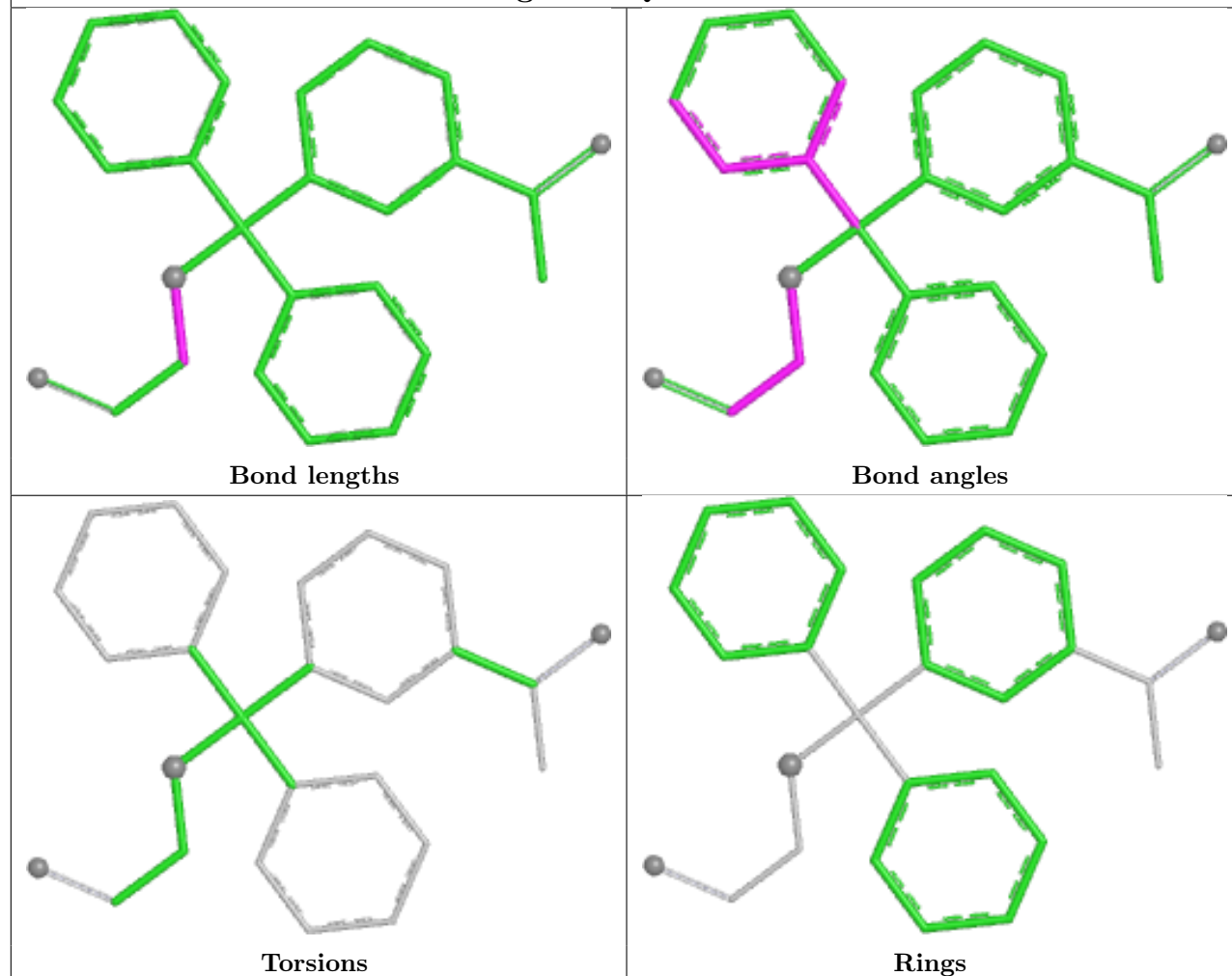
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	DQ8	8	0
4	F	801	DQ8	7	0
4	E	801	DQ8	9	0
2	G	601	ADP	2	0
4	A	801	DQ8	7	0
4	G	801	DQ8	7	0
4	D	801	DQ8	4	0
4	C	801	DQ8	2	0
2	F	601	ADP	3	0
2	E	601	ADP	5	0
2	C	601	ADP	4	0
2	D	601	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

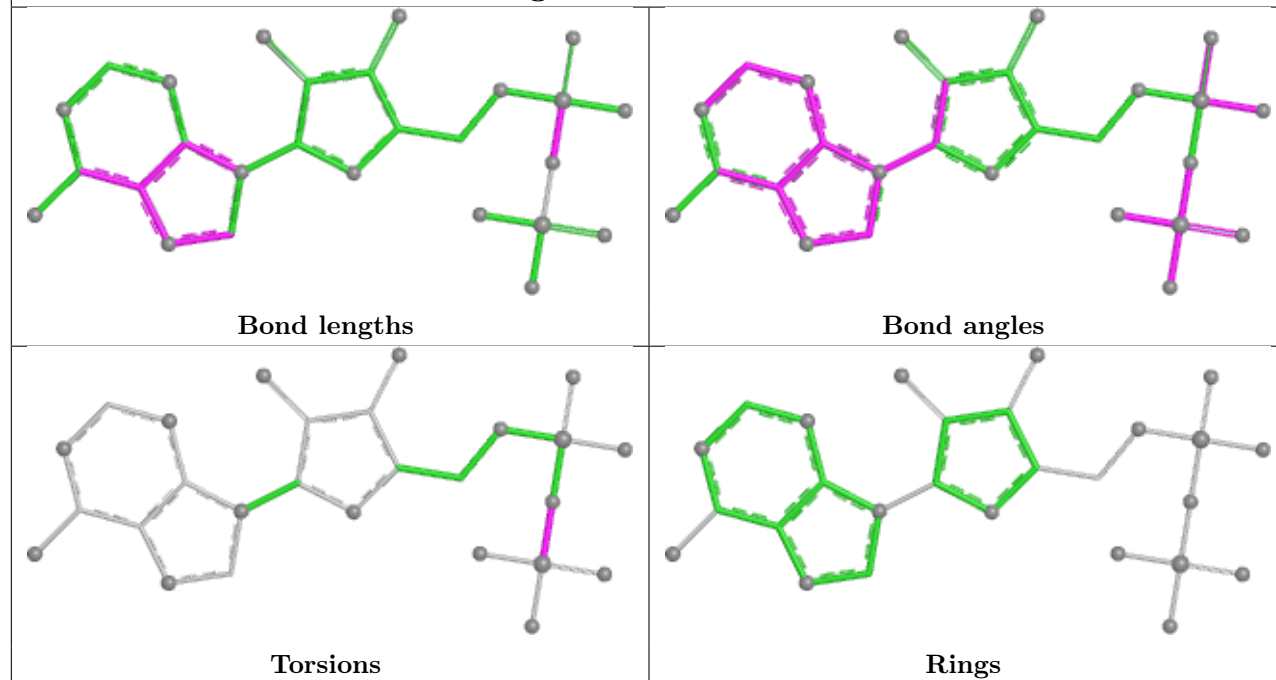
Ligand DQ8 B 801



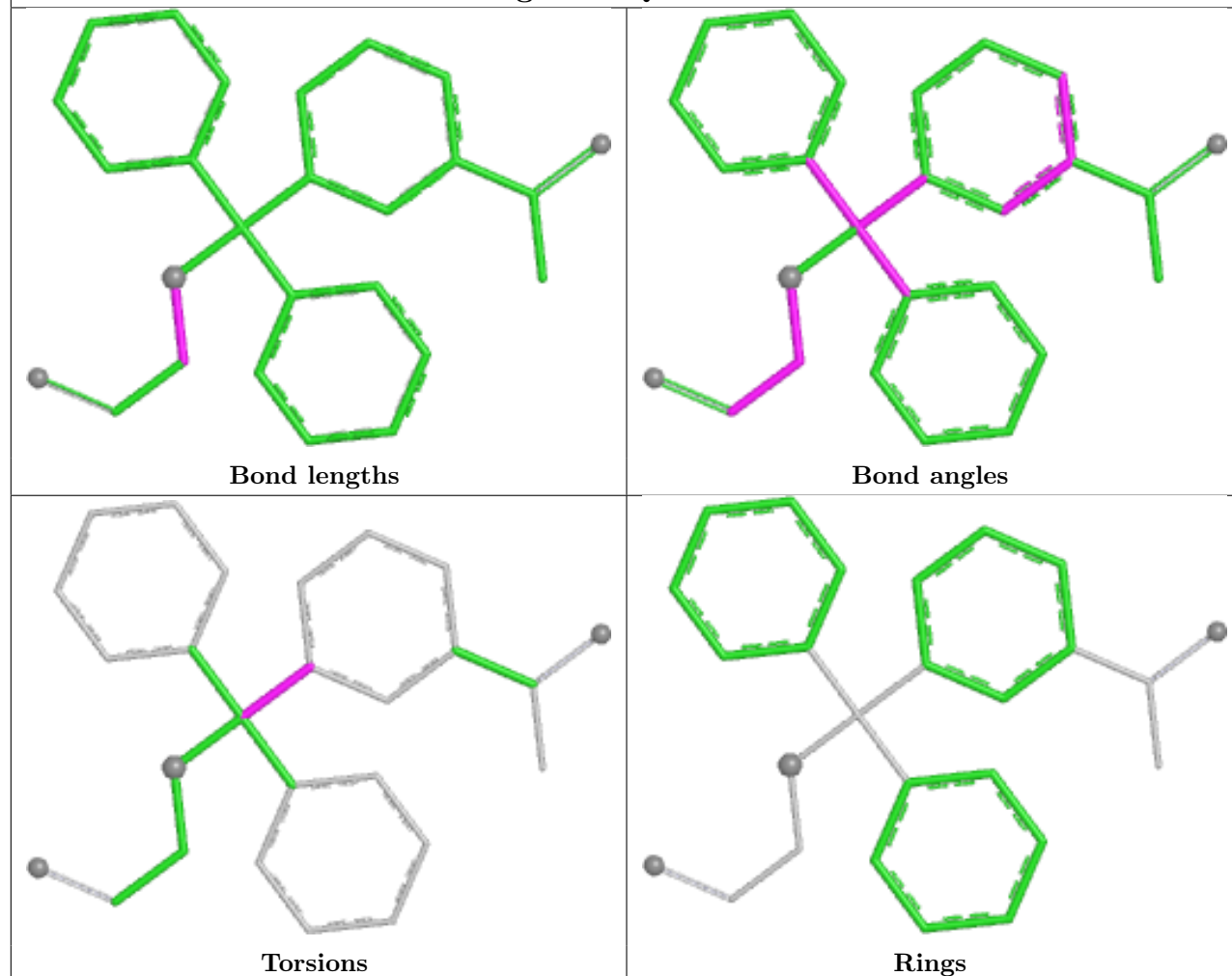
Ligand DQ8 F 801



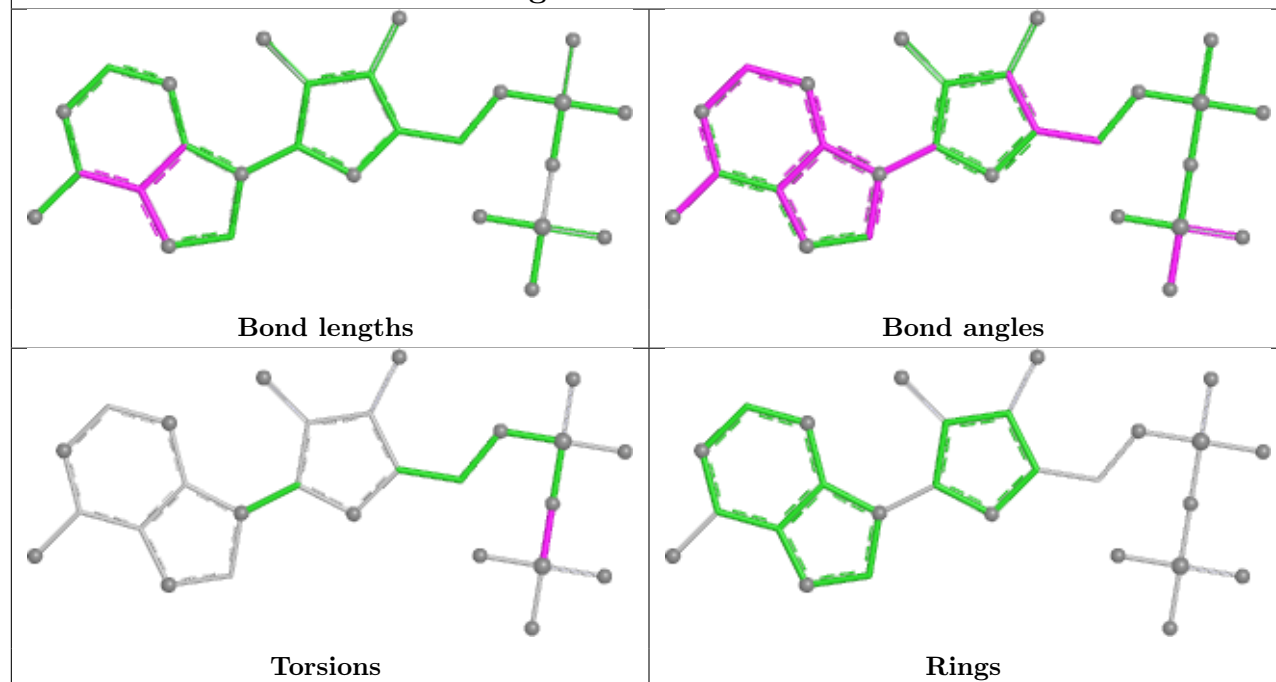
Ligand ADP A 601



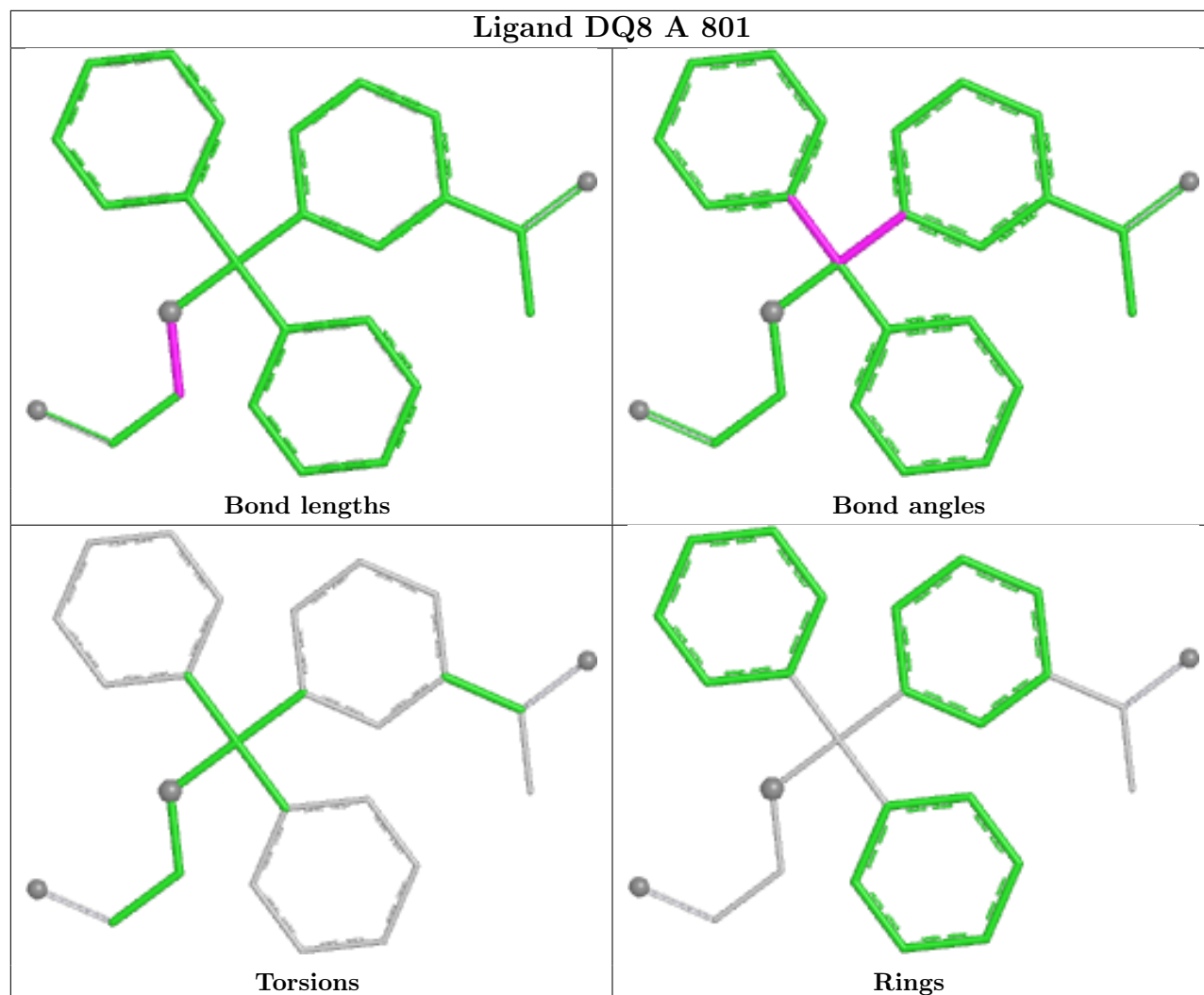
Ligand DQ8 E 801



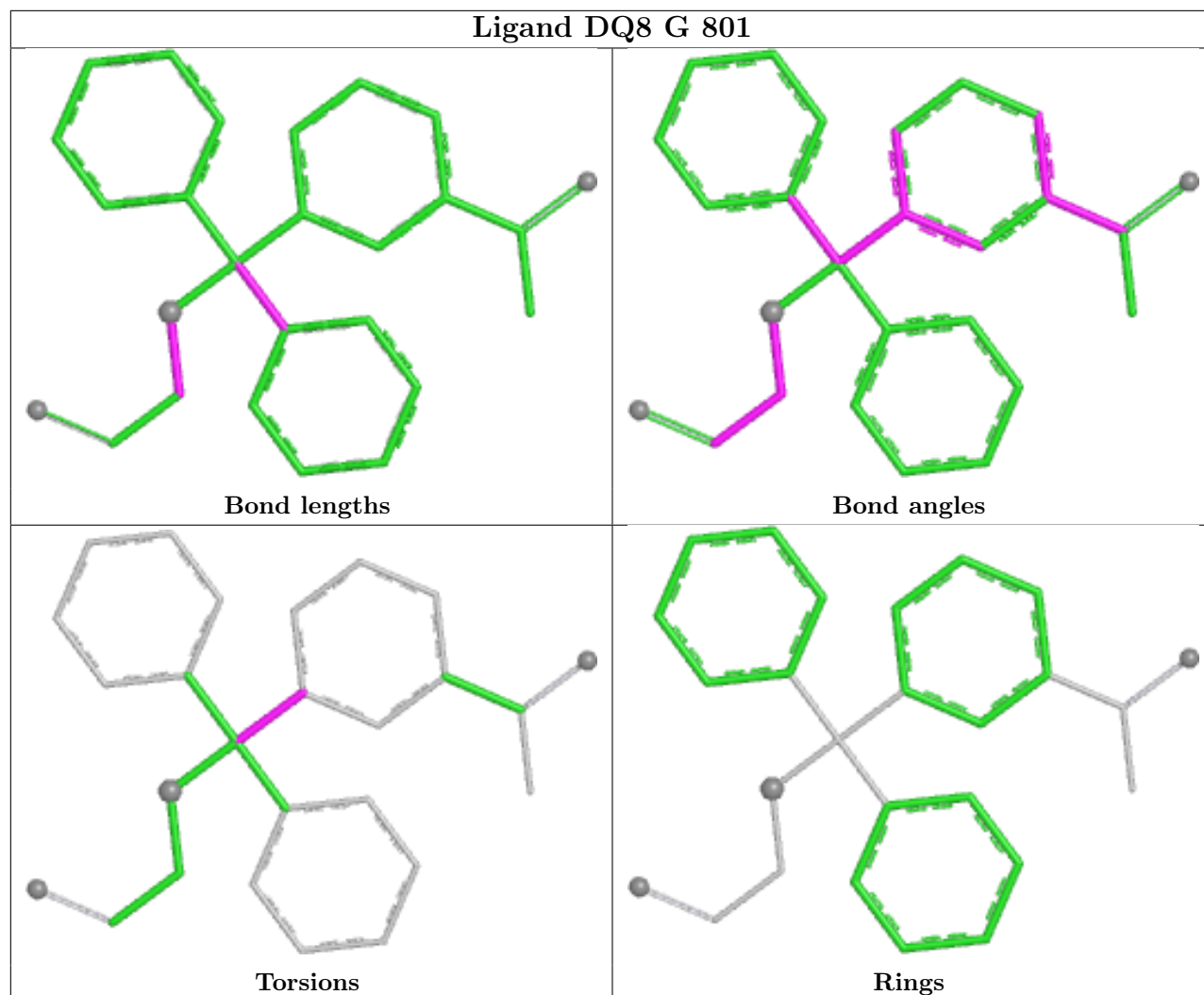
Ligand ADP G 601



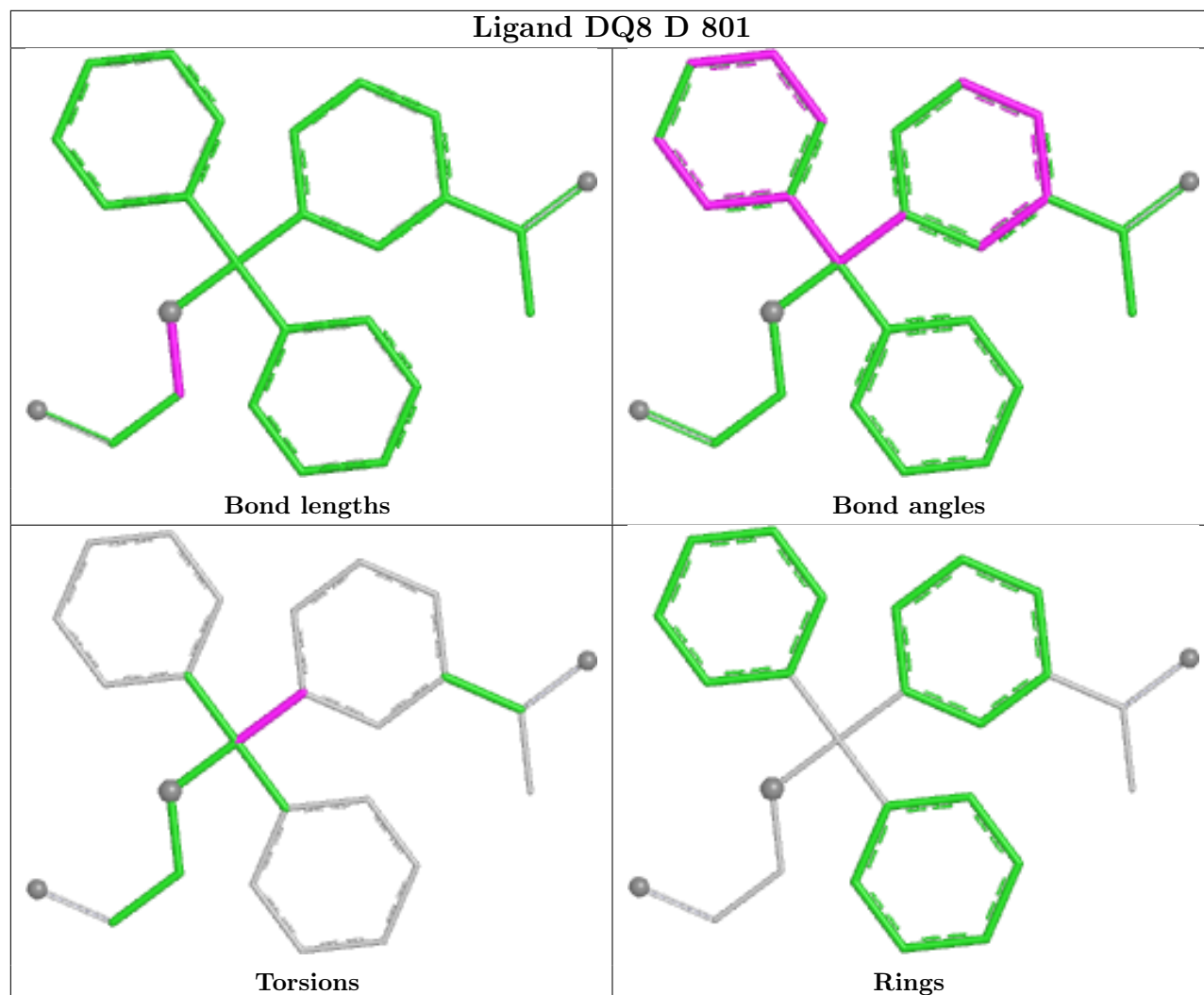
Ligand DQ8 A 801



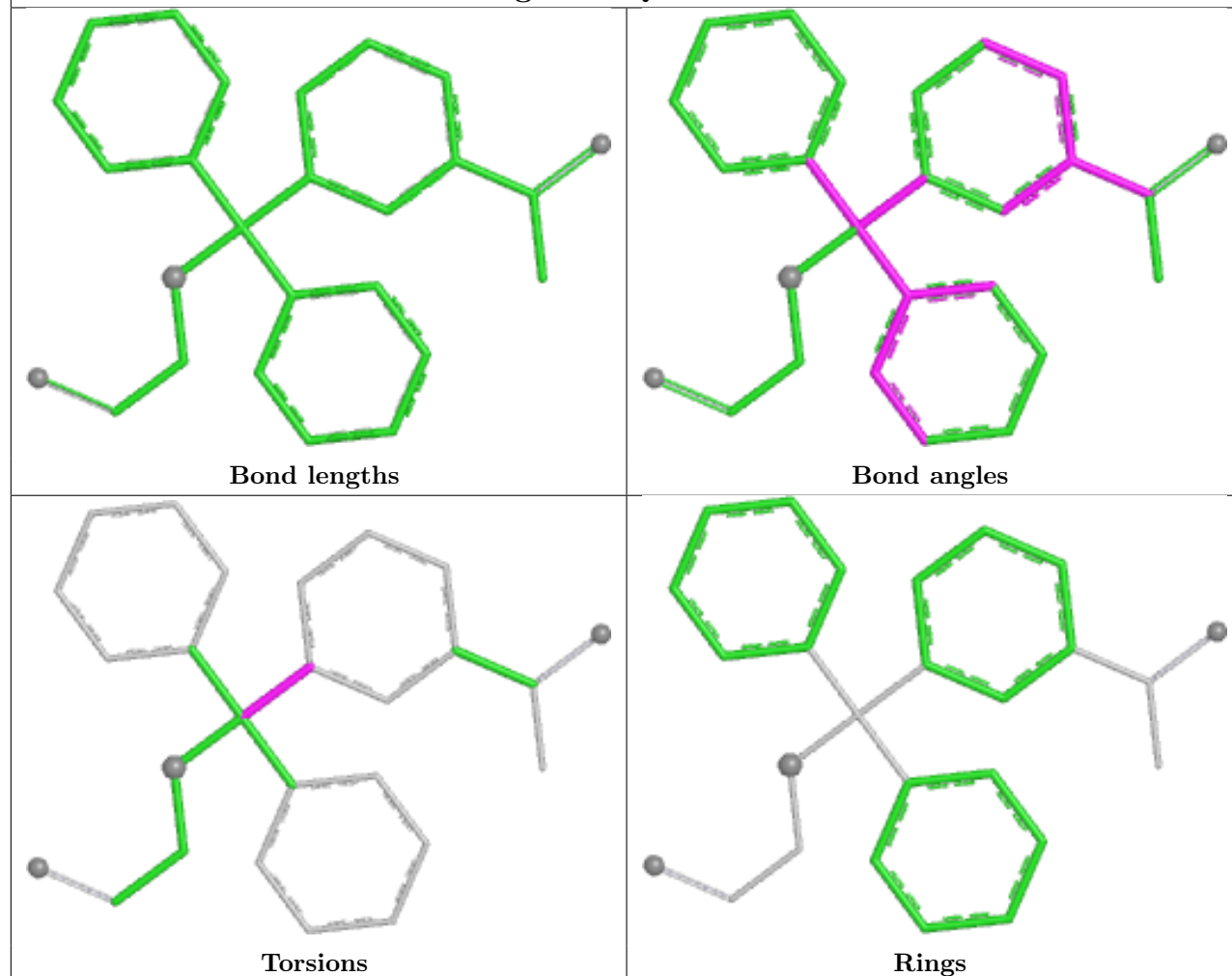
Ligand DQ8 G 801



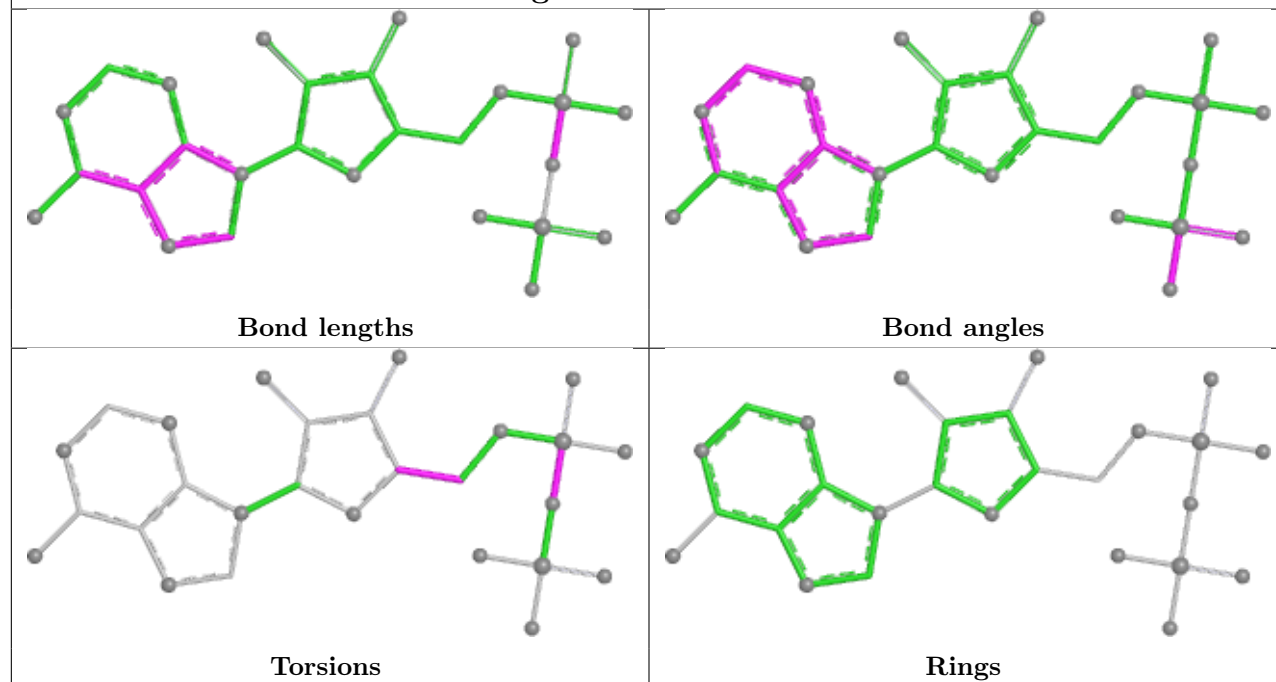
Ligand DQ8 D 801

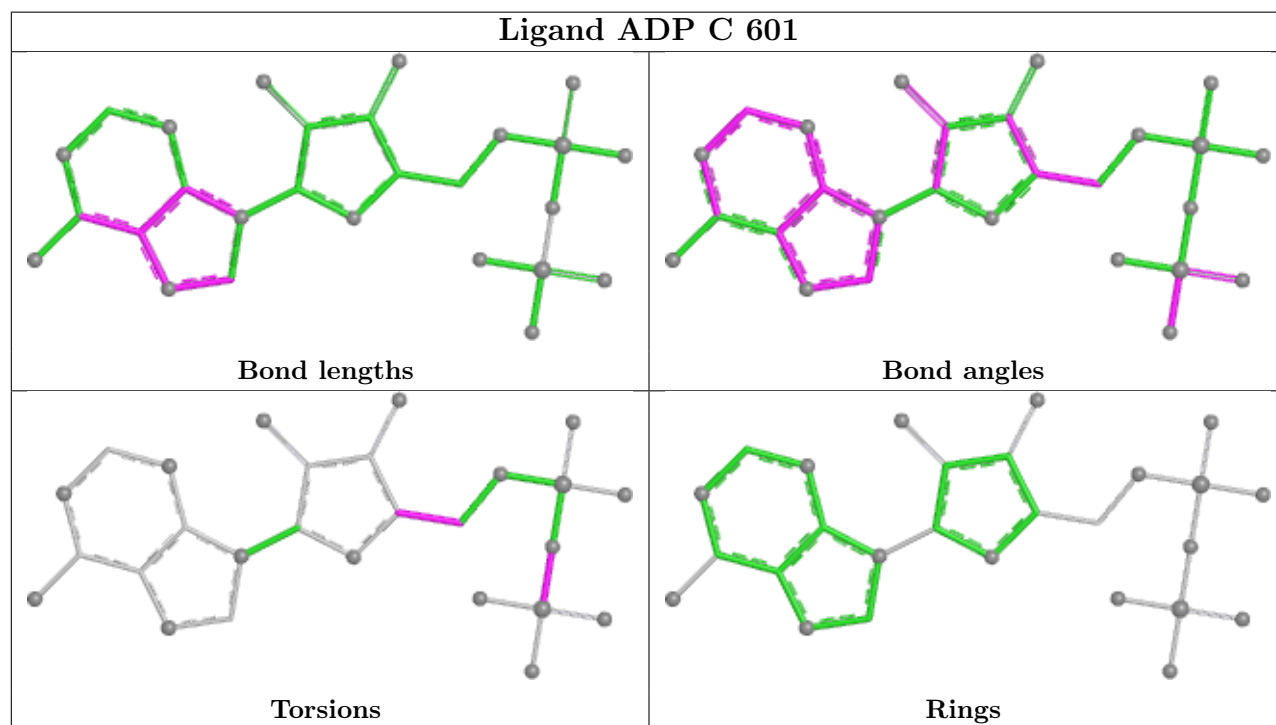
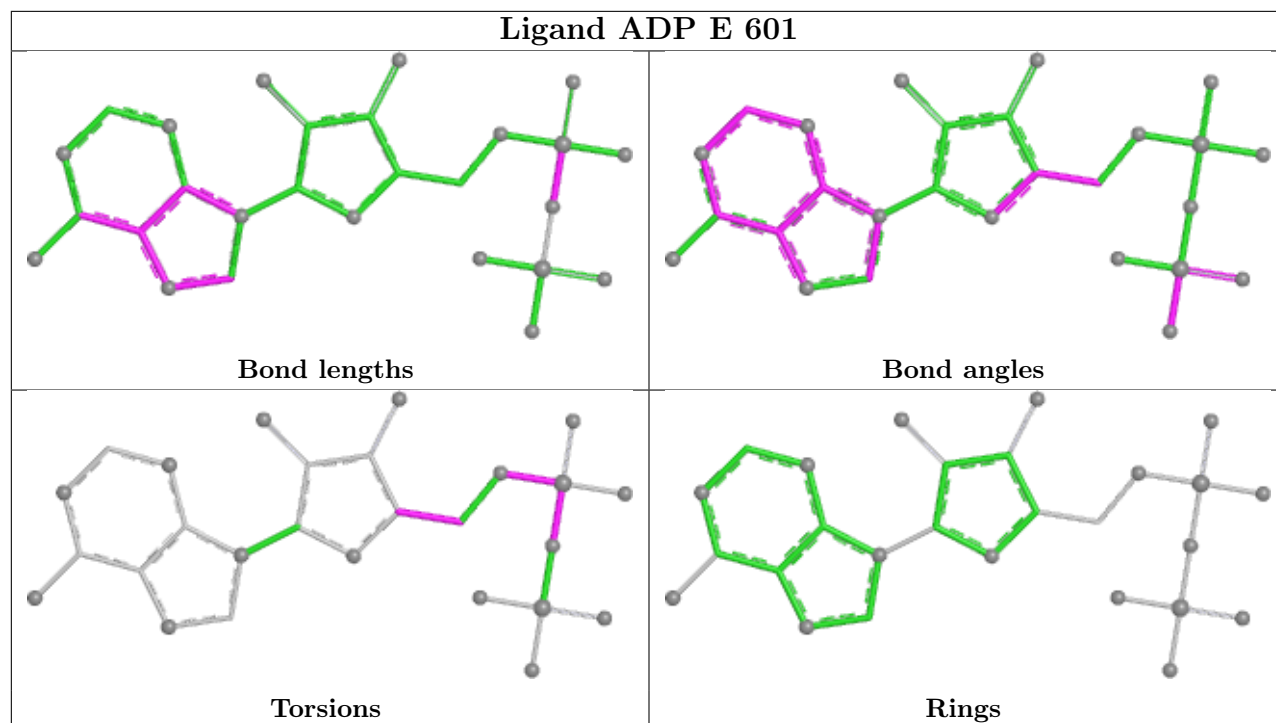


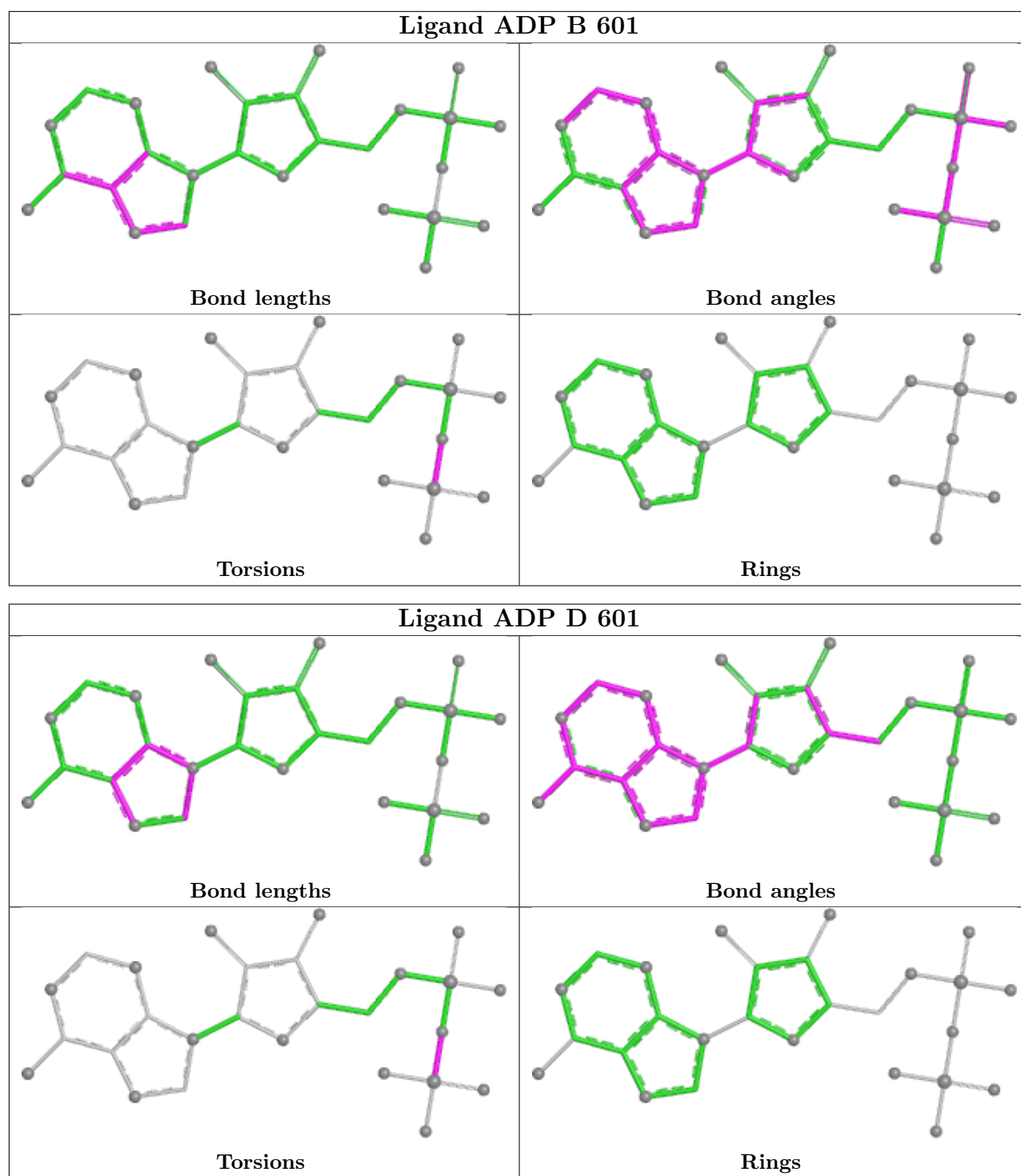
Ligand DQ8 C 801



Ligand ADP F 601







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	322/368 (87%)	0.30	19 (5%)	28 28	25, 54, 90, 112	1 (0%)
1	B	324/368 (88%)	0.18	11 (3%)	48 46	22, 53, 92, 104	1 (0%)
1	C	325/368 (88%)	0.06	10 (3%)	51 49	28, 50, 86, 113	1 (0%)
1	D	322/368 (87%)	0.21	16 (4%)	34 34	20, 50, 92, 114	1 (0%)
1	E	321/368 (87%)	0.54	23 (7%)	21 21	42, 67, 99, 119	0
1	F	319/368 (86%)	0.74	33 (10%)	12 11	41, 71, 106, 117	1 (0%)
1	G	318/368 (86%)	0.91	44 (13%)	6 5	46, 81, 122, 140	0
All	All	2251/2576 (87%)	0.42	156 (6%)	23 22	20, 61, 105, 140	5 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	289	ASN	6.2
1	B	129	GLU	5.2
1	F	93	VAL	5.2
1	G	327	ARG	4.8
1	G	322	ASP	4.5
1	G	309	VAL	4.3
1	F	258	ILE	4.1
1	G	328	THR	4.1
1	C	364	GLU	4.0
1	G	360	LEU	4.0
1	G	154	PHE	4.0
1	E	256	VAL	3.9
1	A	207	LYS	3.8
1	F	148	THR	3.8
1	G	99	CYS	3.8
1	D	358	ASN	3.7
1	F	363	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	152	THR	3.5
1	A	110	GLY	3.5
1	E	325	GLY	3.5
1	F	110	GLY	3.5
1	F	360	LEU	3.5
1	F	326	GLY	3.5
1	E	246	LYS	3.4
1	G	359	ILE	3.4
1	C	246	LYS	3.4
1	A	359	ILE	3.4
1	F	97	TYR	3.3
1	G	291	SER	3.3
1	A	255	LEU	3.3
1	F	362	LYS	3.2
1	A	256	VAL	3.2
1	G	192	ARG	3.2
1	G	102	PHE	3.1
1	E	149	ASP	3.1
1	A	97	TYR	3.1
1	D	256	VAL	3.1
1	D	303	VAL	3.1
1	B	271	ASN	3.1
1	F	203	THR	3.1
1	G	363	PRO	3.0
1	F	133	ALA	3.0
1	G	324	LEU	3.0
1	B	148	THR	3.0
1	B	151	GLY	3.0
1	A	58	ALA	3.0
1	C	365	VAL	3.0
1	D	309	VAL	3.0
1	E	361	ASN	2.9
1	D	152	THR	2.9
1	E	154	PHE	2.9
1	G	153	GLU	2.9
1	B	149	ASP	2.9
1	G	193	GLY	2.9
1	G	308	HIS	2.9
1	F	131	PRO	2.8
1	D	151	GLY	2.8
1	A	125	TYR	2.8
1	F	155	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	2.8
1	F	193	GLY	2.8
1	G	44	ASP	2.8
1	F	301	ALA	2.8
1	E	332	ILE	2.7
1	E	185	PHE	2.7
1	F	149	ASP	2.7
1	G	46	VAL	2.7
1	G	310	PRO	2.7
1	G	19	ILE	2.7
1	G	302	LEU	2.7
1	E	146	LYS	2.7
1	D	128	GLU	2.7
1	A	265	ASP	2.7
1	B	332	ILE	2.6
1	E	188	PRO	2.6
1	F	260	LYS	2.6
1	E	308	HIS	2.6
1	E	59	ASP	2.6
1	G	257	LYS	2.5
1	F	308	HIS	2.5
1	A	304	GLU	2.5
1	C	192	ARG	2.5
1	C	362	LYS	2.5
1	D	258	ILE	2.4
1	G	290	GLN	2.4
1	A	101	ILE	2.4
1	G	162	GLU	2.4
1	E	326	GLY	2.4
1	A	300	THR	2.4
1	G	244	HIS	2.4
1	F	325	GLY	2.4
1	F	327	ARG	2.4
1	A	102	PHE	2.4
1	F	154	PHE	2.4
1	G	231	TYR	2.3
1	C	256	VAL	2.3
1	F	242	THR	2.3
1	G	92	GLU	2.3
1	B	87	CYS	2.3
1	E	99	CYS	2.3
1	G	58	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	67	THR	2.3
1	G	268	GLY	2.3
1	E	263	LEU	2.3
1	G	57	LEU	2.3
1	G	292	LEU	2.3
1	E	35	ALA	2.3
1	E	190	ASN	2.3
1	D	192	ARG	2.3
1	E	119	ARG	2.3
1	B	361	ASN	2.2
1	C	361	ASN	2.2
1	G	303	VAL	2.2
1	D	244	HIS	2.2
1	E	122	ASN	2.2
1	C	303	VAL	2.2
1	B	333	ILE	2.2
1	A	356	ALA	2.2
1	A	123	GLU	2.2
1	G	45	PRO	2.2
1	D	325	GLY	2.2
1	G	95	MET	2.2
1	F	94	ILE	2.2
1	F	300	THR	2.2
1	F	98	ASN	2.2
1	F	157	LYS	2.2
1	F	259	GLY	2.2
1	G	21	VAL	2.2
1	G	62	SER	2.2
1	E	267	ALA	2.1
1	D	254	GLU	2.1
1	F	129	GLU	2.1
1	G	245	MET	2.1
1	D	97	TYR	2.1
1	E	293	LEU	2.1
1	G	55	GLY	2.1
1	C	121	PRO	2.1
1	F	188	PRO	2.1
1	A	271	ASN	2.1
1	G	98	ASN	2.1
1	E	97	TYR	2.1
1	A	309	VAL	2.1
1	F	243	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	322	ASP	2.1
1	G	185	PHE	2.1
1	C	126	THR	2.1
1	F	18	ASN	2.1
1	G	332	ILE	2.1
1	E	148	THR	2.0
1	D	95	MET	2.0
1	F	95	MET	2.0
1	A	361	ASN	2.0
1	D	308	HIS	2.0
1	G	129	GLU	2.0
1	D	360	LEU	2.0
1	B	156	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	G	1364	1/1	0.82	0.12	106,106,106,106	0
5	CL	A	1365	1/1	0.83	0.12	95,95,95,95	0
4	DQ8	F	801	26/26	0.83	0.16	60,75,84,110	0
4	DQ8	E	801	26/26	0.87	0.13	57,67,77,98	0
5	CL	A	1366	1/1	0.88	0.13	89,89,89,89	0
4	DQ8	C	801	26/26	0.90	0.13	39,49,61,83	0
4	DQ8	D	801	26/26	0.91	0.12	38,47,60,79	0
4	DQ8	A	801	26/26	0.91	0.12	43,54,63,85	0
4	DQ8	B	801	26/26	0.92	0.12	44,53,67,82	0
5	CL	B	1365	1/1	0.92	0.13	78,78,78,78	0

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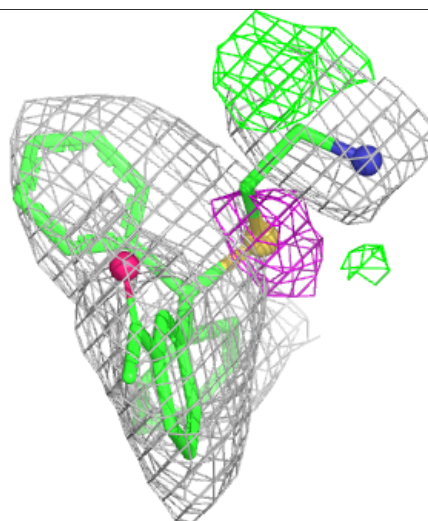
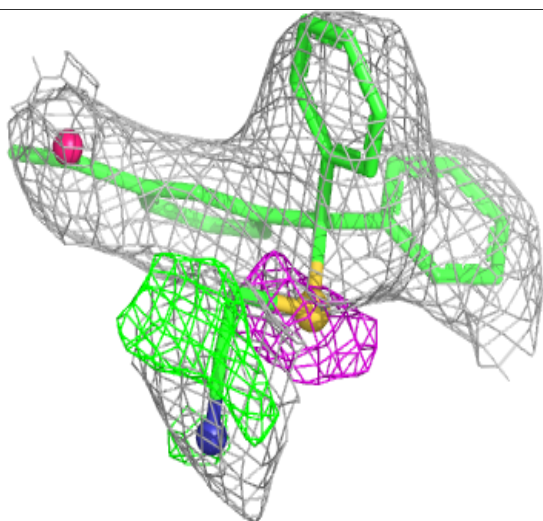
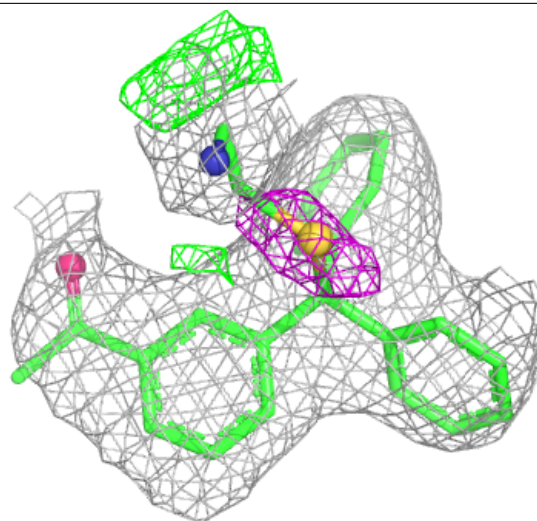
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	1364	1/1	0.92	0.18	77,77,77,77	0
5	CL	E	1364	1/1	0.92	0.10	90,90,90,90	0
5	CL	F	1364	1/1	0.92	0.18	89,89,89,89	0
3	MG	C	701	1/1	0.92	0.09	40,40,40,40	0
4	DQ8	G	801	26/26	0.93	0.12	49,57,68,85	0
5	CL	C	1367	1/1	0.94	0.24	62,62,62,62	0
5	CL	C	1369	1/1	0.94	0.10	97,97,97,97	0
6	SO4	D	1362	5/5	0.94	0.09	54,54,63,68	0
5	CL	A	1364	1/1	0.95	0.12	75,75,75,75	0
3	MG	G	701	1/1	0.95	0.14	45,45,45,45	0
2	ADP	E	601	27/27	0.95	0.09	45,54,61,71	0
5	CL	B	1364	1/1	0.95	0.27	80,80,80,80	0
5	CL	A	1367	1/1	0.96	0.18	73,73,73,73	0
5	CL	C	1368	1/1	0.96	0.06	56,56,56,56	0
2	ADP	F	601	27/27	0.96	0.07	45,55,70,77	0
3	MG	B	701	1/1	0.96	0.08	37,37,37,37	0
2	ADP	B	601	27/27	0.97	0.07	35,42,48,58	0
2	ADP	D	601	27/27	0.97	0.06	28,40,45,51	0
2	ADP	G	601	27/27	0.97	0.06	46,54,59,64	0
5	CL	D	1363	1/1	0.98	0.15	79,79,79,79	0
3	MG	D	701	1/1	0.98	0.08	35,35,35,35	0
3	MG	E	701	1/1	0.98	0.06	50,50,50,50	0
3	MG	F	701	1/1	0.98	0.06	50,50,50,50	0
2	ADP	A	601	27/27	0.98	0.06	34,41,47,50	0
2	ADP	C	601	27/27	0.98	0.06	28,38,42,48	0
3	MG	A	701	1/1	0.99	0.04	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

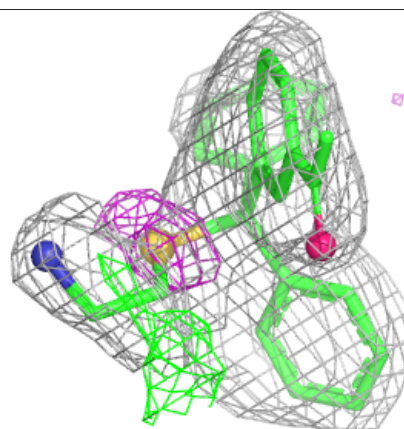
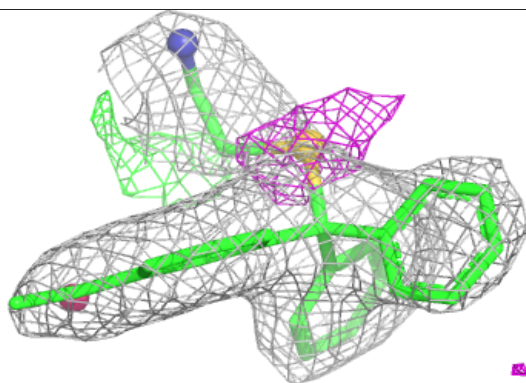
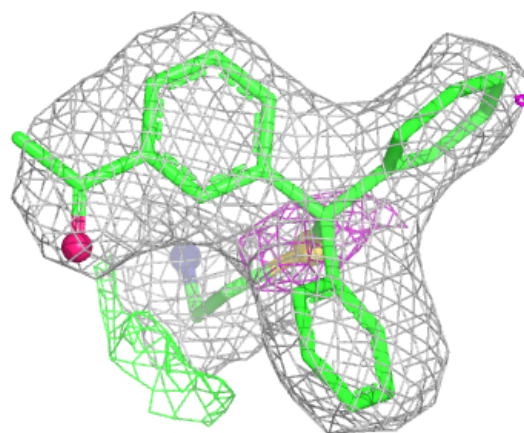
Electron density around DQ8 F 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



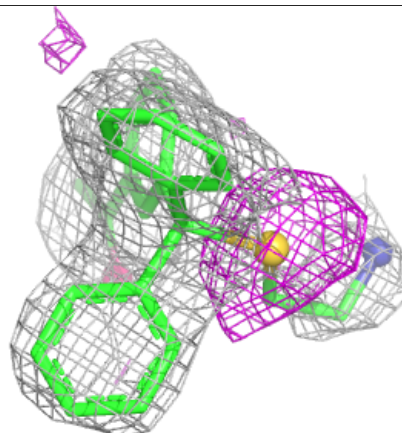
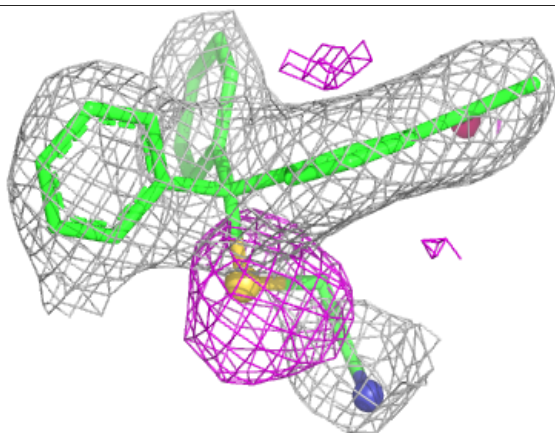
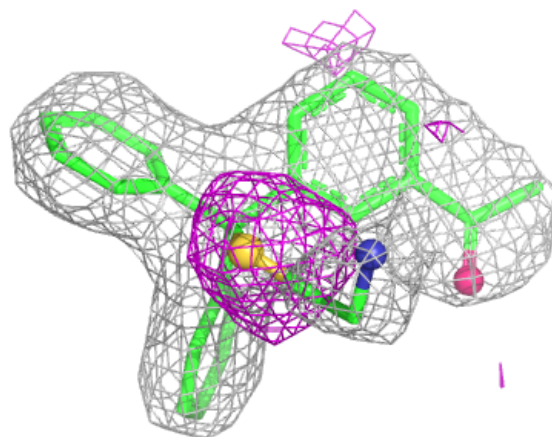
Electron density around DQ8 E 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



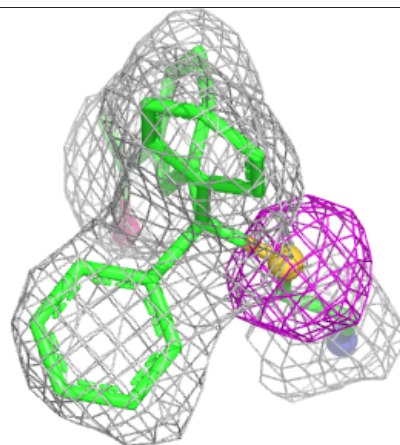
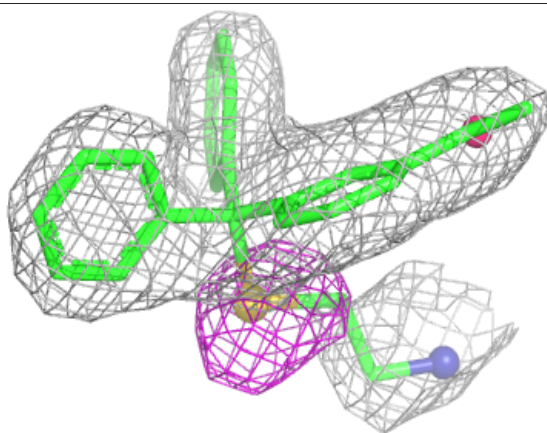
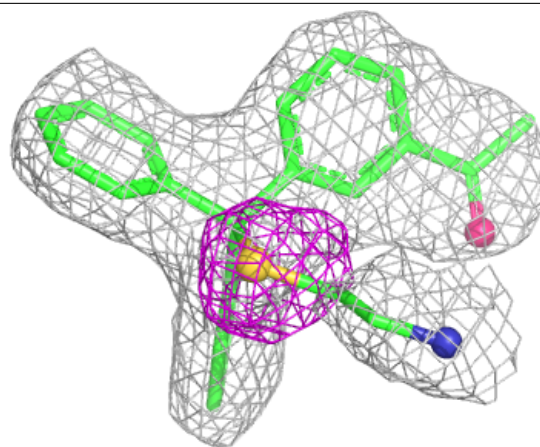
Electron density around DQ8 C 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



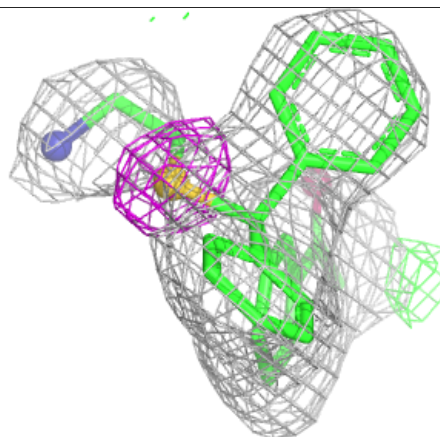
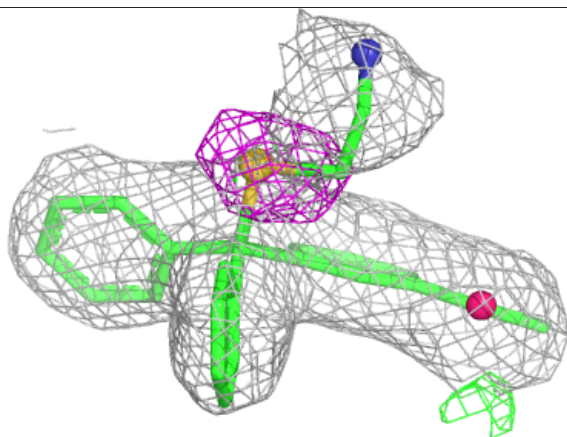
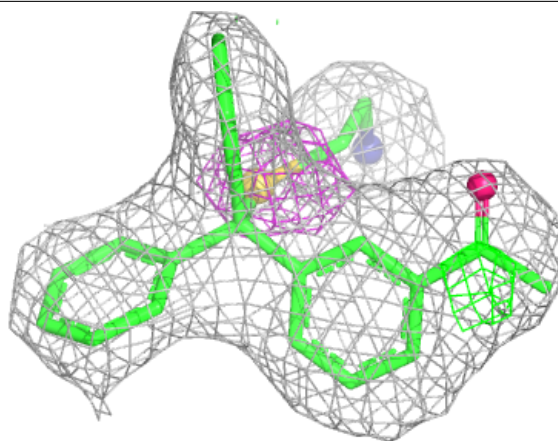
Electron density around DQ8 D 801:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



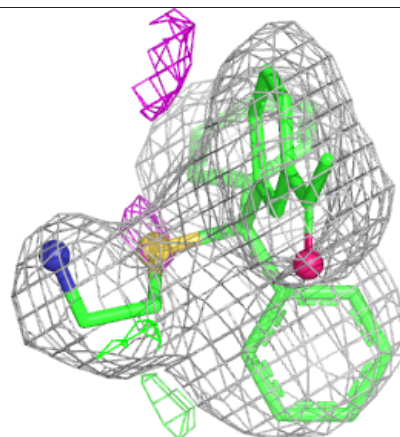
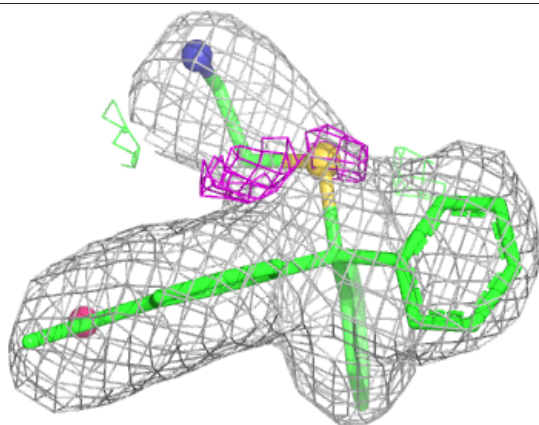
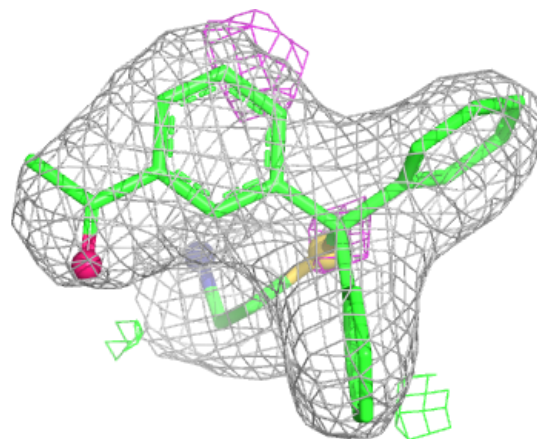
Electron density around DQ8 A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



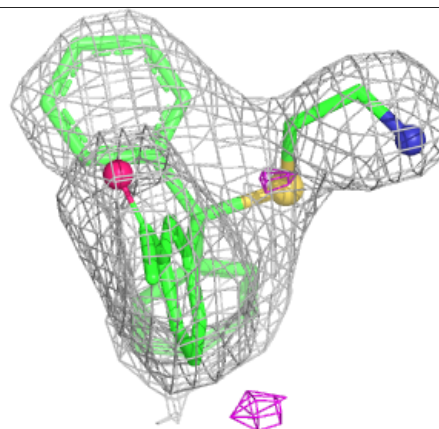
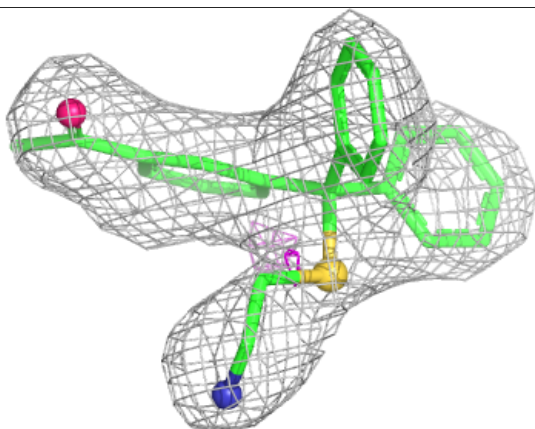
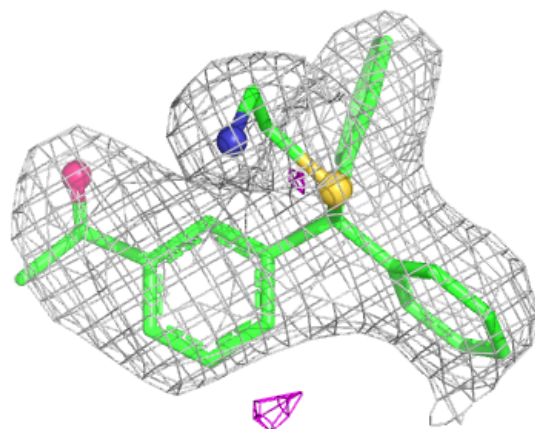
Electron density around DQ8 B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

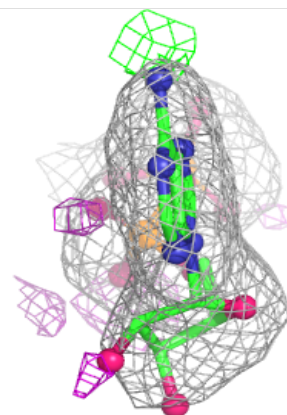
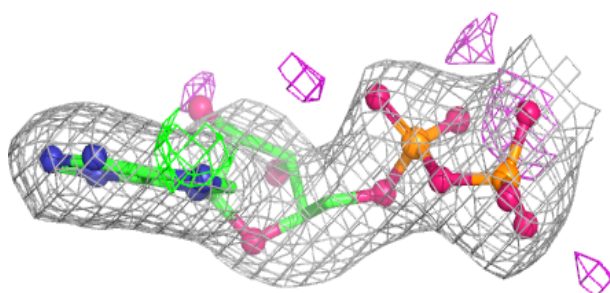
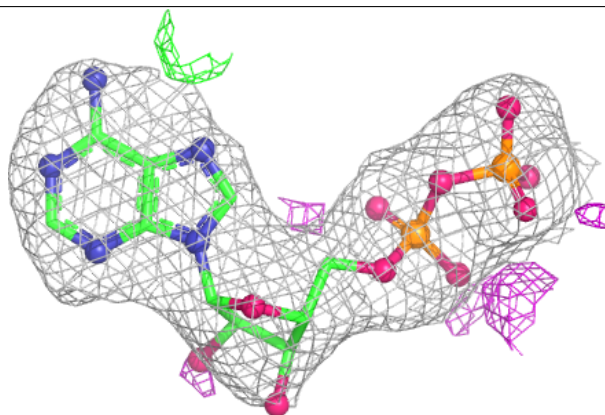


Electron density around DQ8 G 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

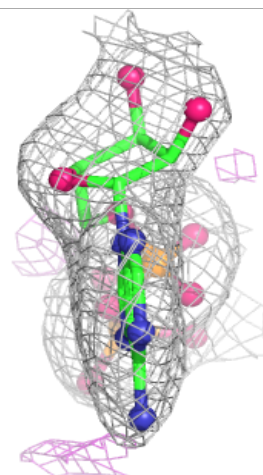
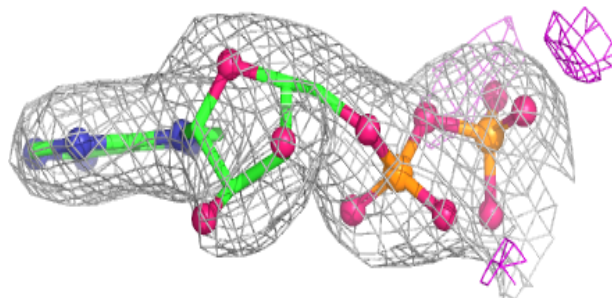
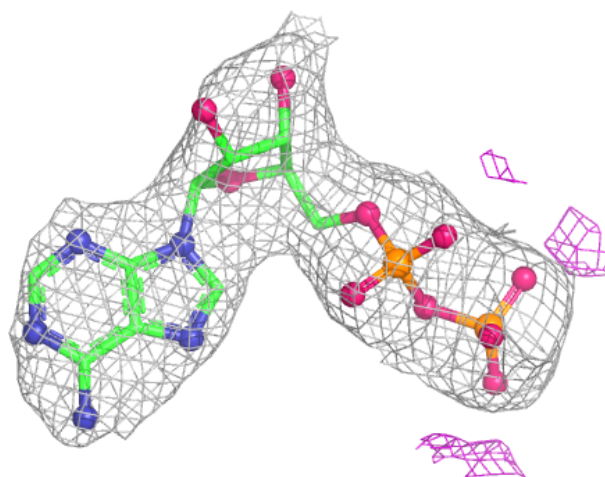
**Electron density around ADP E 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



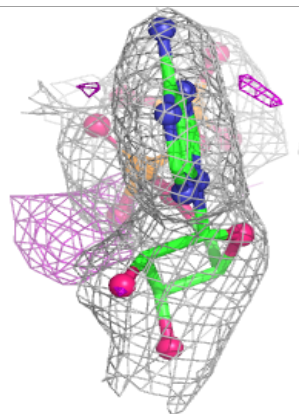
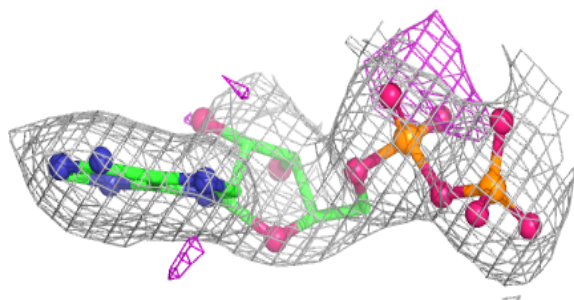
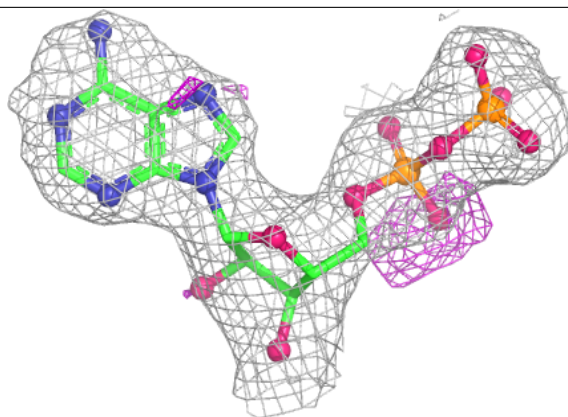
Electron density around ADP F 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

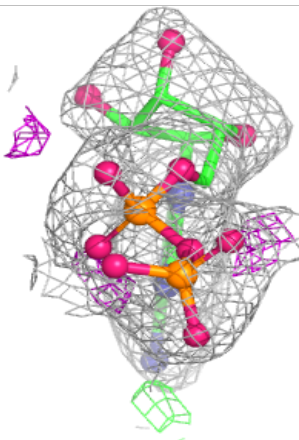
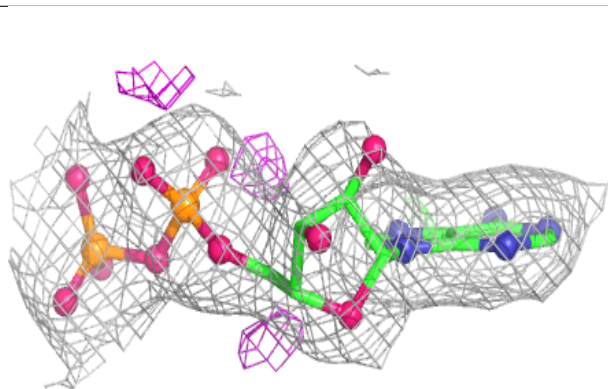
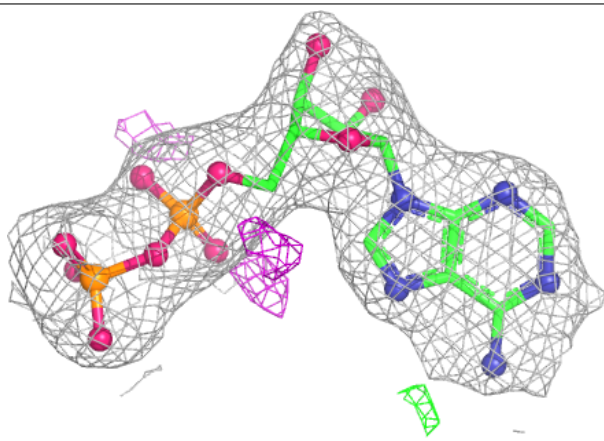


Electron density around ADP B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

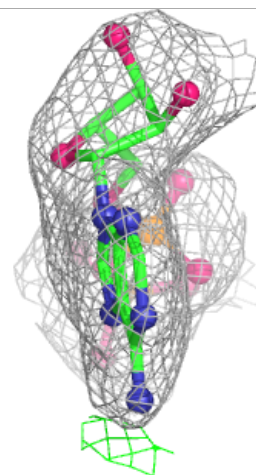
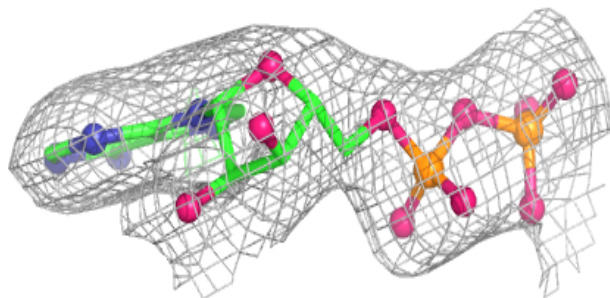
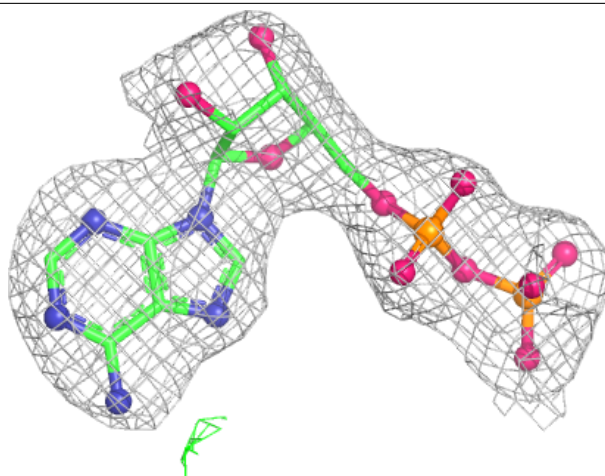
**Electron density around ADP D 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



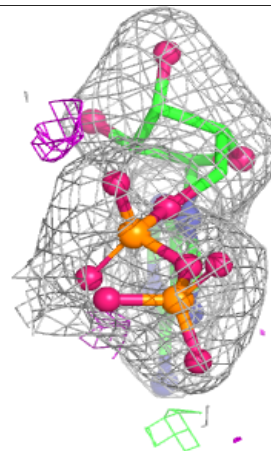
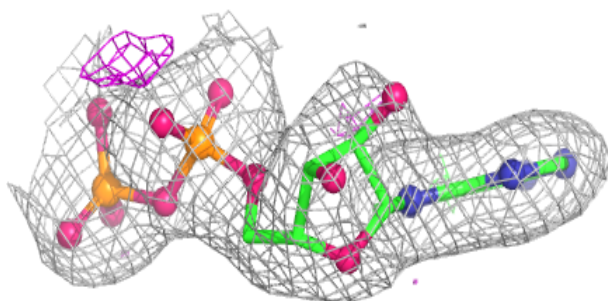
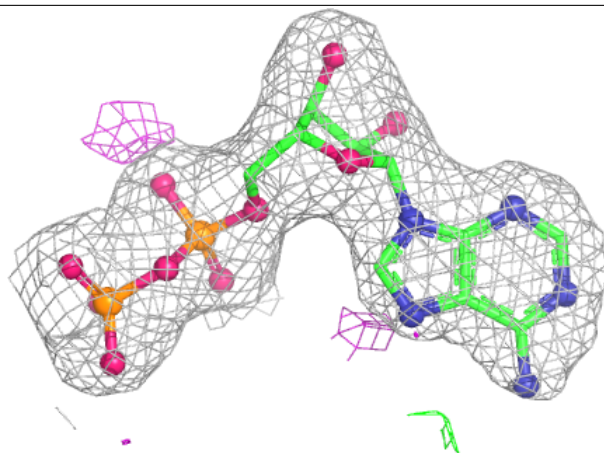
Electron density around ADP G 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



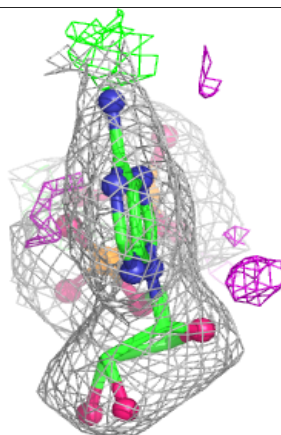
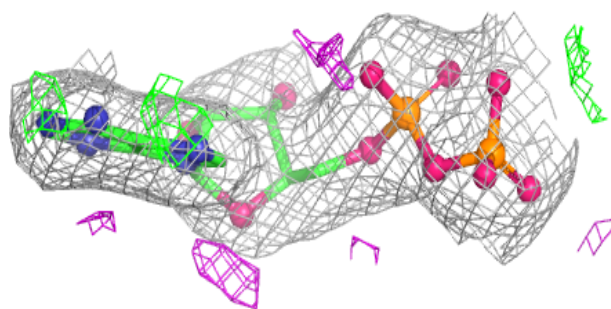
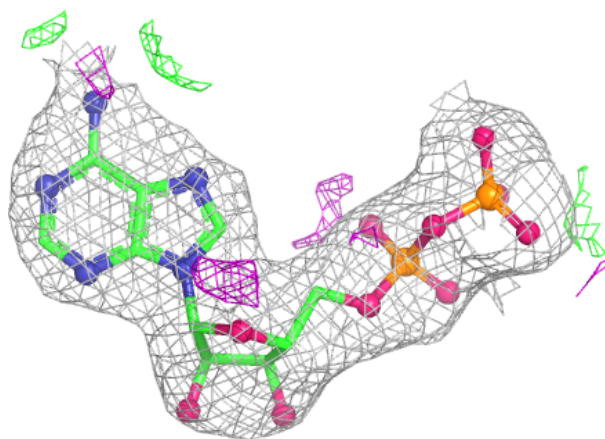
Electron density around ADP A 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.