



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:12 PM UTC

PDB ID : 4KI8 / pdb_00004ki8
Title : Crystal structure of a GroEL-ADP complex in the relaxed allosteric state
Authors : Fei, X.; Yang, D.; LaRonde-LeBlanc, N.; Lorimer, G.H.
Deposited on : 2013-05-01
Resolution : 2.72 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

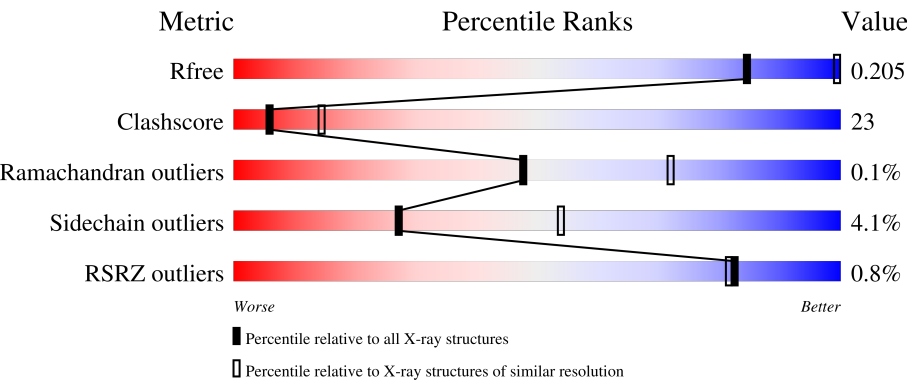
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	548	67%26% . .
1	B	548	% 66%28% . .
1	C	548	% 61%31% . .
1	D	548	% 67%27% . .
1	E	548	% 67%26% . .

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Mol	Chain	Length	Quality of chain
1	F	548	63% 30%
1	G	548	% 59% 34%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27977 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.

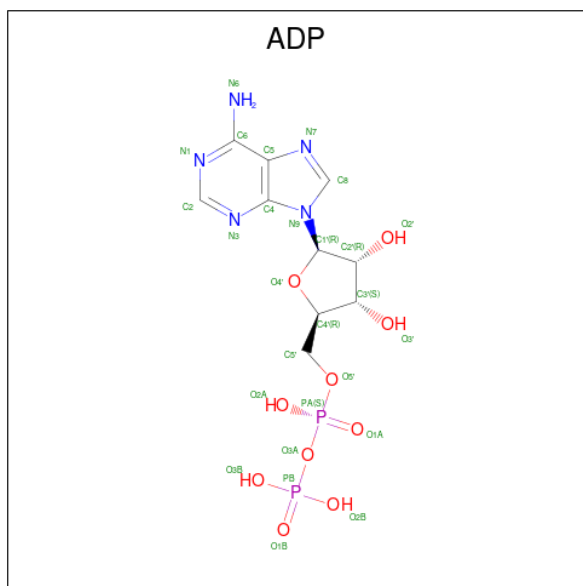
- Molecule 1 is a protein called GroEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			
1	B	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			
1	C	524	Total	C	N	O	S	0	3	0
			3864	2405	668	771	20			
1	D	524	Total	C	N	O	S	0	2	0
			3862	2403	668	771	20			
1	E	524	Total	C	N	O	S	0	1	0
			3851	2396	663	772	20			
1	F	524	Total	C	N	O	S	0	4	0
			3873	2410	668	775	20			
1	G	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	ASP	engineered mutation	UNP Q548M1
A	197	ALA	ARG	engineered mutation	UNP Q548M1
B	83	ALA	ASP	engineered mutation	UNP Q548M1
B	197	ALA	ARG	engineered mutation	UNP Q548M1
C	83	ALA	ASP	engineered mutation	UNP Q548M1
C	197	ALA	ARG	engineered mutation	UNP Q548M1
D	83	ALA	ASP	engineered mutation	UNP Q548M1
D	197	ALA	ARG	engineered mutation	UNP Q548M1
E	83	ALA	ASP	engineered mutation	UNP Q548M1
E	197	ALA	ARG	engineered mutation	UNP Q548M1
F	83	ALA	ASP	engineered mutation	UNP Q548M1
F	197	ALA	ARG	engineered mutation	UNP Q548M1
G	83	ALA	ASP	engineered mutation	UNP Q548M1
G	197	ALA	ARG	engineered mutation	UNP Q548M1

- 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		

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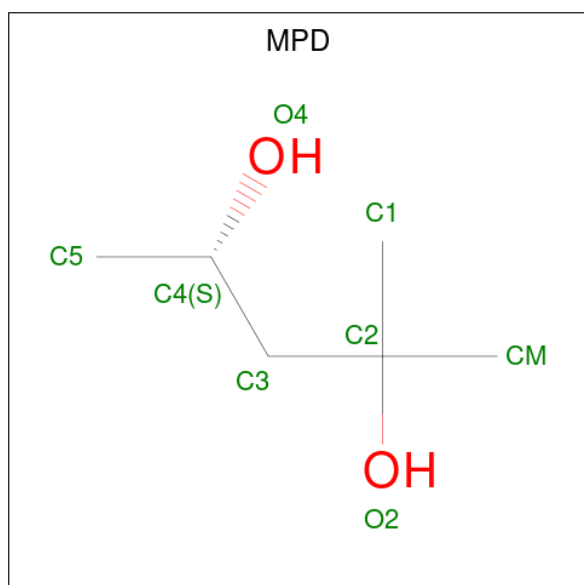
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	F	2	Total K 2 2	0	0
4	G	2	Total K 2 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	F	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0

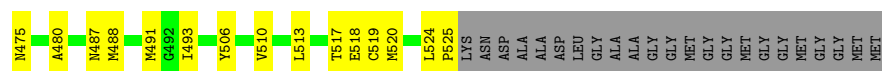
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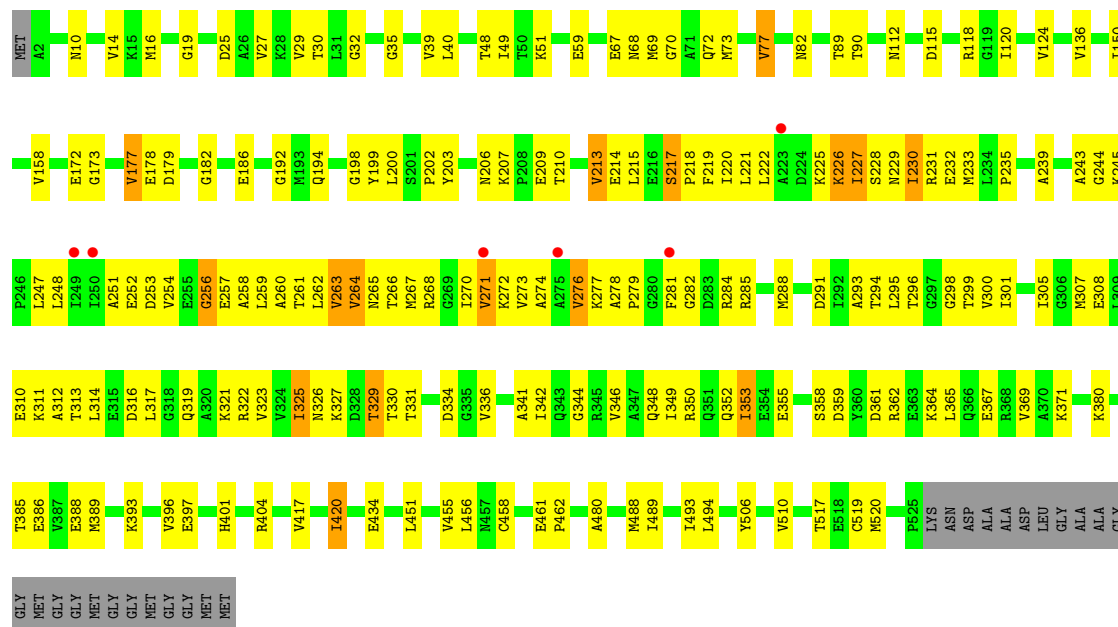
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Ca 1	0	0
6	D	1	Total 1	Ca 1	0	0
6	E	3	Total 3	Ca 3	0	0
6	F	1	Total 1	Ca 1	0	0
6	G	3	Total 3	Ca 3	0	0

- Molecule 7 is water.

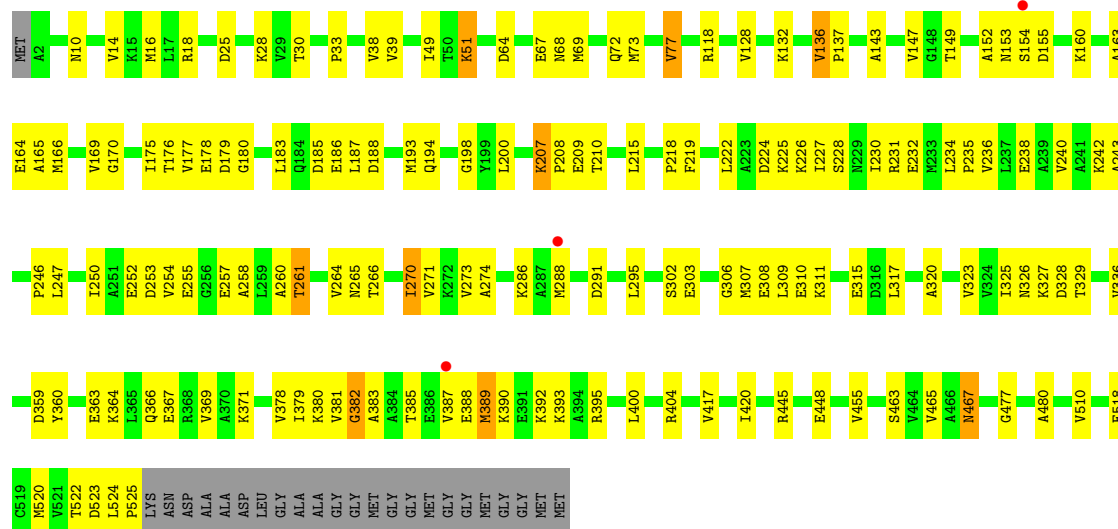
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	90	Total 90	O 90	0	0
7	B	112	Total 112	O 112	0	0
7	C	88	Total 88	O 88	0	0
7	D	90	Total 90	O 90	0	0
7	E	65	Total 65	O 65	0	0
7	F	67	Total 67	O 67	0	0
7	G	85	Total 85	O 85	0	0



• Molecule 1: GroEL protein

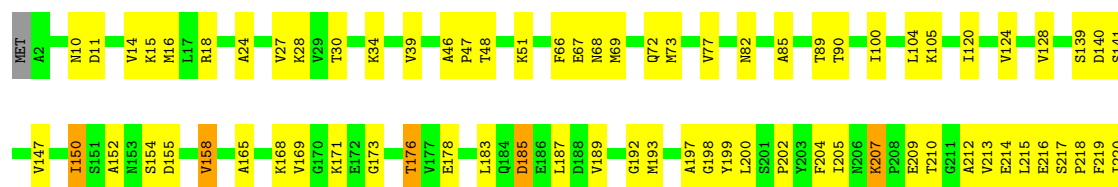


• Molecule 1: GroEL protein



• Molecule 1: GroEL protein







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.22Å 141.66Å 156.69Å 90.00° 113.84° 90.00°	Depositor
Resolution (Å)	46.17 – 2.72 46.17 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.17-2.72) 95.6 (46.17-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.166 , 0.203 0.170 , 0.205	Depositor DCC
R_{free} test set	2000 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27977	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: MPD, ADP, CA, K, MG

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	0.39	0/3885	0.80	0/5246
1	B	0.41	0/3885	0.80	0/5246
1	C	0.43	0/3907	0.84	5/5274 (0.1%)
1	D	0.39	0/3896	0.80	4/5260 (0.1%)
1	E	0.39	0/3882	0.81	3/5243 (0.1%)
1	F	0.39	0/3913	0.80	0/5284
1	G	0.39	0/3885	0.84	4/5246 (0.1%)
All	All	0.40	0/27253	0.81	16/36799 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	278	ALA	CA-C-N	9.13	130.34	120.11
1	G	278	ALA	C-N-CA	9.13	130.34	120.11
1	C	182	GLY	N-CA-C	6.84	120.19	111.09
1	E	207	LYS	CA-C-N	6.38	125.96	119.19
1	E	207	LYS	C-N-CA	6.38	125.96	119.19
1	C	256	GLY	N-CA-C	6.13	118.54	111.36
1	D	382	GLY	N-CA-C	5.91	121.06	112.55
1	C	329	THR	N-CA-C	5.46	118.08	108.75
1	C	217	SER	CA-C-N	5.34	125.80	120.14
1	C	217	SER	C-N-CA	5.34	125.80	120.14
1	G	207	LYS	CA-C-N	5.34	125.66	119.47
1	G	207	LYS	C-N-CA	5.34	125.66	119.47
1	D	383	ALA	N-CA-C	5.21	115.71	108.00
1	E	271	VAL	N-CA-C	5.14	116.64	109.55
1	D	207	LYS	CA-C-N	5.11	124.72	119.05
1	D	207	LYS	C-N-CA	5.11	124.72	119.05

There are no chirality outliers.

There are no planarity outliers.

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	3854	0	3982	162	0
1	B	3854	0	3982	153	0
1	C	3864	0	3994	261	1
1	D	3862	0	3995	134	0
1	E	3851	0	3975	136	0
1	F	3873	0	4005	191	1
1	G	3854	0	3982	271	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	2	0
2	F	27	0	12	0	0
2	G	27	0	12	1	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
5	A	48	0	84	13	0
5	B	40	0	70	5	0
5	C	8	0	14	1	0
5	D	24	0	42	2	0
5	E	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	8	0	14	0	0
5	G	16	0	28	3	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
7	A	90	0	0	4	0
7	B	112	0	0	7	0
7	C	88	0	0	6	0
7	D	90	0	0	4	0
7	E	65	0	0	10	0
7	F	67	0	0	3	0
7	G	85	0	0	6	0
All	All	27977	0	28265	1274	1

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 23.

All (1274) 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:A:230:ILE:HD12	1:A:261:THR:HG21	1.23	1.15
1:G:281:PHE:HB3	1:G:285:ARG:HB3	1.18	1.14
1:A:183:LEU:HA	1:A:383:ALA:HB2	1.14	1.09
1:B:255:GLU:HA	1:B:259:LEU:HD23	1.28	1.07
1:C:225:LYS:HB2	1:C:251:ALA:HB1	1.31	1.07
1:E:183:LEU:HD13	1:E:384:ALA:HB2	1.38	1.05
1:A:383:ALA:HB1	1:A:384:ALA:HA	1.05	1.02
1:C:215:LEU:HD11	1:C:323:VAL:HB	1.39	1.00
1:C:179:ASP:HB3	1:C:389:MET:HE1	1.42	1.00
1:D:226:LYS:HD3	1:D:253:ASP:HB3	1.42	1.00
1:G:284:ARG:HH11	1:G:284:ARG:HG3	1.28	0.98
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.46	0.97
1:E:389:MET:HE2	1:E:390:LYS:HD2	1.47	0.97
1:G:198:GLY:H	1:G:277:LYS:HE3	1.29	0.97
1:C:16:MET:HE2	1:C:73:MET:HE1	1.47	0.96
1:A:383:ALA:HB1	1:A:384:ALA:CA	1.95	0.96
1:G:176:THR:HG22	1:G:378:VAL:HG22	1.46	0.96
1:B:215:LEU:HD22	1:B:246:PRO:HB2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ALA:CB	1:A:384:ALA:HA	1.92	0.95
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.49	0.94
1:G:278:ALA:HB1	1:G:279:PRO:HD2	1.50	0.94
1:A:270:ILE:HD13	1:A:273:VAL:HB	1.48	0.93
1:F:301:ILE:HD12	1:F:307:MET:HB3	1.49	0.93
1:C:225:LYS:C	1:C:227:ILE:HG13	1.93	0.93
1:A:16:MET:HE3	1:A:514:MET:HE3	1.50	0.92
1:A:162:ILE:HG22	1:A:166:MET:HE2	1.49	0.92
1:F:225:LYS:HD2	1:F:309:LEU:HD11	1.49	0.92
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.48	0.91
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.54	0.90
1:A:218:PRO:HG3	1:A:323:VAL:HG12	1.53	0.89
1:A:183:LEU:HA	1:A:383:ALA:CB	2.00	0.89
1:C:222:LEU:HB3	1:C:300:VAL:HG23	1.55	0.89
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.54	0.89
1:A:266:THR:HA	1:A:270:ILE:CG2	2.03	0.88
1:G:352:GLN:HA	1:G:355:GLU:HB3	1.55	0.88
1:C:420:ILE:HD12	1:C:451:LEU:HD13	1.56	0.87
1:C:232:GLU:HB3	1:C:233:MET:CE	2.05	0.87
1:G:222:LEU:HD11	1:G:300:VAL:HA	1.55	0.86
1:F:225:LYS:HG2	1:F:303:GLU:HG3	1.54	0.86
5:A:608:MPD:H11	5:A:608:MPD:H52	1.59	0.85
1:G:281:PHE:HB3	1:G:285:ARG:CB	2.06	0.85
1:A:166:MET:HE1	1:A:403:THR:HG21	1.57	0.85
1:C:225:LYS:HA	1:C:227:ILE:HD11	1.57	0.84
1:C:353:ILE:HG12	1:C:365:LEU:HD22	1.60	0.84
1:E:207:LYS:NZ	1:E:210:THR:HG21	1.92	0.83
1:F:77:VAL:HG13	1:F:506:TYR:HB3	1.58	0.83
1:G:383:ALA:HB2	1:G:392:LYS:HD3	1.60	0.83
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.58	0.83
1:B:259:LEU:HD12	1:B:260:ALA:N	1.92	0.83
1:G:183:LEU:HD12	1:G:384:ALA:HB3	1.59	0.83
1:A:39:VAL:HG21	1:B:16:MET:HE1	1.59	0.83
1:G:279:PRO:HB2	1:G:285:ARG:HB2	1.60	0.82
1:C:225:LYS:HG2	1:C:253:ASP:O	1.79	0.82
1:F:247:LEU:HD21	1:F:249:ILE:HD11	1.60	0.82
1:C:225:LYS:HA	1:C:227:ILE:CD1	2.10	0.81
1:E:444:LEU:HA	1:E:447:MET:HE3	1.61	0.81
1:G:223:ALA:HA	1:G:224:ASP:HB2	1.60	0.81
1:A:39:VAL:HG21	1:B:16:MET:CE	2.11	0.81
1:C:314:LEU:HD12	1:C:314:LEU:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:HG22	1:C:233:MET:HE3	1.63	0.81
1:C:235:PRO:HG2	1:C:310:GLU:HG2	1.63	0.80
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.63	0.80
1:B:227:ILE:HG21	1:B:233:MET:HE3	1.64	0.80
1:G:268:ARG:HG3	1:G:268:ARG:HH11	1.46	0.80
1:F:221:LEU:HD23	1:F:249:ILE:HG23	1.62	0.79
1:G:251:ALA:HB1	1:G:252:GLU:HB2	1.62	0.79
1:A:131:LEU:HD13	1:A:422:VAL:HG21	1.63	0.79
1:C:225:LYS:HD2	1:C:227:ILE:HD12	1.64	0.79
1:E:270:ILE:HG22	1:E:271:VAL:H	1.48	0.78
1:F:204:PHE:HB3	1:F:266:THR:CB	2.12	0.78
1:C:232:GLU:HB3	1:C:233:MET:HE2	1.66	0.78
1:C:284:ARG:HE	1:C:364:LYS:HE2	1.47	0.78
1:G:226:LYS:HB2	1:G:227:ILE:HA	1.66	0.78
1:C:225:LYS:CB	1:C:251:ALA:HB1	2.12	0.77
1:G:221:LEU:HD11	1:G:247:LEU:HD21	1.65	0.77
1:C:314:LEU:O	1:C:317:LEU:HG	1.85	0.77
1:A:183:LEU:HD23	1:A:383:ALA:CB	2.13	0.77
1:A:302:SER:HB2	1:A:305:ILE:HG13	1.66	0.77
1:E:85:ALA:HB1	1:E:499:VAL:HG22	1.65	0.77
1:C:227:ILE:HG22	1:C:228:SER:H	1.47	0.77
1:E:39:VAL:HG21	1:F:16:MET:HE1	1.65	0.77
1:G:250:ILE:HG13	1:G:251:ALA:H	1.50	0.77
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.67	0.77
1:D:308:GLU:HB2	1:D:311:LYS:HE3	1.67	0.77
1:F:301:ILE:CD1	1:F:307:MET:HB3	2.14	0.77
1:G:225:LYS:HB3	1:G:226:LYS:HG2	1.67	0.77
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.68	0.76
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.67	0.76
1:C:230:ILE:HG22	1:C:258:ALA:HB1	1.67	0.76
1:G:385:THR:HB	1:G:388:GLU:HB3	1.67	0.76
1:C:215:LEU:HD11	1:C:323:VAL:CB	2.16	0.76
1:E:183:LEU:CD1	1:E:384:ALA:HB2	2.14	0.76
1:G:16:MET:HE2	1:G:73:MET:SD	2.26	0.76
1:G:281:PHE:CB	1:G:285:ARG:HB3	2.07	0.76
1:A:266:THR:HA	1:A:270:ILE:HG21	1.66	0.76
1:A:270:ILE:HG23	1:A:272:LYS:N	2.01	0.76
1:E:207:LYS:HE3	1:E:214:GLU:CG	2.16	0.76
1:C:178:GLU:HG2	1:C:322:ARG:NH1	2.01	0.76
1:B:222:LEU:HD23	1:B:250:ILE:HB	1.68	0.76
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:HA	1:A:301:ILE:HG23	1.66	0.75
1:F:218:PRO:CA	1:F:246:PRO:HG2	2.17	0.75
1:D:215:LEU:HD22	1:D:246:PRO:HB2	1.66	0.75
1:C:230:ILE:HG13	1:C:262:LEU:HD11	1.69	0.75
1:G:198:GLY:N	1:G:277:LYS:HE3	2.02	0.75
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.69	0.74
5:A:606:MPD:HM2	5:A:606:MPD:H53	1.68	0.74
1:C:16:MET:CE	1:C:73:MET:HE1	2.18	0.74
1:E:183:LEU:HD12	1:E:183:LEU:O	1.87	0.74
1:F:39:VAL:HG21	1:G:16:MET:HE1	1.70	0.74
1:B:305:ILE:HG23	1:B:307:MET:HG3	1.68	0.74
1:G:185:ASP:OD1	1:G:185:ASP:N	2.20	0.74
1:C:199:TYR:OH	1:C:327:LYS:NZ	2.17	0.74
1:G:281:PHE:HB2	1:G:282:GLY:CA	2.19	0.73
1:E:16:MET:HG2	1:E:514:MET:HE3	1.69	0.73
1:E:444:LEU:HD23	1:E:447:MET:CE	2.18	0.73
1:G:249:ILE:O	1:G:275:ALA:HA	1.88	0.73
1:A:230:ILE:HD12	1:A:261:THR:CG2	2.13	0.73
1:C:225:LYS:HD2	1:C:227:ILE:CD1	2.17	0.73
1:C:352:GLN:HB2	1:C:365:LEU:HD11	1.68	0.73
1:E:183:LEU:HD13	1:E:384:ALA:CB	2.18	0.73
1:G:223:ALA:HB3	1:G:252:GLU:H	1.54	0.73
1:C:256:GLY:HA3	1:C:259:LEU:HD12	1.69	0.73
1:G:264:VAL:O	1:G:267:MET:HG2	1.88	0.73
1:G:281:PHE:HB2	1:G:282:GLY:HA2	1.70	0.73
1:A:13:ARG:NH1	7:A:773:HOH:O	2.21	0.73
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.71	0.73
1:C:350:ARG:HE	1:C:369:VAL:HG21	1.53	0.72
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.71	0.72
1:E:444:LEU:HD23	1:E:447:MET:HE1	1.70	0.72
1:F:39:VAL:HG21	1:G:16:MET:CE	2.18	0.72
1:G:226:LYS:H	1:G:227:ILE:HG13	1.53	0.72
1:G:248:LEU:CD2	1:G:250:ILE:HG23	2.19	0.72
1:A:248:LEU:HD22	1:A:323:VAL:HG21	1.71	0.72
1:C:284:ARG:NE	1:C:364:LYS:HE2	2.04	0.72
1:C:227:ILE:HG22	1:C:233:MET:CE	2.20	0.72
1:E:82:ASN:ND2	7:E:743:HOH:O	2.23	0.72
1:G:222:LEU:HD13	1:G:300:VAL:HG13	1.72	0.72
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.71	0.71
1:G:176:THR:CG2	1:G:378:VAL:HG22	2.19	0.71
1:G:223:ALA:HB1	1:G:224:ASP:C	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:HE2	1:B:73:MET:SD	2.29	0.71
1:C:239:ALA:HB1	1:C:314:LEU:HD21	1.71	0.71
1:G:199:TYR:CE2	1:G:327:LYS:HA	2.25	0.71
1:A:266:THR:HA	1:A:270:ILE:HG22	1.72	0.71
1:C:227:ILE:CG2	1:C:233:MET:HE3	2.19	0.71
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.71	0.71
1:G:230:ILE:HD12	1:G:234:LEU:HD21	1.73	0.71
1:G:222:LEU:HD22	1:G:300:VAL:HG22	1.73	0.71
1:B:255:GLU:CA	1:B:259:LEU:HD23	2.15	0.71
1:C:230:ILE:CG2	1:C:258:ALA:HB1	2.20	0.71
1:E:169:VAL:HG13	1:E:173:GLY:HA3	1.73	0.71
1:G:383:ALA:HB1	1:G:388:GLU:HG2	1.72	0.71
1:A:207:LYS:HG3	1:A:214:GLU:HG3	1.72	0.70
1:G:271:VAL:HG12	1:G:273:VAL:HG23	1.73	0.70
1:C:349:ILE:O	1:C:365:LEU:HD21	1.90	0.70
1:E:221:LEU:HD22	1:E:233:MET:HE1	1.72	0.70
1:E:222:LEU:HD13	1:E:293:ALA:HB2	1.73	0.70
1:F:218:PRO:HA	1:F:246:PRO:HG2	1.72	0.70
1:G:223:ALA:HB3	1:G:252:GLU:N	2.06	0.70
1:C:232:GLU:HG2	1:C:310:GLU:OE2	1.91	0.70
1:B:177:VAL:HG11	1:B:397:GLU:HG3	1.72	0.70
1:D:226:LYS:CD	1:D:253:ASP:HB3	2.18	0.70
1:A:304:GLU:N	1:A:304:GLU:OE1	2.25	0.70
1:B:181:THR:HG22	1:B:182:GLY:H	1.56	0.70
1:C:420:ILE:CD1	1:C:451:LEU:HD13	2.22	0.70
1:G:224:ASP:CG	1:G:302:SER:HB2	2.17	0.70
1:C:276:VAL:HG11	1:C:325:ILE:HD13	1.73	0.70
1:C:252:GLU:OE2	1:C:285:ARG:NH2	2.25	0.69
1:C:310:GLU:OE1	1:C:310:GLU:N	2.24	0.69
1:D:179:ASP:HA	1:D:389:MET:HE1	1.74	0.69
1:A:69:MET:HE2	1:G:39:VAL:HG12	1.73	0.69
1:F:359:ASP:OD1	1:F:362:ARG:NH2	2.24	0.69
1:C:325:ILE:HD12	1:C:326:ASN:H	1.57	0.69
1:D:265:ASN:HB3	1:D:270:ILE:HG23	1.72	0.69
1:G:225:LYS:HB3	1:G:226:LYS:CG	2.22	0.69
1:B:248:LEU:HD22	1:B:323:VAL:HG11	1.75	0.69
1:F:383:ALA:HB1	1:F:388:GLU:HB3	1.75	0.69
1:G:183:LEU:CD1	1:G:384:ALA:HB3	2.22	0.69
1:G:217:SER:N	1:G:218:PRO:HD3	2.07	0.69
1:G:268:ARG:NH1	1:G:270:ILE:HB	2.06	0.69
1:B:18:ARG:HD2	7:B:781:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:CG1	1:C:69:MET:HE2	2.23	0.69
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.08	0.69
1:G:222:LEU:CD1	1:G:300:VAL:HA	2.22	0.69
1:G:282:GLY:O	1:G:285:ARG:NH1	2.24	0.69
1:B:232:GLU:HA	1:B:310:GLU:HG2	1.75	0.69
1:E:389:MET:CE	1:E:390:LYS:HD2	2.22	0.69
1:F:204:PHE:HB3	1:F:266:THR:HG21	1.72	0.69
1:A:226:LYS:H	1:A:226:LYS:HD2	1.58	0.69
1:F:233:MET:HG2	1:F:309:LEU:HD23	1.75	0.68
1:D:194:GLN:O	1:D:371:LYS:HE3	1.93	0.68
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.76	0.68
1:F:239:ALA:HB1	1:F:314:LEU:HD21	1.75	0.68
1:A:373:ALA:HA	5:A:604:MPD:H52	1.74	0.68
1:C:213:VAL:HG22	1:C:325:ILE:HG23	1.76	0.68
1:F:246:PRO:HB3	1:F:272:LYS:HE3	1.76	0.68
1:G:268:ARG:HH12	1:G:271:VAL:HG23	1.59	0.68
1:A:183:LEU:HD23	1:A:383:ALA:HB1	1.75	0.68
1:G:230:ILE:HG12	1:G:257:GLU:OE1	1.94	0.68
1:F:284:ARG:O	1:F:288:MET:HG2	1.94	0.67
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.75	0.67
1:D:231:ARG:HA	1:D:234:LEU:HD12	1.76	0.67
1:F:193:MET:HE3	1:F:295:LEU:HD12	1.75	0.67
5:A:606:MPD:HM1	1:G:456:LEU:HG	1.77	0.67
1:G:250:ILE:HA	1:G:276:VAL:HG22	1.77	0.67
1:B:39:VAL:HG12	1:C:69:MET:CE	2.24	0.67
1:C:39:VAL:HG12	1:D:69:MET:HE2	1.76	0.67
1:C:198:GLY:O	1:C:276:VAL:HG12	1.95	0.67
1:B:313:THR:HG22	1:B:314:LEU:H	1.58	0.67
1:G:173:GLY:O	1:G:404:ARG:NH2	2.28	0.67
1:G:221:LEU:HD23	1:G:317:LEU:HG	1.75	0.67
1:A:218:PRO:HG3	1:A:323:VAL:CG1	2.24	0.67
1:B:263:VAL:HG22	1:B:267:MET:HE3	1.76	0.67
1:D:303:GLU:N	1:D:303:GLU:OE1	2.28	0.67
1:G:310:GLU:OE1	1:G:310:GLU:N	2.28	0.66
5:A:606:MPD:CM	1:G:456:LEU:HG	2.25	0.66
1:C:361:ASP:HA	1:C:364:LYS:HE3	1.76	0.66
1:A:270:ILE:N	1:A:271:VAL:HA	2.11	0.66
1:A:350:ARG:HA	1:A:353:ILE:HD12	1.78	0.66
1:A:16:MET:CE	1:A:514:MET:HE3	2.25	0.66
1:G:251:ALA:HB3	1:G:289:LEU:HD21	1.75	0.66
1:A:518:GLU:HG2	7:G:730:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ILE:HG12	1:C:365:LEU:CD2	2.26	0.66
1:F:268:ARG:HE	1:F:268:ARG:HA	1.60	0.66
1:F:235:PRO:CG	1:F:310:GLU:HA	2.26	0.66
1:G:197:ALA:HB3	1:G:330:THR:CG2	2.25	0.66
1:C:259:LEU:HA	1:C:262:LEU:HD13	1.78	0.66
1:C:263:VAL:O	1:C:266:THR:HG22	1.94	0.66
1:D:209:GLU:HG2	1:D:210:THR:H	1.61	0.66
1:A:183:LEU:CA	1:A:383:ALA:HB2	2.09	0.65
1:F:16:MET:HE2	1:F:73:MET:SD	2.36	0.65
1:G:16:MET:HB3	1:G:514:MET:HE3	1.78	0.65
1:C:235:PRO:HG2	1:C:310:GLU:CG	2.26	0.65
1:D:187:LEU:HD23	1:D:379:ILE:HG12	1.77	0.65
1:F:268:ARG:HA	1:F:268:ARG:NE	2.10	0.65
1:C:199:TYR:CE1	1:C:202:PRO:HA	2.31	0.65
1:F:199:TYR:CE1	1:F:202:PRO:HA	2.32	0.65
1:F:386:GLU:HG2	1:F:390:LYS:NZ	2.11	0.65
1:G:287:ALA:HB1	1:G:368:ARG:NH1	2.12	0.65
1:A:381:VAL:HG11	1:A:392:LYS:HB3	1.79	0.65
1:E:207:LYS:HZ3	1:E:210:THR:HG21	1.60	0.65
1:F:131:LEU:HD21	1:F:500:THR:HG22	1.79	0.65
1:G:261:THR:HA	1:G:264:VAL:CG1	2.27	0.65
1:G:268:ARG:HG3	1:G:268:ARG:NH1	2.09	0.65
1:D:30:THR:HB	1:D:51:LYS:O	1.97	0.65
1:G:250:ILE:CA	1:G:276:VAL:HG22	2.27	0.64
1:C:252:GLU:O	1:C:277:LYS:HG3	1.96	0.64
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.78	0.64
1:E:68:ASN:O	1:E:72:GLN:HG2	1.96	0.64
1:E:166:MET:HE1	1:E:403:THR:HG22	1.80	0.64
1:A:242:LYS:NZ	1:B:229:ASN:HB2	2.13	0.64
1:A:270:ILE:HG23	1:A:271:VAL:C	2.22	0.64
1:F:183:LEU:HD13	1:F:184:GLN:HG2	1.78	0.64
1:G:207:LYS:HB3	1:G:209:GLU:OE2	1.98	0.64
1:A:16:MET:HE3	1:A:514:MET:CE	2.24	0.64
1:A:384:ALA:HB3	1:A:388:GLU:OE1	1.97	0.64
1:B:319:GLN:HB2	1:B:336:VAL:HG21	1.79	0.64
1:G:222:LEU:HD11	1:G:301:ILE:H	1.61	0.64
1:F:204:PHE:HB3	1:F:266:THR:CG2	2.26	0.64
1:F:234:LEU:N	1:F:235:PRO:HD2	2.12	0.64
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.78	0.64
1:C:325:ILE:CD1	1:C:326:ASN:H	2.11	0.64
1:A:10:ASN:HB3	7:A:740:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:CD1	1:C:317:LEU:HD11	2.33	0.64
1:D:228:SER:O	1:D:258:ALA:N	2.29	0.64
1:C:215:LEU:HD22	1:C:218:PRO:HB3	1.78	0.63
1:E:301:ILE:HG21	1:E:309:LEU:HD23	1.79	0.63
1:G:367:GLU:O	1:G:371:LYS:HG2	1.98	0.63
1:E:266:THR:OG1	1:E:273:VAL:HG12	1.98	0.63
1:F:301:ILE:HD11	1:F:308:GLU:N	2.13	0.63
1:A:104:LEU:HB3	5:A:605:MPD:HM1	1.81	0.63
1:B:209:GLU:HG2	1:B:210:THR:N	2.14	0.63
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.80	0.63
1:D:225:LYS:HD2	1:D:303:GLU:HG2	1.80	0.63
1:G:284:ARG:HH11	1:G:284:ARG:CG	2.07	0.63
1:G:301:ILE:HG23	1:G:307:MET:HG3	1.80	0.63
1:F:358:SER:HB3	1:F:361:ASP:HB2	1.80	0.63
1:B:513:LEU:O	1:B:517:THR:HG23	1.98	0.63
1:E:247:LEU:HB3	1:E:273:VAL:HG23	1.80	0.63
1:E:445:ARG:NH1	5:E:604:MPD:HM1	2.14	0.63
1:F:221:LEU:HB3	1:F:249:ILE:HD12	1.79	0.63
1:G:278:ALA:CB	1:G:279:PRO:HD2	2.20	0.63
1:C:215:LEU:HD13	1:C:218:PRO:CG	2.28	0.63
1:D:160:LYS:NZ	1:D:164:GLU:OE2	2.23	0.63
1:G:222:LEU:CD2	1:G:300:VAL:HG22	2.29	0.63
1:A:310:GLU:N	1:A:310:GLU:OE1	2.32	0.62
1:B:229:ASN:ND2	1:B:231:ARG:HB2	2.13	0.62
1:D:165:ALA:O	1:D:169:VAL:HG22	1.99	0.62
1:E:215:LEU:HB2	1:E:323:VAL:CG2	2.29	0.62
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.98	0.62
1:F:319:GLN:HB2	1:F:336:VAL:HG21	1.79	0.62
1:B:194:GLN:O	1:B:371:LYS:HE3	2.00	0.62
1:F:213:VAL:HG12	1:F:214:GLU:H	1.65	0.62
1:D:225:LYS:HB2	1:D:303:GLU:CD	2.25	0.62
1:E:39:VAL:HG21	1:F:16:MET:CE	2.30	0.62
1:D:463:SER:HB2	7:D:740:HOH:O	1.99	0.62
1:F:248:LEU:HD13	1:F:325:ILE:HD11	1.81	0.62
1:D:179:ASP:CA	1:D:389:MET:HE1	2.30	0.62
1:E:207:LYS:HE3	1:E:214:GLU:HG3	1.82	0.62
1:F:179:ASP:HB3	1:F:389:MET:SD	2.40	0.62
1:C:232:GLU:HB3	1:C:233:MET:HE1	1.81	0.61
1:C:229:ASN:OD1	1:C:230:ILE:N	2.30	0.61
1:C:359:ASP:OD1	1:C:362:ARG:NH1	2.33	0.61
1:G:150:ILE:HD11	1:G:493:ILE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:O	1:D:404:ARG:HG2	2.00	0.61
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.29	0.61
1:A:284:ARG:HD3	1:A:364:LYS:NZ	2.15	0.61
1:G:279:PRO:CB	1:G:285:ARG:HB2	2.30	0.61
1:A:302:SER:HB2	1:A:305:ILE:CG1	2.30	0.61
1:C:346:VAL:O	1:C:350:ARG:HG2	2.00	0.61
1:G:218:PRO:HG2	1:G:323:VAL:HG22	1.81	0.61
1:G:291:ASP:HB3	1:G:372:LEU:HD11	1.81	0.61
1:F:231:ARG:HG3	1:F:231:ARG:HH11	1.65	0.61
1:B:198:GLY:H	1:B:277:LYS:HE3	1.66	0.61
1:E:310:GLU:N	1:E:310:GLU:OE1	2.32	0.61
1:F:498:LYS:HG3	1:F:501:ARG:NH2	2.16	0.61
1:G:261:THR:O	1:G:264:VAL:HG13	2.01	0.61
1:C:200:LEU:HD12	1:C:254:VAL:CG2	2.31	0.61
1:C:225:LYS:CA	1:C:227:ILE:HG13	2.30	0.61
1:D:308:GLU:O	1:D:311:LYS:HG2	1.99	0.61
1:F:217:SER:HA	1:F:320:ALA:O	2.01	0.61
1:D:152:ALA:HB3	1:D:153:ASN:C	2.27	0.60
1:F:221:LEU:HB3	1:F:249:ILE:CD1	2.32	0.60
1:B:181:THR:HG22	1:B:182:GLY:N	2.15	0.60
1:C:225:LYS:HA	1:C:227:ILE:CG1	2.31	0.60
1:F:247:LEU:CD2	1:F:249:ILE:HD11	2.32	0.60
1:F:348:GLN:O	1:F:352:GLN:HG3	2.02	0.60
1:F:496:PRO:HB2	1:F:499:VAL:HG13	1.84	0.60
1:D:385:THR:CG2	1:D:388:GLU:HG2	2.30	0.60
1:G:233:MET:HA	1:G:233:MET:HE3	1.82	0.60
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.67	0.60
1:D:315:GLU:OE1	1:D:315:GLU:N	2.34	0.60
1:G:197:ALA:HA	1:G:277:LYS:HG2	1.84	0.60
1:B:39:VAL:HG21	1:C:16:MET:CE	2.31	0.60
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.84	0.60
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.83	0.60
1:A:34:LYS:HG3	1:A:458:CYS:SG	2.42	0.60
1:C:16:MET:HE2	1:C:73:MET:CE	2.29	0.60
1:G:222:LEU:HD21	1:G:300:VAL:HA	1.83	0.60
1:B:268:ARG:HG2	1:B:268:ARG:NH1	2.18	0.59
1:E:253:ASP:OD1	1:E:254:VAL:N	2.35	0.59
1:G:284:ARG:HG3	1:G:284:ARG:NH1	2.08	0.59
1:C:215:LEU:CD1	1:C:323:VAL:HB	2.24	0.59
1:E:207:LYS:HZ2	1:E:210:THR:HG21	1.65	0.59
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ILE:HD12	1:F:309:LEU:HD21	1.83	0.59
1:G:200:LEU:HD13	1:G:254:VAL:HG22	1.85	0.59
1:G:221:LEU:HG	1:G:247:LEU:HD11	1.84	0.59
1:B:39:VAL:HG21	1:C:16:MET:HE1	1.85	0.59
1:C:213:VAL:HG22	1:C:325:ILE:CG2	2.33	0.59
1:F:149:THR:HG21	1:F:156:GLU:HG2	1.84	0.59
1:G:276:VAL:HG23	1:G:278:ALA:H	1.67	0.59
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.32	0.59
1:C:253:ASP:OD1	1:C:254:VAL:N	2.35	0.59
1:G:30:THR:HB	1:G:51:LYS:O	2.03	0.59
1:G:221:LEU:CD2	1:G:317:LEU:HG	2.33	0.59
1:B:264:VAL:O	1:B:268:ARG:HG3	2.03	0.59
1:A:198:GLY:HA3	1:A:327:LYS:O	2.03	0.59
1:B:420:ILE:HD13	1:B:448:GLU:HG2	1.85	0.59
1:D:200:LEU:HD12	1:D:254:VAL:HB	1.84	0.59
1:E:235:PRO:CG	1:E:310:GLU:HA	2.32	0.59
1:F:183:LEU:HD12	1:F:184:GLN:H	1.67	0.59
1:F:232:GLU:CD	1:F:309:LEU:HD13	2.28	0.59
1:G:250:ILE:HG13	1:G:251:ALA:N	2.15	0.59
1:D:308:GLU:CB	1:D:311:LYS:HE3	2.33	0.58
1:G:301:ILE:HG12	1:G:307:MET:HG2	1.85	0.58
1:A:242:LYS:CE	1:B:229:ASN:HB2	2.33	0.58
1:E:194:GLN:O	1:E:371:LYS:HE3	2.03	0.58
1:G:154:SER:HB3	7:G:716:HOH:O	2.03	0.58
1:G:281:PHE:HD2	1:G:282:GLY:HA2	1.66	0.58
1:G:346:VAL:O	1:G:350:ARG:HG3	2.03	0.58
1:A:282:GLY:O	1:A:286:LYS:HG2	2.03	0.58
5:G:604:MPD:H51	7:G:748:HOH:O	2.04	0.58
1:C:192:GLY:HA2	1:C:295:LEU:HD21	1.86	0.58
1:A:284:ARG:CZ	1:A:364:LYS:HG2	2.34	0.58
1:D:149:THR:O	1:D:154:SER:N	2.35	0.58
1:F:213:VAL:HG12	1:F:214:GLU:N	2.18	0.58
1:G:197:ALA:HB3	1:G:330:THR:HG21	1.85	0.58
1:B:178:GLU:HA	1:B:393:LYS:HE3	1.86	0.58
1:C:353:ILE:CG1	1:C:365:LEU:HD22	2.33	0.58
1:C:10:ASN:O	1:C:14:VAL:HG23	2.04	0.58
1:C:200:LEU:CD1	1:C:254:VAL:HG23	2.34	0.58
1:C:358:SER:OG	1:C:361:ASP:OD2	2.21	0.58
1:D:235:PRO:HG2	1:D:310:GLU:HA	1.85	0.58
1:E:197:ALA:HB1	1:E:276:VAL:HB	1.85	0.58
1:E:205:ILE:HD12	1:E:211:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:ASN:O	1:F:269:GLY:N	2.35	0.58
1:F:319:GLN:HB2	1:F:336:VAL:CG2	2.34	0.58
7:C:733:HOH:O	1:D:518:GLU:HG2	2.02	0.58
1:E:441:LYS:NZ	7:E:718:HOH:O	2.36	0.58
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.85	0.58
1:G:361:ASP:O	1:G:365:LEU:HG	2.04	0.58
1:A:183:LEU:HD23	1:A:383:ALA:HB2	1.83	0.57
1:C:215:LEU:HD13	1:C:218:PRO:HD3	1.85	0.57
1:G:248:LEU:HD21	1:G:250:ILE:HG23	1.85	0.57
1:A:420:ILE:HD13	1:A:448:GLU:HG2	1.86	0.57
1:C:325:ILE:HD13	1:C:330:THR:OG1	2.03	0.57
1:E:204:PHE:HB3	1:E:266:THR:HG21	1.86	0.57
1:B:347:ALA:O	1:B:351:GLN:HG2	2.04	0.57
1:F:250:ILE:HG22	1:F:289:LEU:HD21	1.85	0.57
1:G:299:THR:HB	1:G:316:ASP:OD1	2.04	0.57
1:A:285:ARG:O	1:A:289:LEU:HG	2.04	0.57
1:A:302:SER:HB2	1:A:305:ILE:CD1	2.34	0.57
1:D:178:GLU:O	1:D:381:VAL:HG23	2.04	0.57
1:A:287:ALA:HB1	1:A:368:ARG:NH1	2.19	0.57
1:C:265:ASN:O	1:C:270:ILE:HG12	2.05	0.57
1:D:388:GLU:O	1:D:392:LYS:N	2.31	0.57
1:E:16:MET:CG	1:E:514:MET:HE3	2.34	0.57
1:G:234:LEU:N	1:G:235:PRO:HD2	2.19	0.57
1:G:271:VAL:CG1	1:G:273:VAL:HG23	2.35	0.57
1:D:136:VAL:HG13	1:D:137:PRO:HD2	1.85	0.57
1:G:230:ILE:CG2	1:G:258:ALA:HA	2.35	0.57
1:C:227:ILE:CG2	1:C:233:MET:CE	2.80	0.57
1:C:215:LEU:CD1	1:C:218:PRO:HG3	2.34	0.57
1:G:215:LEU:HB2	1:G:218:PRO:CG	2.35	0.57
1:G:226:LYS:N	1:G:227:ILE:HG13	2.18	0.57
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.86	0.57
1:G:187:LEU:HD13	1:G:379:ILE:CG2	2.35	0.57
1:G:281:PHE:HB2	1:G:282:GLY:C	2.29	0.57
1:B:169:VAL:HG23	1:B:173:GLY:HA3	1.87	0.56
1:B:209:GLU:HG2	1:B:210:THR:H	1.70	0.56
1:C:261:THR:HA	1:C:264:VAL:HG12	1.87	0.56
1:F:136:VAL:HG13	1:F:137:PRO:HD2	1.86	0.56
1:B:86:GLY:HA2	5:B:608:MPD:H12	1.86	0.56
1:B:215:LEU:CD2	1:B:272:LYS:HG3	2.36	0.56
1:C:69:MET:O	1:C:73:MET:HG3	2.05	0.56
1:C:251:ALA:O	1:C:278:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:HIS:HB2	7:C:760:HOH:O	2.05	0.56
1:A:220:ILE:CD1	1:A:296:THR:HG21	2.35	0.56
1:C:215:LEU:O	1:C:215:LEU:HD12	2.05	0.56
1:D:209:GLU:OE1	1:D:209:GLU:N	2.27	0.56
1:D:225:LYS:HB2	1:D:303:GLU:CG	2.36	0.56
1:E:89:THR:HB	7:E:743:HOH:O	2.05	0.56
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.35	0.56
1:F:242:LYS:HG2	1:G:257:GLU:HB2	1.86	0.56
1:D:225:LYS:HB2	1:D:303:GLU:HG2	1.87	0.56
1:G:395:ARG:HG3	1:G:396:VAL:N	2.21	0.56
1:G:199:TYR:HE1	1:G:202:PRO:HG3	1.71	0.56
1:D:243:ALA:O	1:E:231:ARG:NH1	2.38	0.56
1:E:7:LYS:HG2	1:E:66:PHE:CZ	2.41	0.56
1:E:270:ILE:HG22	1:E:271:VAL:N	2.18	0.56
1:G:257:GLU:HG2	1:G:261:THR:HB	1.86	0.56
1:B:277:LYS:HD2	1:B:277:LYS:O	2.06	0.56
1:C:317:LEU:HD12	1:C:317:LEU:O	2.06	0.56
1:D:238:GLU:O	1:D:242:LYS:HD3	2.05	0.56
1:F:381:VAL:HG21	1:F:392:LYS:HG2	1.87	0.56
1:G:257:GLU:HG2	1:G:261:THR:CB	2.36	0.56
1:B:214:GLU:OE1	1:B:322:ARG:NH2	2.38	0.55
1:C:325:ILE:HD12	1:C:329:THR:O	2.06	0.55
1:F:177:VAL:CG1	1:F:397:GLU:HG2	2.36	0.55
1:F:498:LYS:HG3	1:F:501:ARG:HH21	1.70	0.55
1:G:281:PHE:CB	1:G:285:ARG:HD3	2.36	0.55
1:B:234:LEU:HA	1:B:237:LEU:HD12	1.87	0.55
1:F:204:PHE:CB	1:F:266:THR:HG21	2.37	0.55
1:G:281:PHE:CD2	1:G:282:GLY:HA2	2.40	0.55
1:E:49:ILE:HD11	1:F:73:MET:HE3	1.87	0.55
1:E:445:ARG:HH12	5:E:604:MPD:HM1	1.70	0.55
1:F:225:LYS:HD2	1:F:309:LEU:CD1	2.30	0.55
1:G:265:ASN:HA	1:G:268:ARG:HG2	1.87	0.55
1:A:37:ASN:HB2	1:B:517:THR:HG22	1.88	0.55
1:B:68:ASN:O	1:B:72:GLN:HG2	2.06	0.55
1:A:162:ILE:CG2	1:A:166:MET:HE2	2.30	0.55
7:A:751:HOH:O	1:B:518:GLU:HG2	2.05	0.55
1:C:77:VAL:HG13	1:C:506:TYR:HB3	1.89	0.55
1:C:230:ILE:HG22	1:C:258:ALA:CB	2.35	0.55
1:E:193:MET:HG2	1:E:295:LEU:CD2	2.37	0.55
1:F:215:LEU:HB2	1:F:323:VAL:CG2	2.29	0.55
1:A:401:HIS:HB3	5:A:609:MPD:HM3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:TYR:CG	1:B:267:MET:HE2	2.41	0.55
1:G:152:ALA:HB1	1:G:158:VAL:HG11	1.88	0.55
1:A:69:MET:HE2	1:G:39:VAL:CG1	2.37	0.55
1:B:276:VAL:CG1	1:B:325:ILE:HD13	2.36	0.55
1:D:128:VAL:HG12	1:D:132:LYS:HE3	1.89	0.55
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.07	0.55
1:C:260:ALA:O	1:C:263:VAL:HG13	2.07	0.55
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.89	0.55
1:F:160:LYS:HE2	1:F:164:GLU:OE2	2.06	0.55
1:B:178:GLU:HB2	1:B:322:ARG:NH1	2.22	0.55
1:B:392:LYS:HE3	7:B:806:HOH:O	2.06	0.55
1:E:7:LYS:HD2	1:E:11:ASP:OD1	2.07	0.55
1:G:221:LEU:HD12	1:G:249:ILE:HG12	1.88	0.55
1:A:193:MET:HG3	1:A:371:LYS:HB3	1.89	0.54
1:B:203:TYR:CB	1:B:267:MET:HE2	2.37	0.54
1:C:150:ILE:HB	7:C:787:HOH:O	2.07	0.54
1:C:213:VAL:HG13	1:C:325:ILE:HG23	1.88	0.54
1:F:342:ILE:O	1:F:346:VAL:HG23	2.07	0.54
1:G:85:ALA:HB1	1:G:499:VAL:HG22	1.89	0.54
1:G:205:ILE:HG23	1:G:212:ALA:O	2.06	0.54
1:C:294:THR:HG23	1:C:341:ALA:HB1	1.87	0.54
1:G:365:LEU:HD12	1:G:366:GLN:N	2.22	0.54
1:A:166:MET:HE1	1:A:403:THR:CG2	2.34	0.54
1:A:179:ASP:OD1	1:A:393:LYS:HD2	2.08	0.54
1:B:10:ASN:O	1:B:14:VAL:HG13	2.07	0.54
1:D:265:ASN:C	1:D:271:VAL:HG12	2.32	0.54
1:G:209:GLU:HG2	1:G:210:THR:N	2.22	0.54
1:G:229:ASN:ND2	1:G:231:ARG:HB2	2.21	0.54
1:G:281:PHE:HB2	1:G:282:GLY:O	2.08	0.54
1:A:263:VAL:O	1:A:266:THR:OG1	2.25	0.54
1:B:525:PRO:HD3	7:B:759:HOH:O	2.07	0.54
1:D:260:ALA:O	1:D:264:VAL:HG23	2.06	0.54
1:F:248:LEU:CD1	1:F:325:ILE:HD11	2.38	0.54
1:G:218:PRO:HG2	1:G:323:VAL:CG2	2.37	0.54
1:G:278:ALA:HB1	1:G:279:PRO:CD	2.33	0.54
1:C:215:LEU:HD13	1:C:218:PRO:CD	2.38	0.54
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.90	0.54
7:D:754:HOH:O	1:E:518:GLU:HG2	2.06	0.54
1:A:166:MET:CE	1:A:403:THR:HG21	2.36	0.54
1:A:267:MET:HB2	1:A:268:ARG:HH21	1.73	0.54
1:B:34:LYS:HE2	1:C:118[A]:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:LEU:HD12	1:F:254:VAL:HB	1.89	0.54
1:G:279:PRO:HB2	1:G:285:ARG:CB	2.33	0.54
1:B:441:LYS:HE2	7:B:812:HOH:O	2.08	0.54
1:D:193:MET:HE3	1:D:371:LYS:HB3	1.89	0.54
1:G:200:LEU:HD12	1:G:275:ALA:HB1	1.89	0.54
1:A:177:VAL:HG11	1:A:397:GLU:HG3	1.89	0.54
1:C:215:LEU:HD13	1:C:218:PRO:HG3	1.90	0.54
1:F:39:VAL:HG12	1:G:69:MET:HE2	1.89	0.54
1:F:445[B]:ARG:NH2	7:F:720:HOH:O	2.40	0.54
1:A:200:LEU:CD1	1:A:254:VAL:HB	2.38	0.54
1:C:225:LYS:HA	1:C:227:ILE:HG13	1.89	0.54
1:E:221:LEU:CD2	1:E:233:MET:HE1	2.37	0.54
1:F:173:GLY:O	1:F:404:ARG:NH2	2.41	0.54
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.08	0.54
1:D:310:GLU:OE1	1:D:310:GLU:N	2.30	0.54
1:D:463:SER:O	1:D:467:ASN:HB2	2.08	0.54
1:C:305:ILE:CG2	1:C:307:MET:HG3	2.38	0.53
1:G:383:ALA:O	1:G:389:MET:HE2	2.08	0.53
1:G:384:ALA:O	1:G:385:THR:OG1	2.24	0.53
1:A:184:GLN:OE1	1:A:184:GLN:N	2.32	0.53
1:A:193:MET:HE3	1:A:295:LEU:HD12	1.90	0.53
1:C:199:TYR:HE1	1:C:202:PRO:HA	1.70	0.53
1:C:215:LEU:HD12	1:C:215:LEU:C	2.33	0.53
1:C:385:THR:HG22	1:C:386:GLU:N	2.23	0.53
1:F:30:THR:HB	1:F:51:LYS:O	2.08	0.53
1:F:288:MET:O	1:F:292:ILE:HG13	2.08	0.53
1:F:302:SER:O	1:F:307:MET:HB2	2.08	0.53
1:C:243:ALA:HB3	1:C:244:GLY:C	2.32	0.53
1:D:306:GLY:O	1:D:311:LYS:NZ	2.41	0.53
1:F:414:GLY:O	1:F:417:VAL:HG13	2.08	0.53
1:B:229:ASN:HD21	1:B:231:ARG:HB2	1.73	0.53
1:C:120:ILE:O	1:C:124:VAL:HG23	2.07	0.53
1:E:232:GLU:HG2	1:E:310:GLU:OE2	2.07	0.53
1:E:383:ALA:HB1	1:E:388:GLU:HB2	1.91	0.53
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.89	0.53
1:B:14:VAL:HG12	5:B:604:MPD:H51	1.90	0.53
1:C:213:VAL:CG2	1:C:325:ILE:HG23	2.38	0.53
1:D:152:ALA:HB3	1:D:155:ASP:H	1.72	0.53
1:G:248:LEU:C	1:G:248:LEU:HD23	2.34	0.53
1:A:136:VAL:HG13	1:A:137:PRO:HD2	1.89	0.53
1:D:265:ASN:HB3	1:D:270:ILE:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:PHE:CA	1:F:285:ARG:HB2	2.39	0.53
1:G:221:LEU:HB2	1:G:249:ILE:HG23	1.91	0.53
1:G:224:ASP:OD2	1:G:302:SER:HB2	2.08	0.53
1:B:14:VAL:HG12	5:B:604:MPD:C5	2.39	0.53
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.09	0.53
1:B:359:ASP:OD1	1:B:362:ARG:HD2	2.08	0.53
1:F:231:ARG:O	1:F:231:ARG:HD2	2.08	0.53
1:F:310:GLU:OE1	1:F:310:GLU:N	2.33	0.53
1:G:303:GLU:OE2	1:G:308:GLU:HA	2.08	0.53
1:C:325:ILE:HG13	1:C:326:ASN:N	2.23	0.53
1:D:193:MET:CE	1:D:371:LYS:HD3	2.39	0.53
1:F:221:LEU:HA	1:F:317:LEU:HD23	1.90	0.53
1:G:187:LEU:HD13	1:G:379:ILE:HG23	1.91	0.53
1:B:86:GLY:CA	5:B:608:MPD:H12	2.40	0.52
1:B:217:SER:HB3	1:B:245:LYS:NZ	2.24	0.52
1:C:39:VAL:CG1	1:D:69:MET:HE2	2.39	0.52
1:C:276:VAL:HG11	1:C:325:ILE:CD1	2.37	0.52
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.91	0.52
1:G:326:ASN:HB2	1:G:329:THR:HG23	1.91	0.52
1:A:77:VAL:HG13	1:A:506:TYR:HB3	1.91	0.52
1:A:381:VAL:HG21	1:A:393:LYS:CA	2.37	0.52
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.10	0.52
1:C:39:VAL:HG12	1:D:69:MET:CE	2.38	0.52
1:C:194:GLN:OE1	1:C:331:THR:OG1	2.27	0.52
1:C:243:ALA:HB3	1:C:244:GLY:CA	2.39	0.52
1:C:281:PHE:HA	1:C:285:ARG:HD3	1.91	0.52
1:D:179:ASP:CB	1:D:389:MET:HE1	2.39	0.52
1:E:2:ALA:HB3	7:E:751:HOH:O	2.08	0.52
1:B:177:VAL:CG1	1:B:397:GLU:HG3	2.39	0.52
1:B:263:VAL:HG22	1:B:267:MET:CE	2.40	0.52
1:B:301:ILE:HD13	1:B:312:ALA:HB2	1.91	0.52
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.91	0.52
1:D:230:ILE:HG21	1:D:261:THR:HG21	1.91	0.52
1:G:273:VAL:HG12	1:G:274:ALA:N	2.23	0.52
1:D:236:VAL:O	1:D:240:VAL:HG23	2.10	0.52
1:E:203:TYR:CD1	1:E:267:MET:HE3	2.45	0.52
1:G:171:LYS:HD3	1:G:407:VAL:HG13	1.91	0.52
1:G:219:PHE:C	1:G:220:ILE:HD12	2.35	0.52
1:A:169:VAL:CG1	1:A:173:GLY:HA3	2.40	0.52
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.90	0.52
1:B:111:MET:HE2	7:B:802:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LYS:HE2	1:B:164:GLU:OE2	2.09	0.52
1:C:16:MET:HE3	1:C:520:MET:SD	2.50	0.52
1:C:248:LEU:CD2	1:C:323:VAL:HG11	2.37	0.52
1:C:259:LEU:CA	1:C:262:LEU:HD13	2.40	0.52
1:F:179:ASP:HB3	1:F:389:MET:CE	2.40	0.52
1:G:152:ALA:HB1	1:G:158:VAL:CG1	2.39	0.52
1:G:326:ASN:N	1:G:329:THR:O	2.38	0.52
1:A:288:MET:HE3	1:A:364:LYS:HZ1	1.74	0.52
1:E:180:GLY:HA3	1:E:381:VAL:C	2.35	0.52
1:F:10:ASN:O	1:F:14:VAL:HG13	2.09	0.52
1:G:171:LYS:HD3	1:G:407:VAL:CG1	2.39	0.52
1:G:227:ILE:HD12	1:G:227:ILE:N	2.24	0.52
1:B:256:GLY:O	1:B:259:LEU:HG	2.09	0.52
1:C:229:ASN:HA	1:C:259:LEU:HD11	1.91	0.52
1:C:270:ILE:HG13	1:C:271:VAL:N	2.25	0.52
1:C:279:PRO:HG2	1:C:288:MET:HE2	1.92	0.52
1:C:489:ILE:CD1	1:C:494:LEU:HD22	2.39	0.52
1:E:319:GLN:HG3	1:E:336:VAL:HG21	1.90	0.52
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.92	0.52
1:A:236:VAL:O	1:A:240:VAL:HG23	2.10	0.52
1:C:222:LEU:CB	1:C:300:VAL:HG23	2.35	0.52
1:C:417:VAL:HG21	1:C:488:MET:HG3	1.92	0.52
1:D:38:VAL:HG22	1:E:519:CYS:HB3	1.92	0.52
1:G:222:LEU:HD12	1:G:222:LEU:O	2.09	0.52
1:A:271:VAL:HG23	1:A:272:LYS:HD3	1.91	0.51
1:B:30:THR:HB	1:B:51:LYS:O	2.09	0.51
1:G:193:MET:HB2	1:G:371:LYS:HB3	1.92	0.51
1:G:197:ALA:HA	1:G:277:LYS:CG	2.40	0.51
1:A:397:GLU:O	1:A:401:HIS:ND1	2.32	0.51
1:C:221:LEU:HD13	1:C:222:LEU:N	2.25	0.51
1:C:342:ILE:O	1:C:346:VAL:HG23	2.09	0.51
1:C:346:VAL:HG13	1:C:369:VAL:HG23	1.91	0.51
1:C:194:GLN:O	1:C:371:LYS:HE3	2.09	0.51
1:C:256:GLY:CA	1:C:259:LEU:HB2	2.39	0.51
1:G:285:ARG:HG2	1:G:286:LYS:N	2.24	0.51
1:A:327:LYS:HG3	1:A:328:ASP:OD2	2.10	0.51
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.92	0.51
1:B:308:GLU:CG	1:B:311:LYS:HE2	2.39	0.51
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.10	0.51
1:C:489:ILE:HD13	1:C:494:LEU:HD22	1.93	0.51
1:E:193:MET:CE	1:E:372:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:PRO:HG2	1:E:288:MET:HG2	1.91	0.51
1:F:265:ASN:HA	1:F:268:ARG:HB2	1.93	0.51
1:G:197:ALA:HB3	1:G:330:THR:HG22	1.91	0.51
1:F:200:LEU:HD21	1:F:277:LYS:HB2	1.93	0.51
1:G:260:ALA:O	1:G:263:VAL:HG12	2.10	0.51
1:G:268:ARG:NH1	1:G:271:VAL:HG23	2.26	0.51
1:C:82:ASN:ND2	7:C:737:HOH:O	2.43	0.51
1:C:150:ILE:HD11	1:C:493:ILE:HA	1.92	0.51
1:D:152:ALA:N	1:D:153:ASN:HA	2.25	0.51
1:F:209:GLU:HG2	1:F:210:THR:HG23	1.93	0.51
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.92	0.51
1:G:230:ILE:HG22	1:G:258:ALA:HA	1.91	0.51
1:B:253:ASP:OD1	1:B:254:VAL:N	2.42	0.51
1:C:325:ILE:CG1	1:C:326:ASN:H	2.24	0.51
1:C:112:ASN:HB3	1:C:115:ASP:HB2	1.93	0.50
1:D:193:MET:HE3	1:D:371:LYS:HD3	1.93	0.50
1:G:150:ILE:CD1	1:G:493:ILE:HA	2.41	0.50
1:A:270:ILE:CG2	1:A:271:VAL:C	2.84	0.50
1:C:344:GLY:O	1:C:348:GLN:HG3	2.11	0.50
1:G:120:ILE:O	1:G:124:VAL:HG23	2.11	0.50
1:G:251:ALA:HB2	1:G:279:PRO:HD2	1.92	0.50
1:G:268:ARG:HH11	1:G:268:ARG:CG	2.22	0.50
1:C:314:LEU:H	1:C:314:LEU:CD1	2.21	0.50
1:E:204:PHE:O	1:E:213:VAL:HG22	2.11	0.50
1:B:458:CYS:SG	1:B:480:ALA:HB1	2.52	0.50
1:C:364:LYS:HG3	1:C:365:LEU:N	2.27	0.50
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.77	0.50
1:F:270:ILE:O	1:F:270:ILE:HD12	2.11	0.50
1:A:16:MET:HG2	1:A:514:MET:HE3	1.94	0.50
1:C:225:LYS:HZ3	1:C:259:LEU:HD22	1.77	0.50
1:G:222:LEU:HD11	1:G:301:ILE:N	2.27	0.50
1:G:385:THR:HG22	1:G:386:GLU:N	2.27	0.50
1:B:77:VAL:HG13	1:B:506:TYR:HB3	1.93	0.50
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.94	0.50
1:E:366:GLN:O	1:E:369:VAL:HG22	2.12	0.50
1:G:215:LEU:HB2	1:G:218:PRO:HG3	1.94	0.50
1:G:363:GLU:O	1:G:367:GLU:HG3	2.12	0.50
1:C:32:GLY:HA3	7:C:740:HOH:O	2.11	0.50
1:C:219:PHE:O	1:C:247:LEU:HD12	2.11	0.50
1:C:313:THR:HG23	1:C:316:ASP:H	1.76	0.50
1:D:209:GLU:HG2	1:D:210:THR:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:O	1:D:252:GLU:HB2	2.12	0.50
1:D:226:LYS:HD2	1:D:255:GLU:CD	2.37	0.50
1:E:234:LEU:N	1:E:235:PRO:HD2	2.27	0.50
1:F:359:ASP:O	1:F:363:GLU:HG3	2.12	0.50
5:C:604:MPD:HM1	5:C:604:MPD:H52	1.94	0.50
1:D:180:GLY:HA3	1:D:380:LYS:HB3	1.93	0.50
1:D:385:THR:CG2	1:D:387:VAL:HG12	2.42	0.50
1:E:345:ARG:O	1:E:349:ILE:HG13	2.12	0.50
1:F:225:LYS:CG	1:F:303:GLU:HG3	2.34	0.50
1:F:363:GLU:O	1:F:367:GLU:HG3	2.11	0.50
1:G:261:THR:C	1:G:264:VAL:HG13	2.36	0.50
1:C:173:GLY:O	1:C:404:ARG:NH2	2.35	0.49
1:C:229:ASN:OD1	1:C:259:LEU:HG	2.12	0.49
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.12	0.49
1:G:284:ARG:CG	1:G:284:ARG:NH1	2.71	0.49
1:G:366:GLN:HA	1:G:369:VAL:HG22	1.94	0.49
1:G:458:CYS:HB3	7:G:719:HOH:O	2.11	0.49
1:B:227:ILE:HG21	1:B:233:MET:CE	2.38	0.49
1:C:30:THR:HB	1:C:51:LYS:O	2.12	0.49
1:F:235:PRO:HG3	1:F:310:GLU:CB	2.42	0.49
1:G:257:GLU:OE2	1:G:261:THR:HB	2.12	0.49
1:B:231:ARG:HA	1:B:234:LEU:HG	1.93	0.49
1:F:153:ASN:OD1	7:F:706:HOH:O	2.20	0.49
1:F:164:GLU:HA	1:F:167[B]:ASP:OD2	2.12	0.49
1:G:281:PHE:CB	1:G:282:GLY:HA2	2.41	0.49
1:B:259:LEU:HD12	1:B:260:ALA:H	1.76	0.49
1:C:217:SER:N	1:C:321:LYS:O	2.39	0.49
1:C:288:MET:HA	1:C:291:ASP:HB2	1.93	0.49
1:D:198:GLY:HA3	1:D:327:LYS:O	2.13	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.94	0.49
1:F:183:LEU:CD1	1:F:184:GLN:H	2.25	0.49
1:G:178:GLU:O	1:G:381:VAL:HG23	2.11	0.49
1:G:385:THR:HG22	1:G:387:VAL:H	1.77	0.49
1:D:25:ASP:OD1	1:D:28:LYS:HE2	2.13	0.49
1:D:224:ASP:OD1	1:D:286:LYS:HD3	2.12	0.49
1:E:261:THR:O	1:E:264:VAL:HB	2.12	0.49
1:F:203:TYR:HD2	1:F:263:VAL:HG13	1.76	0.49
1:B:392:LYS:HA	1:B:395:ARG:HE	1.77	0.49
1:C:49:ILE:HD11	1:D:73:MET:HE3	1.95	0.49
1:D:128:VAL:CG1	1:D:132:LYS:HE3	2.43	0.49
1:E:383:ALA:O	1:E:384:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:TYR:HD2	1:F:263:VAL:CG1	2.24	0.49
1:A:383:ALA:CB	1:A:384:ALA:CA	2.69	0.49
1:C:200:LEU:HD12	1:C:254:VAL:HG23	1.94	0.49
1:C:259:LEU:C	1:C:262:LEU:HD13	2.38	0.49
1:C:305:ILE:HG23	1:C:307:MET:HG3	1.95	0.49
1:C:352:GLN:HA	1:C:355:GLU:CD	2.38	0.49
1:D:152:ALA:CB	1:D:155:ASP:H	2.25	0.49
1:B:157:THR:HB	7:B:806:HOH:O	2.13	0.49
1:D:385:THR:HG23	1:D:387:VAL:HG12	1.93	0.49
1:E:217:SER:HA	1:E:320:ALA:O	2.12	0.49
1:F:186:GLU:HG3	1:F:187:LEU:N	2.27	0.49
1:G:171:LYS:HB3	1:G:407:VAL:HG11	1.95	0.49
1:G:248:LEU:HD21	1:G:250:ILE:CG2	2.42	0.49
1:G:301:ILE:CG2	1:G:307:MET:HG3	2.43	0.49
1:C:202:PRO:O	1:C:203:TYR:HB2	2.13	0.49
1:D:118[A]:ARG:NH2	7:D:785:HOH:O	2.46	0.49
1:D:200:LEU:CD1	1:D:254:VAL:HB	2.42	0.49
1:E:258:ALA:O	1:E:262:LEU:HD13	2.13	0.49
1:F:221:LEU:CD2	1:F:249:ILE:HD12	2.42	0.49
1:G:10:ASN:HB3	7:G:736:HOH:O	2.12	0.49
1:G:24:ALA:O	1:G:28:LYS:HG2	2.12	0.49
1:G:279:PRO:HB2	1:G:285:ARG:HA	1.94	0.49
1:B:181:THR:CG2	1:B:182:GLY:H	2.24	0.49
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.94	0.49
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.95	0.49
1:C:349:ILE:HG22	1:C:365:LEU:CD2	2.43	0.49
1:E:321:LYS:O	1:E:321:LYS:HD3	2.13	0.49
1:G:197:ALA:CA	1:G:277:LYS:HG2	2.43	0.49
1:B:225:LYS:HD2	1:B:303:GLU:OE2	2.13	0.48
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.94	0.48
1:F:259:LEU:O	1:F:263:VAL:HG23	2.13	0.48
1:G:420:ILE:HD13	1:G:448:GLU:HG2	1.94	0.48
1:G:493:ILE:HD13	2:G:601:ADP:C6	2.48	0.48
1:A:358:SER:HB3	1:A:361:ASP:OD2	2.13	0.48
1:B:198:GLY:N	1:B:277:LYS:HE3	2.28	0.48
1:C:458:CYS:SG	1:C:480:ALA:HB1	2.53	0.48
1:F:186:GLU:CD	1:F:187:LEU:H	2.22	0.48
1:F:219:PHE:CE2	1:F:245:LYS:HD2	2.48	0.48
1:D:33:PRO:HG2	1:D:480:ALA:HB3	1.94	0.48
1:D:385:THR:HG22	1:D:388:GLU:OE2	2.12	0.48
1:D:420:ILE:HD13	1:D:448:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:HG22	1:A:386:GLU:N	2.28	0.48
1:C:225:LYS:HE2	1:C:254:VAL:HA	1.95	0.48
1:F:16:MET:HE3	1:F:520:MET:HE3	1.96	0.48
1:E:403:THR:O	1:E:407:VAL:HG23	2.13	0.48
1:C:293:ALA:HB1	1:C:298:GLY:O	2.13	0.48
1:C:326:ASN:OD1	1:C:327:LYS:HG2	2.13	0.48
1:E:140:ASP:OD1	1:E:140:ASP:N	2.46	0.48
1:F:201:SER:HB2	1:F:204:PHE:HE2	1.77	0.48
1:G:124:VAL:O	1:G:128:VAL:HG23	2.13	0.48
1:G:248:LEU:HD23	1:G:249:ILE:N	2.28	0.48
1:G:279:PRO:CG	1:G:285:ARG:HB2	2.44	0.48
1:A:144:ILE:HG23	1:A:166:MET:HE1	1.95	0.48
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.49	0.48
1:B:381:VAL:CG1	1:B:392:LYS:HD3	2.43	0.48
1:C:265:ASN:HB2	1:C:270:ILE:HD11	1.95	0.48
1:C:325:ILE:CG1	1:C:326:ASN:N	2.76	0.48
1:F:171:LYS:O	1:F:404:ARG:NH1	2.44	0.48
1:C:199:TYR:HE1	1:C:202:PRO:CA	2.26	0.48
1:E:217:SER:O	1:E:245:LYS:NZ	2.38	0.48
1:F:281:PHE:N	1:F:285:ARG:HB2	2.29	0.48
1:B:232:GLU:HA	1:B:310:GLU:CG	2.44	0.48
1:C:172:GLU:OE1	1:C:172:GLU:N	2.40	0.48
1:C:206:ASN:OD1	1:C:214:GLU:N	2.47	0.48
1:C:243:ALA:HB3	1:C:244:GLY:HA2	1.96	0.48
1:D:288:MET:O	1:D:291:ASP:HB2	2.13	0.48
1:E:386:GLU:O	1:E:390:LYS:HG2	2.14	0.48
1:G:18[A]:ARG:HG2	1:G:67:GLU:CD	2.38	0.48
1:G:216:GLU:OE2	1:G:321:LYS:NZ	2.47	0.48
1:C:35:GLY:O	1:C:51:LYS:HE2	2.14	0.48
1:G:222:LEU:CD2	1:G:300:VAL:HA	2.44	0.48
1:G:242:LYS:O	1:G:243:ALA:HB3	2.14	0.48
1:G:385:THR:CG2	1:G:387:VAL:HG12	2.43	0.48
1:B:263:VAL:O	1:B:267:MET:HG3	2.14	0.47
1:C:172:GLU:H	1:C:172:GLU:CD	2.22	0.47
1:E:218:PRO:CB	1:E:246:PRO:HG2	2.32	0.47
1:E:383:ALA:HB2	1:E:389:MET:HA	1.95	0.47
1:F:186:GLU:CG	1:F:187:LEU:N	2.77	0.47
1:F:313:THR:HG22	1:F:314:LEU:N	2.29	0.47
1:C:203:TYR:HB3	1:C:267:MET:SD	2.55	0.47
1:C:206:ASN:ND2	1:C:214:GLU:H	2.12	0.47
1:F:217:SER:N	1:F:321:LYS:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ALA:HB1	1:G:225:LYS:N	2.28	0.47
1:G:383:ALA:HB1	1:G:388:GLU:CG	2.43	0.47
1:B:150:ILE:HD11	1:B:493:ILE:HA	1.97	0.47
1:G:383:ALA:HB2	1:G:392:LYS:CD	2.40	0.47
1:G:455:VAL:O	1:G:458:CYS:HB2	2.15	0.47
1:A:229:ASN:HB3	1:A:232:GLU:OE1	2.14	0.47
1:A:261:THR:HG23	1:A:265:ASN:ND2	2.29	0.47
1:A:381:VAL:HG13	1:A:392:LYS:HD3	1.95	0.47
1:B:34:LYS:HE2	1:C:118[A]:ARG:HH22	1.79	0.47
1:B:38:VAL:HG22	1:C:519:CYS:HB3	1.97	0.47
1:E:264:VAL:O	1:E:268:ARG:HG3	2.13	0.47
1:F:204:PHE:HB3	1:F:266:THR:OG1	2.13	0.47
1:F:225:LYS:NZ	1:F:308:GLU:HA	2.29	0.47
1:F:345:ARG:O	1:F:349:ILE:HG13	2.14	0.47
1:G:257:GLU:HG2	1:G:261:THR:OG1	2.15	0.47
1:G:281:PHE:HB3	1:G:285:ARG:HD3	1.96	0.47
1:A:242:LYS:HE2	1:B:229:ASN:HB2	1.96	0.47
1:C:68:ASN:O	1:C:72:GLN:HG2	2.15	0.47
1:C:227:ILE:HG22	1:C:228:SER:N	2.22	0.47
1:F:192:GLY:C	1:F:376:VAL:HG23	2.39	0.47
1:A:16:MET:CG	1:A:514:MET:HE3	2.45	0.47
1:A:253:ASP:HB3	7:A:725:HOH:O	2.14	0.47
1:A:284:ARG:O	1:A:288:MET:HG3	2.15	0.47
1:B:149:THR:OG1	1:B:156:GLU:HA	2.14	0.47
1:B:288:MET:O	1:B:292:ILE:HG13	2.14	0.47
1:C:270:ILE:HG13	1:C:271:VAL:H	1.80	0.47
1:C:349:ILE:HG22	1:C:365:LEU:HD23	1.96	0.47
1:C:489:ILE:HD13	1:C:494:LEU:CD2	2.44	0.47
1:D:219:PHE:O	1:D:247:LEU:HD12	2.14	0.47
1:D:385:THR:HG23	1:D:388:GLU:HG2	1.97	0.47
1:E:417:VAL:HG21	1:E:488:MET:HG3	1.96	0.47
1:F:227:ILE:CD1	1:F:309:LEU:HD21	2.44	0.47
1:G:15:LYS:HD3	1:G:66:PHE:HB2	1.97	0.47
1:G:325:ILE:HD12	1:G:325:ILE:N	2.30	0.47
1:A:69:MET:CE	1:G:39:VAL:HG12	2.42	0.47
1:A:108:ALA:HB2	5:A:605:MPD:HM2	1.95	0.47
1:A:266:THR:HG22	1:A:270:ILE:HG21	1.96	0.47
1:B:276:VAL:HG11	1:B:325:ILE:HD13	1.97	0.47
1:B:475:ASN:O	1:B:488:MET:HG2	2.14	0.47
1:E:420:ILE:HD13	1:E:448:GLU:HG2	1.96	0.47
1:F:204:PHE:HB3	1:F:266:THR:HB	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:PHE:CB	1:G:317:LEU:HD23	2.39	0.47
1:G:222:LEU:HD11	1:G:300:VAL:CA	2.37	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.15	0.47
1:C:206:ASN:HD21	1:C:214:GLU:H	1.62	0.47
1:C:243:ALA:N	1:C:244:GLY:HA2	2.29	0.47
1:F:383:ALA:CB	1:F:388:GLU:HB3	2.44	0.47
1:A:498:LYS:NZ	5:A:609:MPD:C5	2.78	0.47
1:C:336:VAL:HG12	1:C:336:VAL:O	2.15	0.47
1:A:176:THR:OG1	1:A:177:VAL:N	2.49	0.46
1:B:222:LEU:HD13	1:B:293:ALA:HB2	1.97	0.46
5:B:605:MPD:HM2	5:B:605:MPD:O4	2.15	0.46
1:C:16:MET:SD	1:C:73:MET:HE1	2.54	0.46
1:D:257:GLU:O	1:D:261:THR:OG1	2.23	0.46
1:F:224:ASP:O	1:F:252:GLU:HG3	2.15	0.46
1:G:14:VAL:O	1:G:18[B]:ARG:HG3	2.14	0.46
1:G:359:ASP:HA	1:G:362:ARG:NH2	2.30	0.46
1:G:392:LYS:O	1:G:396:VAL:HG23	2.14	0.46
1:A:262:LEU:O	1:A:266:THR:OG1	2.18	0.46
1:A:349:ILE:HB	1:A:369:VAL:HG12	1.96	0.46
1:A:381:VAL:CG1	1:A:392:LYS:HD3	2.45	0.46
1:B:203:TYR:HB3	1:B:267:MET:HE2	1.96	0.46
1:D:187:LEU:HD13	1:D:187:LEU:C	2.40	0.46
1:D:445:ARG:NH2	7:D:730:HOH:O	2.48	0.46
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.15	0.46
1:C:16:MET:HE1	1:C:517:THR:HG21	1.98	0.46
1:C:266:THR:OG1	1:C:272:LYS:HA	2.14	0.46
1:F:179:ASP:OD1	1:F:393:LYS:HD2	2.15	0.46
1:G:221:LEU:HD12	1:G:249:ILE:CG1	2.45	0.46
1:G:251:ALA:HB2	1:G:279:PRO:CD	2.45	0.46
1:D:160:LYS:O	1:D:163:ALA:N	2.46	0.46
1:D:164:GLU:OE1	1:D:164:GLU:N	2.44	0.46
1:E:122:LYS:NZ	1:E:430:ARG:O	2.40	0.46
1:E:381:VAL:O	1:E:381:VAL:HG22	2.16	0.46
1:E:460:GLU:OE2	7:E:754:HOH:O	2.21	0.46
1:F:215:LEU:HB3	1:F:218:PRO:HB3	1.97	0.46
1:G:433:ASN:ND2	7:G:785:HOH:O	2.40	0.46
1:B:487:ASN:O	1:B:491:MET:HG3	2.16	0.46
1:D:360:TYR:O	1:D:364:LYS:HG2	2.16	0.46
1:B:204:PHE:HE1	1:B:263:VAL:HA	1.81	0.46
1:B:227:ILE:CD1	1:B:309:LEU:HD22	2.46	0.46
1:C:200:LEU:CD1	1:C:254:VAL:CG2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:THR:HA	1:C:264:VAL:CG1	2.45	0.46
1:D:166:MET:O	1:D:170:GLY:N	2.49	0.46
1:E:49:ILE:HD12	1:F:513:LEU:HD13	1.98	0.46
1:E:444:LEU:HD23	1:E:447:MET:HE3	1.94	0.46
1:F:165:ALA:O	1:F:169:VAL:HG22	2.16	0.46
1:F:222:LEU:O	1:F:301:ILE:HG22	2.15	0.46
1:G:205:ILE:HA	1:G:213:VAL:CG2	2.45	0.46
1:G:105:LYS:HG2	5:G:604:MPD:O4	2.14	0.46
1:A:498:LYS:NZ	5:A:609:MPD:H53	2.31	0.46
1:B:227:ILE:HD12	1:B:309:LEU:CD2	2.46	0.46
1:C:231:ARG:NH1	1:C:258:ALA:HB1	2.31	0.46
1:C:348:GLN:O	1:C:352:GLN:HG3	2.15	0.46
1:C:385:THR:HG22	1:C:386:GLU:H	1.81	0.46
1:E:219:PHE:CE2	1:E:245:LYS:HD3	2.51	0.46
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.56	0.46
1:F:381:VAL:CG2	1:F:392:LYS:HD3	2.45	0.46
1:D:166:MET:HG2	1:D:175:ILE:HD11	1.98	0.46
1:E:308:GLU:HB2	1:E:311:LYS:HD3	1.98	0.46
1:E:351:GLN:O	1:E:355:GLU:HG3	2.15	0.46
1:F:264:VAL:O	1:F:268:ARG:HB2	2.16	0.46
1:F:310:GLU:H	1:F:310:GLU:CD	2.21	0.46
1:G:264:VAL:HG22	1:G:265:ASN:N	2.30	0.46
1:A:169:VAL:HG23	1:A:377:ALA:HB2	1.97	0.46
1:A:381:VAL:CG1	1:A:392:LYS:HB3	2.45	0.46
1:B:305:ILE:CG2	1:B:307:MET:HG3	2.42	0.46
1:G:34:LYS:HG3	1:G:458:CYS:SG	2.56	0.46
1:G:221:LEU:O	1:G:250:ILE:HG12	2.16	0.46
1:G:268:ARG:HH22	1:G:271:VAL:CG2	2.29	0.46
1:B:15:LYS:NZ	1:B:64:ASP:OD2	2.49	0.45
1:C:230:ILE:HD12	1:C:262:LEU:HD12	1.98	0.45
1:G:321:LYS:HG3	1:G:322:ARG:N	2.30	0.45
1:B:233:MET:HE2	1:B:249:ILE:HD13	1.97	0.45
1:B:363:GLU:O	1:B:367:GLU:HG3	2.15	0.45
1:C:206:ASN:CG	1:C:214:GLU:H	2.24	0.45
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.98	0.45
1:D:253:ASP:OD1	1:D:254:VAL:N	2.49	0.45
1:G:247:LEU:HD12	1:G:248:LEU:H	1.81	0.45
1:A:224:ASP:OD1	1:A:286:LYS:HD2	2.17	0.45
1:B:16:MET:HE3	1:B:520:MET:HE3	1.99	0.45
1:C:243:ALA:HB3	1:C:245:LYS:N	2.31	0.45
1:C:265:ASN:ND2	1:C:270:ILE:HD11	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:VAL:O	1:F:18[B]:ARG:HG3	2.16	0.45
1:G:301:ILE:HG23	1:G:307:MET:CG	2.44	0.45
1:G:321:LYS:HZ2	1:G:322:ARG:HB2	1.81	0.45
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.99	0.45
1:B:123:ALA:HB2	1:B:440:ILE:HG23	1.97	0.45
1:F:242:LYS:O	1:G:257:GLU:HB2	2.17	0.45
1:G:281:PHE:CB	1:G:282:GLY:CA	2.86	0.45
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	0.45
1:A:38:VAL:HG22	1:B:519:CYS:HB3	1.99	0.45
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.99	0.45
1:C:16:MET:CE	1:C:520:MET:HE3	2.47	0.45
1:D:385:THR:HG22	1:D:388:GLU:HG2	1.96	0.45
1:E:39:VAL:HG12	1:F:69:MET:HE2	1.99	0.45
1:G:385:THR:HB	1:G:388:GLU:CB	2.41	0.45
1:C:353:ILE:CD1	1:C:365:LEU:HD22	2.46	0.45
1:B:215:LEU:HB3	1:B:218:PRO:HB3	1.99	0.45
1:C:308:GLU:O	1:C:311:LYS:HB3	2.17	0.45
1:E:19:GLY:HA3	1:E:67:GLU:O	2.17	0.45
1:E:102:GLU:HB2	1:E:442:VAL:HG13	1.98	0.45
1:G:220:ILE:HD12	1:G:220:ILE:N	2.32	0.45
1:A:366:GLN:O	1:A:369:VAL:HG22	2.16	0.45
1:C:231:ARG:HH12	1:C:258:ALA:HB1	1.82	0.45
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.41	0.45
1:G:192:GLY:HA2	1:G:295:LEU:HD21	1.99	0.45
1:G:350:ARG:O	1:G:353:ILE:HG12	2.17	0.45
1:B:248:LEU:HD13	1:B:325:ILE:HD11	1.99	0.45
1:C:257:GLU:O	1:C:261:THR:HG23	2.17	0.45
1:F:28:LYS:NZ	7:F:750:HOH:O	2.47	0.45
1:F:381:VAL:HG22	1:F:392:LYS:HD3	1.97	0.45
1:G:100:ILE:HD13	1:G:514:MET:SD	2.56	0.45
1:G:155:ASP:HB3	1:G:158:VAL:CG1	2.46	0.45
1:G:215:LEU:HB2	1:G:218:PRO:HG2	1.97	0.45
1:G:262:LEU:HD12	1:G:262:LEU:O	2.17	0.45
1:B:188:ASP:OD1	1:B:188:ASP:N	2.49	0.45
1:C:200:LEU:CD1	1:C:254:VAL:HB	2.47	0.45
1:D:270:ILE:O	1:D:270:ILE:HG12	2.17	0.45
1:D:273:VAL:HG22	1:D:274:ALA:N	2.32	0.45
1:D:392:LYS:O	1:D:395:ARG:HB3	2.16	0.45
1:F:25:ASP:OD1	1:F:28:LYS:HE2	2.16	0.45
1:G:68:ASN:O	1:G:72:GLN:HG2	2.17	0.45
1:G:104:LEU:HB3	5:G:604:MPD:H12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:LYS:O	1:G:278:ALA:HB3	2.16	0.45
1:A:230:ILE:O	1:A:230:ILE:HG12	2.16	0.44
1:B:140:ASP:OD2	1:B:142:LYS:HB3	2.16	0.44
1:B:214:GLU:CD	1:B:322:ARG:HH21	2.24	0.44
1:C:259:LEU:HA	1:C:262:LEU:CD1	2.44	0.44
1:F:177:VAL:HG13	1:F:397:GLU:HG2	1.98	0.44
1:F:225:LYS:HZ2	1:F:309:LEU:HD12	1.82	0.44
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.99	0.44
1:A:344:GLY:O	1:A:348:GLN:HG3	2.17	0.44
1:A:401:HIS:O	1:A:404:ARG:HB2	2.16	0.44
1:B:455:VAL:HG21	1:B:465:VAL:HG11	1.98	0.44
1:C:198:GLY:HA3	1:C:327:LYS:O	2.17	0.44
1:C:213:VAL:CG1	1:C:325:ILE:HG23	2.47	0.44
1:F:235:PRO:HG3	1:F:310:GLU:CA	2.48	0.44
1:G:16:MET:HE3	1:G:520:MET:HE3	1.99	0.44
1:A:124:VAL:O	1:A:128:VAL:HG23	2.17	0.44
1:A:456:LEU:HG	5:A:608:MPD:H12	2.00	0.44
1:A:475:ASN:O	1:A:488:MET:HG2	2.17	0.44
1:C:25:ASP:O	1:C:29:VAL:HG13	2.17	0.44
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.17	0.44
1:G:285:ARG:HG3	1:G:289:LEU:HD12	2.00	0.44
1:A:193:MET:HG2	1:A:194:GLN:N	2.31	0.44
1:A:231:ARG:HA	1:A:234:LEU:HD23	1.99	0.44
1:B:181:THR:CG2	1:B:182:GLY:N	2.81	0.44
1:C:225:LYS:O	1:C:227:ILE:HG13	2.13	0.44
1:D:218:PRO:HD2	1:D:320:ALA:O	2.17	0.44
1:D:359:ASP:O	1:D:363:GLU:HG3	2.18	0.44
1:F:309:LEU:HD12	1:F:309:LEU:N	2.32	0.44
1:F:420:ILE:HD13	1:F:448:GLU:HG2	1.99	0.44
1:G:268:ARG:HH22	1:G:271:VAL:HG23	1.82	0.44
1:G:301:ILE:HD13	1:G:307:MET:HE3	1.99	0.44
1:C:230:ILE:HG21	1:C:258:ALA:HB1	1.98	0.44
1:C:456:LEU:HD13	1:C:462:PRO:HG2	1.99	0.44
1:D:136:VAL:HG13	1:D:137:PRO:CD	2.47	0.44
1:A:498:LYS:HZ1	5:A:609:MPD:H53	1.82	0.44
1:B:260:ALA:HA	1:B:263:VAL:CG1	2.48	0.44
1:C:219:PHE:CG	1:C:245:LYS:HD2	2.53	0.44
1:D:152:ALA:HB3	1:D:154:SER:N	2.33	0.44
5:D:605:MPD:O4	5:D:605:MPD:H11	2.17	0.44
1:F:225:LYS:HZ2	1:F:308:GLU:HA	1.83	0.44
1:F:391:GLU:HG2	1:F:392:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:THR:HG21	1:G:387:VAL:HG12	2.00	0.44
1:B:225:LYS:NZ	1:B:232:GLU:OE2	2.27	0.44
1:B:319:GLN:O	1:B:336:VAL:HG23	2.18	0.44
1:C:177:VAL:HG21	1:C:397:GLU:CG	2.47	0.44
1:D:325:ILE:HD12	1:D:325:ILE:N	2.32	0.44
1:E:219:PHE:HE2	1:E:245:LYS:HD3	1.83	0.44
1:F:214:GLU:O	1:F:215:LEU:HD23	2.18	0.44
1:G:214:GLU:HA	1:G:323:VAL:O	2.17	0.44
1:G:225:LYS:HA	1:G:226:LYS:HA	1.50	0.44
1:A:348:GLN:O	1:A:352:GLN:HG3	2.18	0.44
1:C:232:GLU:CD	1:C:233:MET:HE1	2.43	0.44
1:E:117:LYS:NZ	7:E:750:HOH:O	2.51	0.44
1:F:349:ILE:O	1:F:353:ILE:HG12	2.18	0.44
1:A:365:LEU:CD2	1:A:368:ARG:HH21	2.31	0.44
5:A:608:MPD:HM1	1:B:518:GLU:HG3	2.00	0.44
1:B:238:GLU:O	1:B:242:LYS:HG3	2.18	0.44
1:D:326:ASN:OD1	1:D:329:THR:N	2.46	0.44
1:D:389:MET:HG3	1:D:390:LYS:N	2.33	0.44
1:E:200:LEU:CD1	1:E:254:VAL:HB	2.47	0.44
1:E:201:SER:HA	1:E:202:PRO:HD3	1.89	0.44
1:A:140:ASP:OD1	1:A:140:ASP:N	2.50	0.43
1:B:332:ILE:N	1:B:332:ILE:HD12	2.33	0.43
1:E:177:VAL:CG1	1:E:397:GLU:HG2	2.48	0.43
1:G:226:LYS:CB	1:G:227:ILE:HA	2.31	0.43
1:C:488:MET:HE3	1:C:493:ILE:HB	2.00	0.43
1:E:81:ALA:HB1	7:E:719:HOH:O	2.17	0.43
2:E:601:ADP:O1B	2:E:601:ADP:O2A	2.36	0.43
1:G:207:LYS:HB3	1:G:209:GLU:CD	2.44	0.43
1:B:361:ASP:O	1:B:365:LEU:HD13	2.18	0.43
1:F:153:ASN:O	1:F:154:SER:HB2	2.18	0.43
1:F:195:PHE:CE2	1:F:330:THR:HG21	2.53	0.43
1:F:313:THR:HG22	1:F:314:LEU:H	1.84	0.43
1:B:205:ILE:HG22	1:B:207:LYS:H	1.83	0.43
1:B:260:ALA:HA	1:B:263:VAL:HG12	2.00	0.43
1:C:326:ASN:OD1	1:C:327:LYS:N	2.44	0.43
1:D:25:ASP:HA	1:D:28:LYS:HE2	2.00	0.43
1:D:522:THR:OG1	1:D:523:ASP:N	2.52	0.43
1:E:183:LEU:HD12	1:E:183:LEU:C	2.43	0.43
1:F:49:ILE:CD1	1:G:73:MET:HE3	2.48	0.43
1:C:301:ILE:HD11	1:C:312:ALA:CB	2.48	0.43
1:D:49:ILE:HD11	1:E:73:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:GLU:O	1:D:367:GLU:HG3	2.19	0.43
1:E:193:MET:HE3	1:E:295:LEU:HD22	2.00	0.43
1:E:219:PHE:HB3	1:E:317:LEU:HD23	2.00	0.43
1:G:392:LYS:HE3	1:G:395:ARG:HH21	1.84	0.43
1:C:220:ILE:HD12	1:C:296:THR:CG2	2.46	0.43
1:C:258:ALA:O	1:C:261:THR:OG1	2.22	0.43
1:F:192:GLY:HA3	1:F:376:VAL:HG23	2.00	0.43
1:F:215:LEU:HD12	1:F:323:VAL:HG21	2.00	0.43
1:G:155:ASP:CG	1:G:158:VAL:HG12	2.44	0.43
1:G:251:ALA:CB	1:G:289:LEU:HD21	2.47	0.43
1:A:37:ASN:CB	1:B:517:THR:HG22	2.49	0.43
1:A:393:LYS:NZ	1:A:397:GLU:OE2	2.38	0.43
1:B:362:ARG:O	1:B:366:GLN:HB2	2.18	0.43
1:C:230:ILE:CG1	1:C:262:LEU:HD11	2.41	0.43
1:C:256:GLY:CA	1:C:259:LEU:HD12	2.45	0.43
1:D:232:GLU:CD	1:D:309:LEU:HD12	2.43	0.43
1:D:302:SER:O	1:D:307:MET:HB2	2.19	0.43
1:E:193:MET:HE1	1:E:372:LEU:HD12	1.99	0.43
1:F:246:PRO:CB	1:F:272:LYS:HE3	2.46	0.43
1:G:27:VAL:HG12	1:G:90:THR:HG23	2.00	0.43
1:B:359:ASP:O	1:B:363:GLU:HG3	2.18	0.43
1:D:176:THR:CG2	1:D:378:VAL:HG22	2.49	0.43
1:D:385:THR:O	1:D:389:MET:HB3	2.18	0.43
1:E:160:LYS:O	1:E:164:GLU:HG3	2.19	0.43
1:C:19:GLY:HA3	1:C:67:GLU:O	2.19	0.43
1:C:200:LEU:HD12	1:C:254:VAL:HB	2.01	0.43
1:C:219:PHE:CD2	1:C:245:LYS:HD2	2.53	0.43
1:C:385:THR:HB	1:C:388:GLU:HB3	2.01	0.43
1:C:493:ILE:C	1:C:494:LEU:HD23	2.43	0.43
1:F:230:ILE:O	1:F:234:LEU:HG	2.19	0.43
1:F:383:ALA:HB1	1:F:388:GLU:CB	2.46	0.43
1:G:291:ASP:OD2	1:G:368:ARG:NH1	2.52	0.43
1:A:350:ARG:O	1:A:353:ILE:HB	2.19	0.43
1:B:198:GLY:H	1:B:277:LYS:CE	2.32	0.43
1:C:385:THR:O	1:C:389:MET:HB2	2.19	0.43
1:E:451:LEU:C	1:E:451:LEU:HD23	2.44	0.43
1:F:46:ALA:HA	1:F:47:PRO:HD3	1.83	0.43
1:F:252:GLU:O	1:F:253:ASP:HB2	2.18	0.43
1:C:272:LYS:HD2	1:C:272:LYS:N	2.34	0.42
1:C:434:GLU:HG2	7:C:763:HOH:O	2.19	0.42
1:D:177:VAL:HG12	1:D:393:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:LYS:O	1:F:164:GLU:HG3	2.18	0.42
1:F:221:LEU:CB	1:F:249:ILE:HD12	2.47	0.42
1:G:219:PHE:HE1	1:G:245:LYS:HD3	1.83	0.42
1:C:233:MET:N	1:C:233:MET:SD	2.92	0.42
1:C:352:GLN:HA	1:C:355:GLU:CG	2.50	0.42
1:F:185:ASP:OD1	1:F:185:ASP:N	2.39	0.42
1:G:321:LYS:HB3	1:G:334:ASP:HB3	2.00	0.42
1:C:16:MET:HE3	1:C:520:MET:HE3	2.01	0.42
1:F:192:GLY:CA	1:F:376:VAL:HG23	2.48	0.42
1:F:200:LEU:CD1	1:F:254:VAL:HB	2.48	0.42
1:A:106:ALA:O	1:A:111:MET:HG3	2.19	0.42
1:A:169:VAL:CG2	1:A:377:ALA:HB2	2.48	0.42
1:A:363:GLU:O	1:A:367:GLU:HG3	2.19	0.42
1:B:222:LEU:HD22	1:B:289:LEU:HD22	2.00	0.42
1:D:152:ALA:HB1	1:D:155:ASP:HB3	2.00	0.42
1:D:225:LYS:NZ	1:D:232:GLU:OE2	2.39	0.42
1:E:339:GLU:O	1:E:343:GLN:HG2	2.20	0.42
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.19	0.42
1:F:281:PHE:C	1:F:285:ARG:HB2	2.44	0.42
1:F:417:VAL:O	1:F:421:ARG:HG2	2.19	0.42
1:G:264:VAL:HG22	1:G:265:ASN:ND2	2.34	0.42
1:B:269:GLY:O	1:B:270:ILE:HB	2.19	0.42
1:B:364:LYS:HD2	1:B:364:LYS:HA	1.84	0.42
1:C:227:ILE:CG2	1:C:228:SER:H	2.16	0.42
1:D:180:GLY:CA	1:D:380:LYS:HB3	2.49	0.42
1:E:260:ALA:O	1:E:264:VAL:HG23	2.19	0.42
1:E:383:ALA:HB1	1:E:388:GLU:CB	2.50	0.42
1:G:251:ALA:CB	1:G:279:PRO:HD2	2.50	0.42
1:A:195:PHE:CE1	1:A:330:THR:HB	2.55	0.42
1:B:268:ARG:HH11	1:B:268:ARG:CG	2.29	0.42
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.42
1:C:456:LEU:HD13	1:C:462:PRO:CG	2.50	0.42
1:D:14:VAL:O	1:D:18[B]:ARG:HG3	2.19	0.42
1:D:222:LEU:HD23	1:D:250:ILE:HB	2.01	0.42
1:D:232:GLU:OE2	1:D:309:LEU:HD12	2.19	0.42
1:F:349:ILE:HG21	1:F:369:VAL:HG13	2.01	0.42
1:A:272:LYS:HE2	1:A:272:LYS:HB2	1.92	0.42
1:C:207:LYS:HG3	1:C:207:LYS:O	2.20	0.42
1:C:226:LYS:HD3	1:C:252:GLU:OE2	2.19	0.42
1:D:143:ALA:O	1:D:147:VAL:HG23	2.20	0.42
1:D:266:THR:HA	1:D:271:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:LEU:CA	1:E:447:MET:HE3	2.40	0.42
1:G:183:LEU:HA	1:G:384:ALA:HB2	2.02	0.42
1:A:391:GLU:O	1:A:394:ALA:HB3	2.20	0.42
1:C:206:ASN:O	1:C:207:LYS:HG2	2.19	0.42
1:C:215:LEU:HD11	1:C:323:VAL:N	2.35	0.42
1:D:336:VAL:O	1:D:336:VAL:HG12	2.18	0.42
1:G:279:PRO:HG2	1:G:285:ARG:HB2	2.01	0.42
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.60	0.42
1:A:194:GLN:O	1:A:371:LYS:HE3	2.20	0.42
1:A:288:MET:CE	1:A:364:LYS:HZ1	2.33	0.42
1:C:299:THR:HB	1:C:316:ASP:OD1	2.20	0.42
1:F:232:GLU:OE1	1:F:309:LEU:HD13	2.19	0.42
1:F:367:GLU:O	1:F:371:LYS:HG3	2.20	0.42
1:G:16:MET:HB3	1:G:514:MET:CE	2.49	0.42
1:A:325:ILE:N	1:A:325:ILE:HD12	2.35	0.42
1:C:27:VAL:HG12	1:C:90:THR:HG23	2.01	0.42
1:C:256:GLY:HA3	1:C:259:LEU:HB2	2.01	0.42
1:D:366:GLN:O	1:D:369:VAL:HG22	2.19	0.42
1:D:417:VAL:HG21	1:D:477:GLY:HA3	2.01	0.42
1:E:263:VAL:HG12	1:E:263:VAL:O	2.20	0.42
1:F:232:GLU:HG3	1:F:309:LEU:HD22	2.02	0.42
1:G:46:ALA:HA	1:G:47:PRO:HD3	1.84	0.42
1:G:187:LEU:HD13	1:G:379:ILE:HG22	2.02	0.42
1:G:230:ILE:HA	1:G:233:MET:HG2	2.02	0.42
1:A:245:LYS:HE3	1:B:255:GLU:OE1	2.19	0.41
1:A:257:GLU:O	1:A:261:THR:HB	2.20	0.41
1:B:217:SER:HA	1:B:320:ALA:O	2.19	0.41
1:C:282:GLY:H	1:C:285:ARG:HH11	1.67	0.41
1:D:49:ILE:CD1	1:E:73:MET:HE3	2.50	0.41
1:F:350:ARG:HA	1:F:353:ILE:HG13	2.02	0.41
1:F:389:MET:HE3	1:F:389:MET:HB3	1.79	0.41
1:F:501:ARG:HG2	1:F:505:GLN:OE1	2.20	0.41
1:G:352:GLN:HA	1:G:355:GLU:CB	2.38	0.41
1:B:217:SER:HB3	1:B:245:LYS:HZ1	1.85	0.41
1:B:220:ILE:CD1	1:B:296:THR:HG21	2.50	0.41
1:C:209:GLU:HG2	1:C:210:THR:N	2.35	0.41
1:C:217:SER:O	1:C:245:LYS:HG3	2.20	0.41
1:E:184:GLN:OE1	1:E:184:GLN:HA	2.20	0.41
1:F:183:LEU:HD12	1:F:183:LEU:N	2.35	0.41
1:G:219:PHE:CE1	1:G:245:LYS:HD3	2.55	0.41
1:C:229:ASN:O	1:C:233:MET:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:MET:HG3	1:D:520:MET:SD	2.60	0.41
1:E:102:GLU:OE1	1:E:445:ARG:NH1	2.53	0.41
1:F:253:ASP:OD1	1:F:277:LYS:HE2	2.20	0.41
1:G:360:TYR:CE2	1:G:364:LYS:HE2	2.55	0.41
1:A:144:ILE:CG2	1:A:166:MET:HE1	2.50	0.41
1:D:207:LYS:HA	1:D:208:PRO:HD2	1.93	0.41
1:D:225:LYS:CB	1:D:303:GLU:CD	2.92	0.41
1:E:49:ILE:CD1	1:F:513:LEU:HD13	2.50	0.41
1:E:325:ILE:HD12	1:E:325:ILE:N	2.36	0.41
1:F:225:LYS:HE2	1:F:303:GLU:CG	2.51	0.41
1:G:204:PHE:C	1:G:213:VAL:HG22	2.44	0.41
1:G:321:LYS:HG3	1:G:322:ARG:HB2	2.02	0.41
1:A:266:THR:CG2	1:A:270:ILE:HG21	2.50	0.41
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.81	0.41
1:B:118[A]:ARG:HD2	7:B:786:HOH:O	2.20	0.41
1:C:215:LEU:CD1	1:C:323:VAL:H	2.33	0.41
1:C:393:LYS:NZ	1:C:397:GLU:OE2	2.53	0.41
1:D:39:VAL:HG12	1:E:69:MET:CE	2.51	0.41
7:E:745:HOH:O	1:F:518:GLU:HG2	2.18	0.41
1:F:364:LYS:HD3	1:F:367:GLU:OE1	2.21	0.41
1:A:270:ILE:CD1	1:A:273:VAL:HB	2.36	0.41
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.61	0.41
1:B:221:LEU:HD23	1:B:249:ILE:HG23	2.02	0.41
1:C:215:LEU:HD11	1:C:218:PRO:HG3	2.02	0.41
1:C:226:LYS:HA	1:C:226:LYS:CE	2.50	0.41
1:C:282:GLY:H	1:C:285:ARG:NH1	2.18	0.41
1:C:317:LEU:HD12	1:C:317:LEU:C	2.45	0.41
1:D:183:LEU:HD12	1:D:183:LEU:N	2.36	0.41
1:E:342:ILE:O	1:E:346:VAL:HG23	2.19	0.41
1:F:294:THR:HG23	1:F:341:ALA:HB1	2.02	0.41
1:F:295:LEU:O	1:F:295:LEU:HD23	2.21	0.41
1:A:234:LEU:N	1:A:235:PRO:HD2	2.36	0.41
1:A:247:LEU:HB3	1:A:273:VAL:CG2	2.45	0.41
1:B:259:LEU:HD12	1:B:260:ALA:CA	2.51	0.41
1:C:326:ASN:CG	1:C:327:LYS:H	2.26	0.41
1:D:227:ILE:HG22	1:D:258:ALA:CB	2.50	0.41
1:E:16:MET:HG2	1:E:514:MET:CE	2.44	0.41
1:E:75:LYS:NZ	7:E:721:HOH:O	2.53	0.41
1:F:16:MET:HB3	1:F:514:MET:HE3	2.02	0.41
1:G:168:LYS:HD2	1:G:189:VAL:HG21	2.02	0.41
1:G:524:LEU:HD23	1:G:524:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:HA	1:A:47:PRO:HD3	1.93	0.41
1:A:177:VAL:HG11	1:A:397:GLU:CG	2.49	0.41
1:A:281:PHE:N	1:A:285:ARG:HB2	2.36	0.41
1:B:234:LEU:N	1:B:235:PRO:HD2	2.35	0.41
1:B:287:ALA:HB1	1:B:368:ARG:NH1	2.36	0.41
1:C:256:GLY:O	1:C:260:ALA:N	2.53	0.41
1:E:366:GLN:HG2	7:E:742:HOH:O	2.20	0.41
1:A:16:MET:SD	1:A:73:MET:HE1	2.61	0.41
1:A:131:LEU:CD1	1:A:422:VAL:HG21	2.43	0.41
1:C:350:ARG:O	1:C:353:ILE:HB	2.20	0.41
1:D:68:ASN:O	1:D:72:GLN:HG2	2.21	0.41
1:D:160:LYS:HG2	1:D:164:GLU:OE2	2.21	0.41
1:E:293:ALA:HB1	1:E:298:GLY:O	2.19	0.41
1:F:127:ALA:O	1:F:131:LEU:HB2	2.21	0.41
1:G:178:GLU:OE2	1:G:322:ARG:HD3	2.20	0.41
1:G:222:LEU:HD12	1:G:222:LEU:C	2.46	0.41
1:G:284:ARG:NH1	1:G:364:LYS:HE3	2.35	0.41
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.51	0.41
1:F:193:MET:HB2	1:F:371:LYS:HB3	2.03	0.41
1:G:223:ALA:CA	1:G:224:ASP:HB2	2.43	0.41
1:G:279:PRO:HB2	1:G:285:ARG:CA	2.51	0.41
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.41
1:A:162:ILE:HD11	1:A:399:ALA:HB3	2.03	0.40
1:A:222:LEU:O	1:A:301:ILE:HG22	2.21	0.40
1:C:225:LYS:HZ3	1:C:259:LEU:CD2	2.33	0.40
1:C:259:LEU:O	1:C:262:LEU:HD13	2.21	0.40
1:D:381:VAL:HG12	1:D:382:GLY:N	2.36	0.40
1:D:455:VAL:HG21	1:D:465:VAL:HG11	2.03	0.40
1:D:524:LEU:HA	1:D:525:PRO:HD3	1.97	0.40
1:E:124:VAL:O	1:E:128:VAL:HG23	2.21	0.40
1:E:381:VAL:CG2	1:E:392:LYS:HD3	2.51	0.40
1:F:308:GLU:HB3	1:F:310:GLU:OE2	2.20	0.40
1:A:30:THR:HB	1:A:51:LYS:O	2.21	0.40
1:A:225:LYS:HD2	1:A:303:GLU:OE1	2.21	0.40
1:C:364:LYS:O	1:C:367:GLU:HB2	2.21	0.40
1:C:420:ILE:HD12	1:C:451:LEU:CD1	2.38	0.40
1:D:64:ASP:CG	1:D:67:GLU:HG3	2.46	0.40
5:D:604:MPD:O4	5:D:604:MPD:H12	2.21	0.40
1:E:33:PRO:HG3	2:E:601:ADP:C6	2.55	0.40
1:E:163:ALA:O	1:E:167:ASP:HB2	2.22	0.40
1:E:203:TYR:O	1:E:267:MET:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.21	0.40
1:F:231:ARG:HG3	1:F:231:ARG:NH1	2.33	0.40
1:F:234:LEU:N	1:F:235:PRO:CD	2.82	0.40
1:F:326:ASN:HB3	1:F:329:THR:HB	2.02	0.40
1:G:232:GLU:CD	1:G:309:LEU:HD12	2.46	0.40
1:C:273:VAL:HG22	1:C:274:ALA:N	2.35	0.40
1:C:455:VAL:O	1:C:458:CYS:HB2	2.21	0.40
1:E:22:VAL:HG11	1:E:62:LEU:HD21	2.02	0.40
1:E:365:LEU:CD2	1:E:368:ARG:HH21	2.34	0.40
1:G:165:ALA:O	1:G:169:VAL:HG22	2.21	0.40
1:B:202:PRO:O	1:B:205:ILE:HG13	2.22	0.40
1:B:270:ILE:O	1:B:270:ILE:HG22	2.21	0.40
1:G:139:SER:HA	1:G:171:LYS:NZ	2.36	0.40
1:G:226:LYS:HB2	1:G:227:ILE:CA	2.44	0.40
1:A:49:ILE:HD11	1:B:73:MET:HE3	2.03	0.40
1:B:5:ASP:HB2	1:B:524:LEU:HD23	2.04	0.40
1:B:16:MET:HG3	1:B:520:MET:CE	2.52	0.40
1:B:222:LEU:HD22	1:B:289:LEU:CD2	2.52	0.40
1:C:229:ASN:HA	1:C:259:LEU:CD1	2.51	0.40
1:D:381:VAL:HG12	1:D:392:LYS:HD3	2.04	0.40
1:D:420:ILE:CD1	1:D:448:GLU:HG2	2.51	0.40
1:F:77:VAL:HG21	1:F:510:VAL:HB	2.03	0.40
1:F:314:LEU:HA	1:F:317:LEU:HD12	2.03	0.40
1:G:204:PHE:HB3	1:G:213:VAL:HG21	2.02	0.40
1:G:451:LEU:HD23	1:G:451:LEU:C	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:GLU:OE2	1:F:463:SER:OG[2_959]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	523/548 (95%)	512 (98%)	11 (2%)	0	100	100
1	B	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	66
1	C	525/548 (96%)	505 (96%)	19 (4%)	1 (0%)	43	66
1	D	524/548 (96%)	509 (97%)	15 (3%)	0	100	100
1	E	523/548 (95%)	512 (98%)	10 (2%)	1 (0%)	43	66
1	F	526/548 (96%)	512 (97%)	13 (2%)	1 (0%)	43	66
1	G	523/548 (95%)	502 (96%)	21 (4%)	0	100	100
All	All	3667/3836 (96%)	3561 (97%)	102 (3%)	4 (0%)	48	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	ILE
1	F	270	ILE
1	E	270	ILE
1	C	227	ILE

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	403/413 (98%)	386 (96%)	17 (4%)	26	53
1	B	403/413 (98%)	391 (97%)	12 (3%)	36	64
1	C	405/413 (98%)	388 (96%)	17 (4%)	26	53
1	D	404/413 (98%)	391 (97%)	13 (3%)	34	62
1	E	403/413 (98%)	387 (96%)	16 (4%)	28	55
1	F	406/413 (98%)	387 (95%)	19 (5%)	23	49
1	G	403/413 (98%)	383 (95%)	20 (5%)	22	46
All	All	2827/2891 (98%)	2713 (96%)	114 (4%)	27	55

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	77	VAL
1	A	131	LEU
1	A	138	CYS
1	A	176	THR
1	A	177	VAL
1	A	226	LYS
1	A	230	ILE
1	A	261	THR
1	A	264	VAL
1	A	266	THR
1	A	273	VAL
1	A	301	ILE
1	A	305	ILE
1	A	328	ASP
1	A	329	THR
1	A	353	ILE
1	B	10	ASN
1	B	14	VAL
1	B	48	THR
1	B	77	VAL
1	B	125	THR
1	B	136	VAL
1	B	196	ASP
1	B	213	VAL
1	B	268	ARG
1	B	277	LYS
1	B	389	MET
1	B	473	ASP
1	C	48	THR
1	C	77	VAL
1	C	136	VAL
1	C	177	VAL
1	C	213	VAL
1	C	226	LYS
1	C	230	ILE
1	C	263	VAL
1	C	264	VAL
1	C	268	ARG
1	C	271	VAL
1	C	276	VAL
1	C	319	GLN

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Mol	Chain	Res	Type
1	C	325	ILE
1	C	334	ASP
1	C	353	ILE
1	C	420	ILE
1	D	10	ASN
1	D	51	LYS
1	D	77	VAL
1	D	136	VAL
1	D	185	ASP
1	D	186	GLU
1	D	188	ASP
1	D	261	THR
1	D	270	ILE
1	D	295	LEU
1	D	328	ASP
1	D	389	MET
1	D	467	ASN
1	E	16	MET
1	E	34	LYS
1	E	89	THR
1	E	105	LYS
1	E	136	VAL
1	E	169	VAL
1	E	177	VAL
1	E	183	LEU
1	E	204	PHE
1	E	210	THR
1	E	273	VAL
1	E	321	LYS
1	E	359	ASP
1	E	372	LEU
1	E	381	VAL
1	E	422	VAL
1	F	10	ASN
1	F	14	VAL
1	F	48	THR
1	F	77	VAL
1	F	94	VAL
1	F	118	ARG
1	F	131	LEU
1	F	136	VAL
1	F	177	VAL

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Mol	Chain	Res	Type
1	F	183	LEU
1	F	196	ASP
1	F	264	VAL
1	F	268	ARG
1	F	270	ILE
1	F	301	ILE
1	F	353	ILE
1	F	389	MET
1	F	417	VAL
1	F	499	VAL
1	G	11	ASP
1	G	48	THR
1	G	77	VAL
1	G	140	ASP
1	G	141	SER
1	G	147	VAL
1	G	150	ILE
1	G	158	VAL
1	G	176	THR
1	G	185	ASP
1	G	249	ILE
1	G	253	ASP
1	G	254	VAL
1	G	264	VAL
1	G	268	ARG
1	G	284	ARG
1	G	305	ILE
1	G	326	ASN
1	G	330	THR
1	G	350	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	D	10	ASN
1	D	82	ASN
1	D	184	GLN
1	D	194	GLN
1	E	37	ASN
1	E	146	GLN
1	F	401	HIS

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Mol	Chain	Res	Type
1	F	432	GLN
1	G	37	ASN
1	G	326	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 53 ligands modelled in this entry, 27 are monoatomic - leaving 26 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	$\# Z > 2$
5	MPD	D	605	-	7,7,7	0.34	0	9,10,10	0.46	0
2	ADP	A	601	3,4	28,29,29	1.42	5 (17%)	43,45,45	1.95	12 (27%)
5	MPD	A	604	-	7,7,7	0.41	0	9,10,10	0.38	0
5	MPD	G	604	-	7,7,7	0.38	0	9,10,10	0.49	0
5	MPD	A	608	-	7,7,7	0.32	0	9,10,10	0.77	0
2	ADP	C	601	3,4	28,29,29	1.45	5 (17%)	43,45,45	1.98	11 (25%)
5	MPD	A	606	-	7,7,7	0.37	0	9,10,10	0.73	0
5	MPD	E	604	-	7,7,7	0.39	0	9,10,10	0.50	0
5	MPD	B	608	-	7,7,7	0.37	0	9,10,10	0.43	0
5	MPD	D	604	-	7,7,7	0.35	0	9,10,10	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	601	3,4	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
5	MPD	G	605	-	7,7,7	0.83	0	9,10,10	0.92	0
5	MPD	B	604	-	7,7,7	0.42	0	9,10,10	0.44	0
5	MPD	B	605	-	7,7,7	0.34	0	9,10,10	0.57	0
2	ADP	G	601	3,4	28,29,29	1.45	6 (21%)	43,45,45	1.98	11 (25%)
5	MPD	D	606	-	7,7,7	0.43	0	9,10,10	0.68	0
5	MPD	B	607	-	7,7,7	0.34	0	9,10,10	0.42	0
2	ADP	F	601	3,4	28,29,29	1.38	4 (14%)	43,45,45	1.89	10 (23%)
5	MPD	B	606	-	7,7,7	0.39	0	9,10,10	0.48	0
5	MPD	A	605	-	7,7,7	0.37	0	9,10,10	0.62	0
5	MPD	C	604	-	7,7,7	0.43	0	9,10,10	0.82	0
5	MPD	A	609	-	7,7,7	0.27	0	9,10,10	0.44	0
5	MPD	F	604	-	7,7,7	0.35	0	9,10,10	0.43	0
2	ADP	E	601	3,4	28,29,29	1.38	4 (14%)	43,45,45	1.94	11 (25%)
2	ADP	D	601	3,4	28,29,29	1.44	6 (21%)	43,45,45	1.97	12 (27%)
5	MPD	A	607	-	7,7,7	0.37	0	9,10,10	0.33	0

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
5	MPD	D	605	-	-	1/5/5/5	-
2	ADP	A	601	3,4	-	2/16/32/32	0/3/3/3
5	MPD	A	604	-	-	2/5/5/5	-
5	MPD	G	604	-	-	1/5/5/5	-
5	MPD	A	608	-	-	4/5/5/5	-
2	ADP	C	601	3,4	-	2/16/32/32	0/3/3/3
5	MPD	A	606	-	-	2/5/5/5	-
5	MPD	E	604	-	-	1/5/5/5	-
5	MPD	B	608	-	-	4/5/5/5	-
5	MPD	D	604	-	-	2/5/5/5	-
2	ADP	B	601	3,4	-	6/16/32/32	0/3/3/3
5	MPD	G	605	-	-	0/5/5/5	-
5	MPD	B	604	-	-	1/5/5/5	-
5	MPD	B	605	-	-	3/5/5/5	-
2	ADP	G	601	3,4	-	3/16/32/32	0/3/3/3
5	MPD	D	606	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	B	607	-	-	2/5/5/5	-
2	ADP	F	601	3,4	-	7/16/32/32	0/3/3/3
5	MPD	B	606	-	-	1/5/5/5	-
5	MPD	A	605	-	-	3/5/5/5	-
5	MPD	C	604	-	-	2/5/5/5	-
5	MPD	A	609	-	-	2/5/5/5	-
5	MPD	F	604	-	-	2/5/5/5	-
2	ADP	E	601	3,4	-	6/16/32/32	0/3/3/3
2	ADP	D	601	3,4	-	2/16/32/32	0/3/3/3
5	MPD	A	607	-	-	0/5/5/5	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	4.55	1.47	1.39
2	F	601	ADP	C5-C4	4.52	1.47	1.39
2	G	601	ADP	C5-C4	4.46	1.47	1.39
2	E	601	ADP	C5-C4	4.42	1.47	1.39
2	A	601	ADP	C5-C4	4.32	1.46	1.39
2	D	601	ADP	C5-C4	4.29	1.46	1.39
2	C	601	ADP	C5-C4	4.20	1.46	1.39
2	C	601	ADP	PA-O3A	3.37	1.63	1.59
2	B	601	ADP	C8-N7	3.15	1.37	1.31
2	D	601	ADP	PA-O3A	3.07	1.62	1.59
2	D	601	ADP	C8-N7	2.95	1.37	1.31
2	A	601	ADP	PA-O3A	2.92	1.62	1.59
2	E	601	ADP	C5-C6	2.74	1.48	1.41
2	F	601	ADP	C8-N7	2.65	1.36	1.31
2	A	601	ADP	C8-N7	2.63	1.36	1.31
2	F	601	ADP	C5-C6	2.56	1.48	1.41
2	G	601	ADP	C8-N7	2.54	1.36	1.31
2	A	601	ADP	C5-C6	2.50	1.48	1.41
2	C	601	ADP	C8-N7	2.50	1.36	1.31
2	B	601	ADP	C5-C6	2.41	1.47	1.41
2	G	601	ADP	PA-O3A	2.40	1.62	1.59
2	G	601	ADP	C5-N7	-2.38	1.34	1.39
2	E	601	ADP	C8-N7	2.29	1.36	1.31
2	C	601	ADP	C5-C6	2.28	1.47	1.41
2	G	601	ADP	C5-C6	2.27	1.47	1.41
2	C	601	ADP	C5-N7	-2.25	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	ADP	C5-N7	-2.23	1.35	1.39
2	D	601	ADP	C4-N9	-2.22	1.33	1.37
2	D	601	ADP	C5-C6	2.21	1.47	1.41
2	F	601	ADP	C5-N7	-2.16	1.35	1.39
2	B	601	ADP	C5-N7	-2.13	1.35	1.39
2	E	601	ADP	C5-N7	-2.11	1.35	1.39
2	G	601	ADP	C4-N9	-2.07	1.33	1.37
2	A	601	ADP	C5-N7	-2.06	1.35	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	ADP	C5-C4-N3	-5.90	118.60	126.72
2	C	601	ADP	C5-C4-N3	-5.69	118.88	126.72
2	F	601	ADP	C5-C4-N3	-5.55	119.07	126.72
2	B	601	ADP	C5-C4-N3	-5.53	119.10	126.72
2	E	601	ADP	C5-C4-N3	-5.39	119.29	126.72
2	D	601	ADP	C5-C4-N3	-5.29	119.43	126.72
2	A	601	ADP	C5-C4-N3	-5.23	119.51	126.72
2	D	601	ADP	O4'-C1'-N9	4.82	117.34	108.09
2	G	601	ADP	N3-C4-N9	4.74	135.23	127.17
2	E	601	ADP	N3-C4-N9	4.63	135.04	127.17
2	C	601	ADP	N3-C4-N9	4.59	134.98	127.17
2	F	601	ADP	N3-C4-N9	4.56	134.93	127.17
2	A	601	ADP	N3-C4-N9	4.47	134.77	127.17
2	C	601	ADP	O4'-C1'-N9	4.14	116.05	108.09
2	G	601	ADP	O4'-C1'-N9	4.04	115.86	108.09
2	B	601	ADP	N3-C4-N9	4.00	133.97	127.17
2	E	601	ADP	C4-N9-C8	3.83	109.76	105.74
2	A	601	ADP	C4-N9-C8	3.81	109.74	105.74
2	D	601	ADP	N3-C4-N9	3.81	133.65	127.17
2	A	601	ADP	N3-C2-N1	-3.78	122.85	128.58
2	F	601	ADP	C2-N3-C4	3.72	120.92	111.83
2	E	601	ADP	N3-C2-N1	-3.70	122.98	128.58
2	E	601	ADP	C2-N3-C4	3.68	120.82	111.83
2	C	601	ADP	C2-N3-C4	3.67	120.79	111.83
2	A	601	ADP	C2-N3-C4	3.64	120.72	111.83
2	F	601	ADP	N3-C2-N1	-3.60	123.13	128.58
2	D	601	ADP	C2-N3-C4	3.54	120.49	111.83
2	B	601	ADP	O4'-C1'-N9	3.51	114.82	108.09
2	C	601	ADP	N3-C2-N1	-3.48	123.31	128.58
2	D	601	ADP	N3-C2-N1	-3.46	123.34	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C4-C5-N7	-3.46	106.62	110.58
2	E	601	ADP	C4-C5-N7	-3.45	106.64	110.58
2	B	601	ADP	C2-N3-C4	3.44	120.24	111.83
2	D	601	ADP	C4-C5-N7	-3.38	106.72	110.58
2	F	601	ADP	C4-N9-C8	3.33	109.24	105.74
2	F	601	ADP	C4-C5-N7	-3.29	106.82	110.58
2	G	601	ADP	C4-C5-N7	-3.26	106.85	110.58
2	G	601	ADP	C2-N3-C4	3.26	119.79	111.83
2	C	601	ADP	C4-C5-N7	-3.18	106.94	110.58
2	A	601	ADP	C4-C5-N7	-3.17	106.96	110.58
2	C	601	ADP	C4-N9-C8	3.16	109.06	105.74
2	B	601	ADP	N3-C2-N1	-3.12	123.86	128.58
2	A	601	ADP	O4'-C1'-N9	3.08	114.00	108.09
2	E	601	ADP	O4'-C1'-N9	3.07	113.98	108.09
2	G	601	ADP	C4-N9-C8	3.06	108.95	105.74
2	E	601	ADP	C5-N7-C8	2.98	108.13	103.45
2	E	601	ADP	N9-C8-N7	-2.92	109.80	113.94
2	G	601	ADP	N6-C6-N1	2.83	124.69	118.38
2	A	601	ADP	N9-C8-N7	-2.82	109.93	113.94
2	D	601	ADP	C4-N9-C8	2.74	108.61	105.74
2	F	601	ADP	C5-N7-C8	2.73	107.74	103.45
2	A	601	ADP	C5-N7-C8	2.67	107.64	103.45
2	G	601	ADP	N3-C2-N1	-2.66	124.55	128.58
2	B	601	ADP	C4-N9-C8	2.64	108.51	105.74
2	F	601	ADP	N9-C8-N7	-2.64	110.20	113.94
2	C	601	ADP	C5-N7-C8	2.56	107.48	103.45
2	B	601	ADP	C5-N7-C8	2.55	107.45	103.45
2	D	601	ADP	N9-C8-N7	-2.52	110.37	113.94
2	C	601	ADP	N9-C8-N7	-2.51	110.37	113.94
2	D	601	ADP	C5-N7-C8	2.50	107.37	103.45
2	G	601	ADP	C5-N7-C8	2.49	107.36	103.45
2	B	601	ADP	N9-C8-N7	-2.43	110.48	113.94
2	G	601	ADP	N9-C8-N7	-2.32	110.65	113.94
2	D	601	ADP	C4-N9-C1'	-2.29	121.27	126.63
2	E	601	ADP	C6-C5-N7	2.24	136.40	132.09
2	C	601	ADP	O2A-PA-O1A	2.18	122.59	112.44
2	A	601	ADP	O2A-PA-O1A	2.15	122.47	112.44
2	G	601	ADP	C5-C6-N6	-2.15	117.96	123.29
2	F	601	ADP	C6-C5-N7	2.13	136.20	132.09
2	D	601	ADP	O2A-PA-O1A	2.09	122.15	112.44
2	A	601	ADP	C6-C5-N7	2.07	136.07	132.09
2	E	601	ADP	C2-N1-C6	2.06	122.12	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	ADP	O2A-PA-O1A	2.06	122.03	112.44
2	D	601	ADP	C6-C5-N7	2.04	136.03	132.09
2	C	601	ADP	N6-C6-N1	2.04	122.92	118.38
2	A	601	ADP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O3A
2	E	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	C5'-O5'-PA-O1A
2	E	601	ADP	C5'-O5'-PA-O2A
2	E	601	ADP	C5'-O5'-PA-O3A
2	F	601	ADP	PA-O3A-PB-O2B
2	F	601	ADP	C5'-O5'-PA-O3A
5	A	605	MPD	C2-C3-C4-C5
5	A	606	MPD	C2-C3-C4-C5
5	B	604	MPD	C2-C3-C4-C5
5	B	605	MPD	C2-C3-C4-O4
5	C	604	MPD	C2-C3-C4-C5
5	D	604	MPD	C2-C3-C4-C5
2	F	601	ADP	C3'-C4'-C5'-O5'
2	E	601	ADP	C3'-C4'-C5'-O5'
2	F	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	PA-O3A-PB-O1B
2	A	601	ADP	PB-O3A-PA-O1A
2	E	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O2A
5	B	605	MPD	O2-C2-C3-C4
5	B	606	MPD	O2-C2-C3-C4
5	B	607	MPD	O2-C2-C3-C4
5	D	605	MPD	O2-C2-C3-C4
5	A	608	MPD	C2-C3-C4-O4
5	E	604	MPD	C2-C3-C4-O4
5	A	608	MPD	C1-C2-C3-C4
5	A	608	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	B	608	MPD	C1-C2-C3-C4
5	D	606	MPD	C1-C2-C3-C4
5	D	606	MPD	CM-C2-C3-C4
2	B	601	ADP	C3'-C4'-C5'-O5'
2	F	601	ADP	C5'-O5'-PA-O1A
5	A	608	MPD	C2-C3-C4-C5
5	B	605	MPD	C2-C3-C4-C5
2	D	601	ADP	PB-O3A-PA-O1A
2	G	601	ADP	PB-O3A-PA-O1A
2	G	601	ADP	PB-O3A-PA-O2A
2	G	601	ADP	PA-O3A-PB-O1B
2	B	601	ADP	PA-O3A-PB-O3B
2	F	601	ADP	PA-O3A-PB-O3B
5	A	609	MPD	O2-C2-C3-C4
5	B	608	MPD	O2-C2-C3-C4
5	F	604	MPD	O2-C2-C3-C4
5	G	604	MPD	O2-C2-C3-C4
5	A	605	MPD	C2-C3-C4-O4
5	A	609	MPD	C2-C3-C4-O4
5	B	607	MPD	C2-C3-C4-O4
5	B	608	MPD	C2-C3-C4-O4
5	C	604	MPD	C2-C3-C4-O4
5	D	604	MPD	C2-C3-C4-O4
5	F	604	MPD	C2-C3-C4-O4
2	F	601	ADP	PA-O3A-PB-O1B
5	A	604	MPD	C1-C2-C3-C4
5	A	604	MPD	CM-C2-C3-C4
5	A	605	MPD	CM-C2-C3-C4
5	A	606	MPD	C1-C2-C3-C4
5	B	608	MPD	CM-C2-C3-C4

There are no ring outliers.

15 monomers are involved in 29 short contacts:

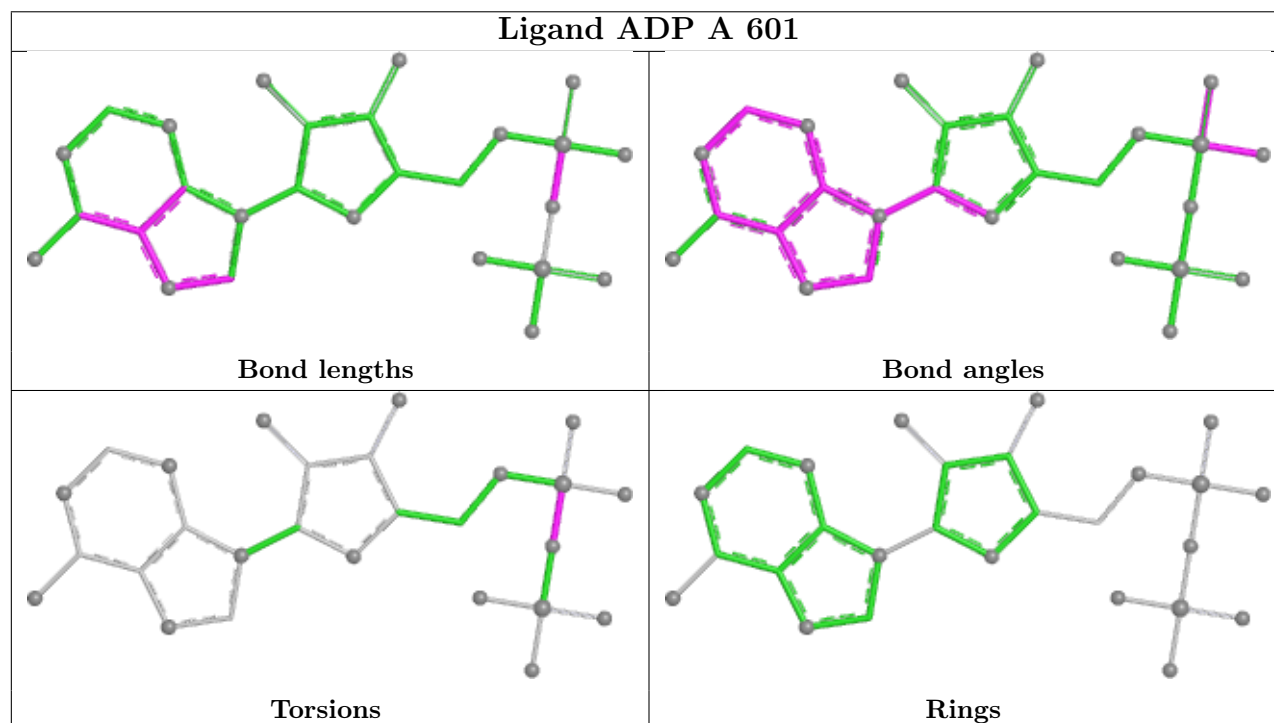
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	605	MPD	1	0
5	A	604	MPD	1	0
5	G	604	MPD	3	0
5	A	608	MPD	3	0
5	A	606	MPD	3	0
5	E	604	MPD	2	0
5	B	608	MPD	2	0

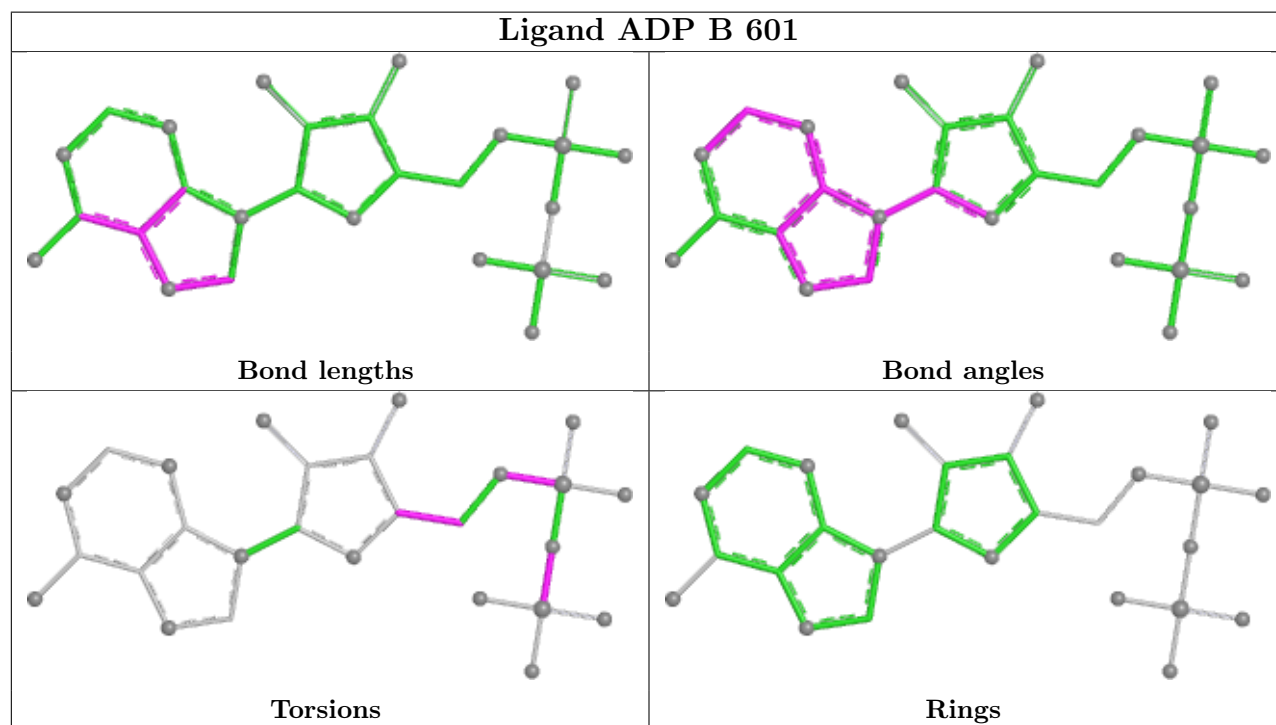
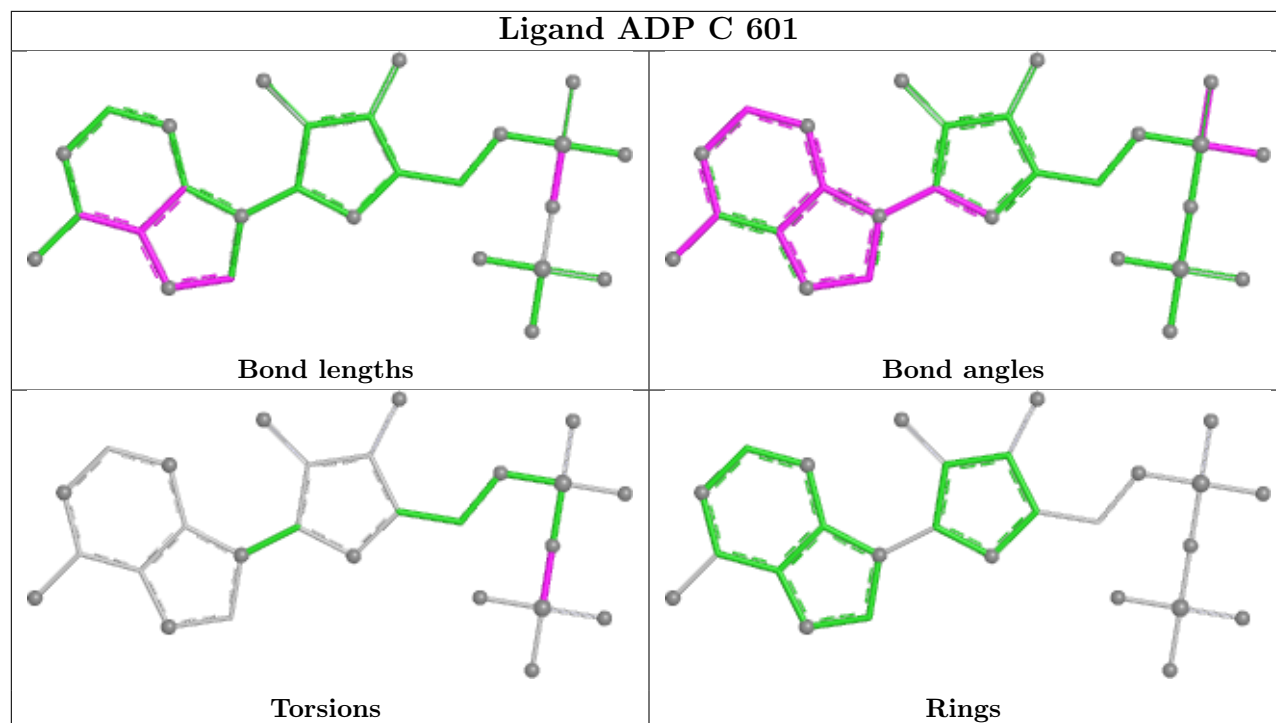
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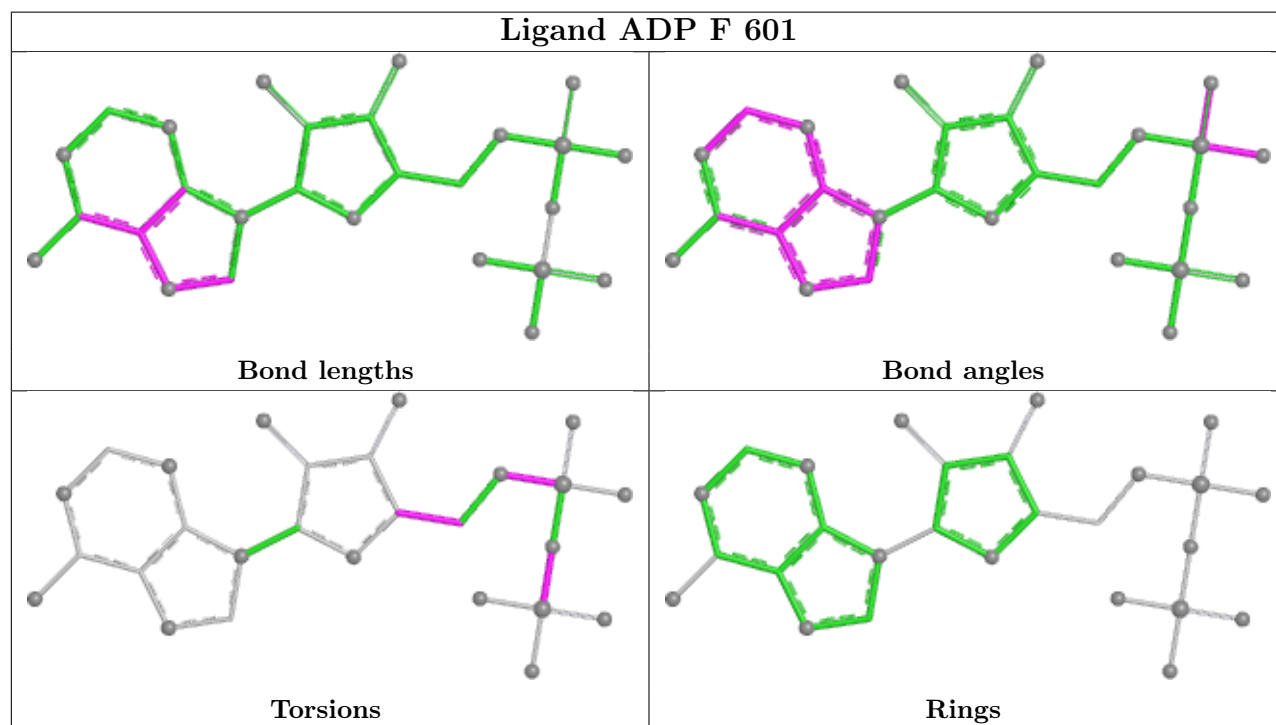
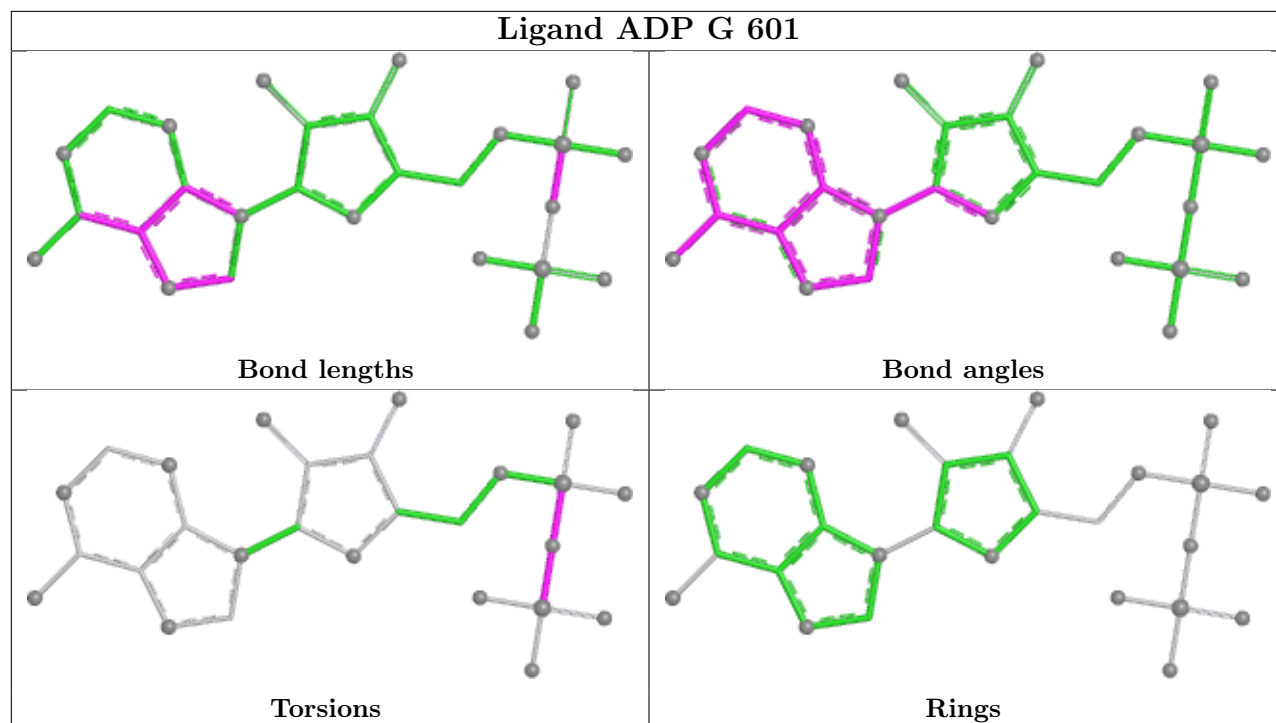
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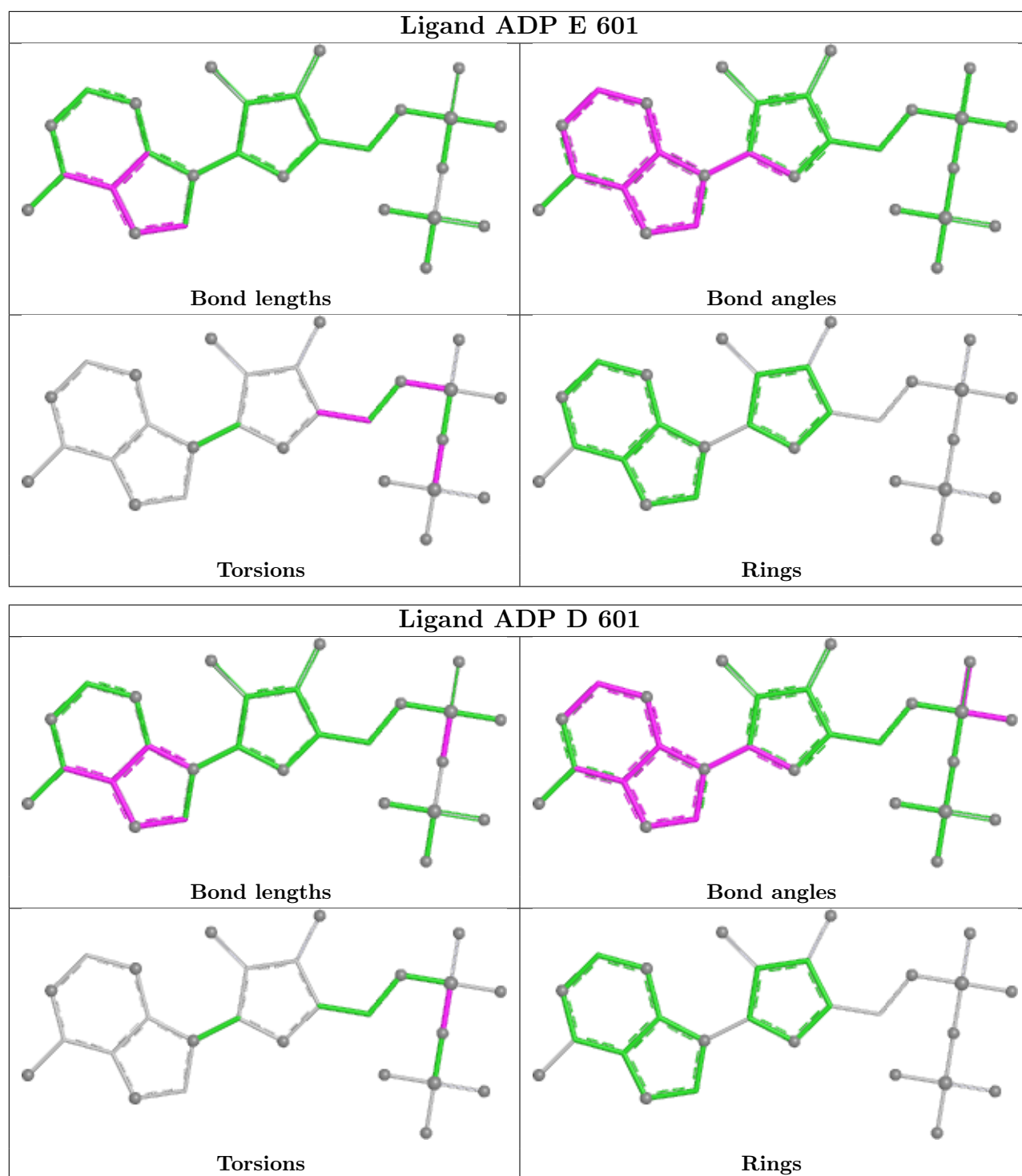
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	604	MPD	1	0
5	B	604	MPD	2	0
5	B	605	MPD	1	0
2	G	601	ADP	1	0
5	A	605	MPD	2	0
5	C	604	MPD	1	0
5	A	609	MPD	4	0
2	E	601	ADP	2	0

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.









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	524/548 (95%)	-0.32	2 (0%) 88 88	26, 69, 168, 196	1 (0%)
1	B	524/548 (95%)	-0.32	6 (1%) 78 76	24, 60, 160, 190	1 (0%)
1	C	524/548 (95%)	-0.15	6 (1%) 78 76	26, 68, 202, 243	3 (0%)
1	D	524/548 (95%)	-0.32	3 (0%) 85 85	29, 71, 155, 181	2 (0%)
1	E	524/548 (95%)	-0.28	4 (0%) 82 81	31, 79, 141, 187	1 (0%)
1	F	524/548 (95%)	-0.19	2 (0%) 88 88	31, 74, 178, 223	4 (0%)
1	G	524/548 (95%)	-0.17	6 (1%) 78 76	25, 71, 211, 243	1 (0%)
All	All	3668/3836 (95%)	-0.25	29 (0%) 82 81	24, 72, 181, 243	13 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	271	VAL	4.2
1	G	251	ALA	3.1
1	B	233	MET	2.9
1	D	288	MET	2.8
1	C	249	ILE	2.7
1	C	250	ILE	2.7
1	G	379	ILE	2.6
1	B	254	VAL	2.6
1	E	85	ALA	2.6
1	G	270	ILE	2.5
1	F	233	MET	2.5
1	G	223	ALA	2.5
1	A	44	PHE	2.4
1	C	275	ALA	2.4
1	E	44	PHE	2.3
1	B	271	VAL	2.3
1	D	387	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	357	THR	2.2
1	E	270	ILE	2.2
1	F	347	ALA	2.2
1	B	44	PHE	2.2
1	G	280	GLY	2.2
1	C	281	PHE	2.2
1	A	271	VAL	2.1
1	D	154	SER	2.1
1	B	208	PRO	2.1
1	C	223	ALA	2.0
1	B	259	LEU	2.0
1	C	271	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.

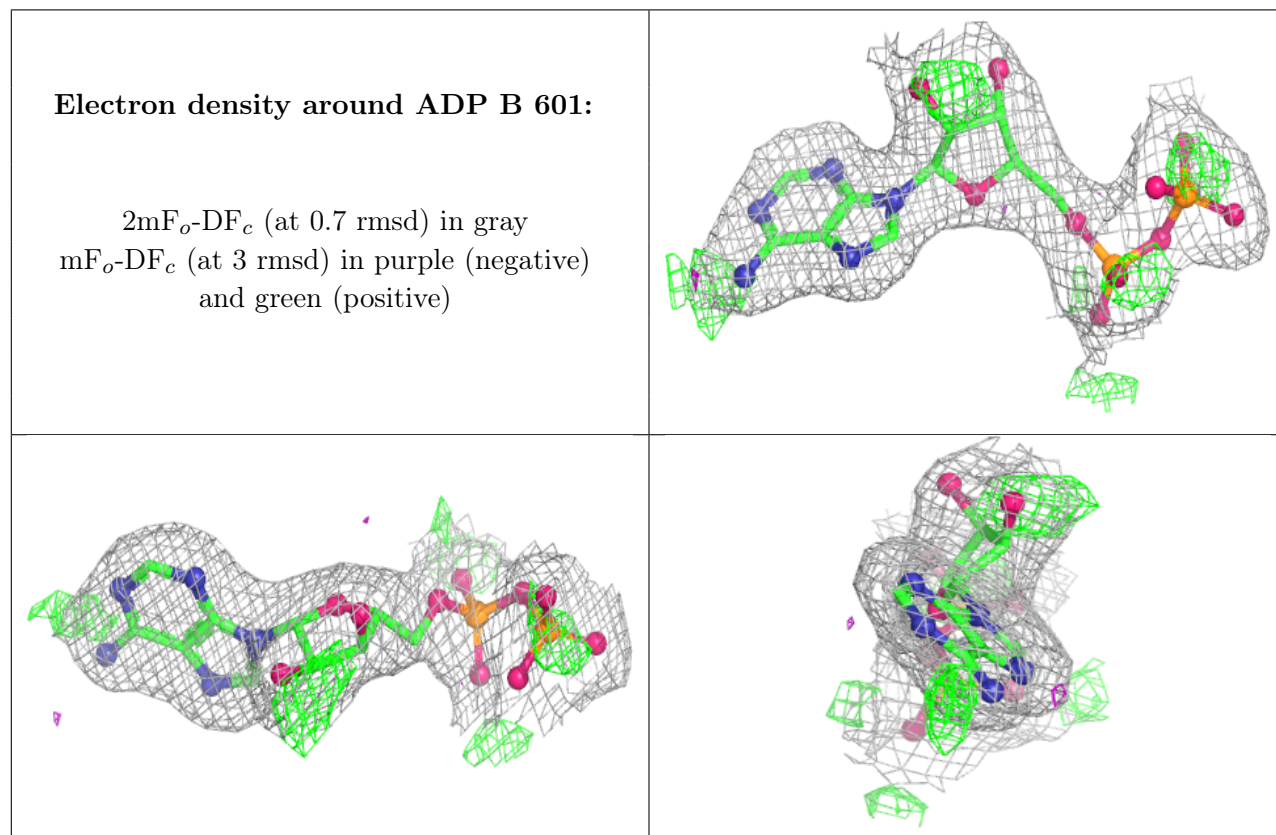
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	F	605	1/1	0.51	0.13	166,166,166,166	0
4	K	G	608	1/1	0.66	0.15	154,154,154,154	0
5	MPD	B	608	8/8	0.81	0.22	93,98,109,118	0
6	CA	B	609	1/1	0.81	0.12	141,141,141,141	0
5	MPD	A	607	8/8	0.82	0.22	83,95,97,104	0
5	MPD	A	604	8/8	0.83	0.20	106,109,115,123	0
6	CA	G	609	1/1	0.83	0.24	123,123,123,123	0
5	MPD	G	604	8/8	0.84	0.28	78,99,109,117	0
5	MPD	D	605	8/8	0.85	0.25	108,112,116,116	0
5	MPD	B	606	8/8	0.86	0.22	74,90,103,111	0
5	MPD	A	609	8/8	0.88	0.20	110,122,129,134	0

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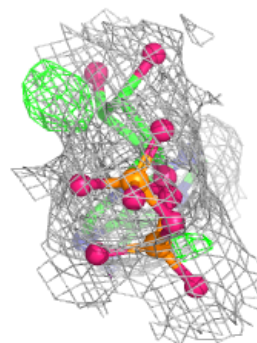
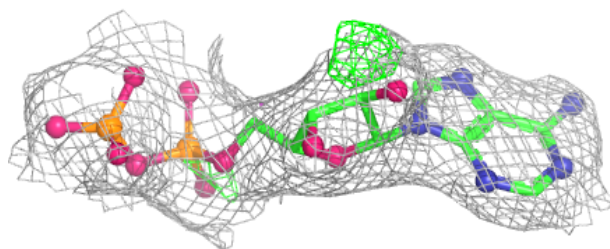
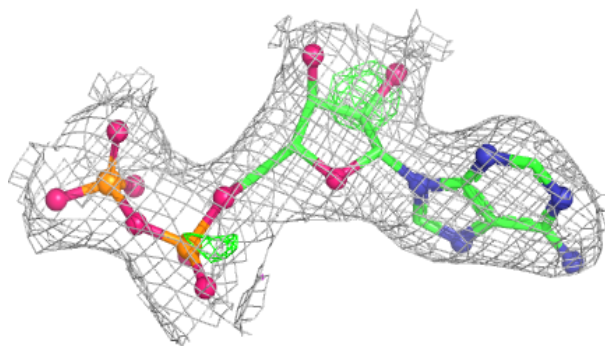
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	E	607	1/1	0.88	0.10	126,126,126,126	0
5	MPD	C	604	8/8	0.88	0.25	102,107,112,117	0
5	MPD	E	604	8/8	0.89	0.25	120,123,127,127	0
5	MPD	D	606	8/8	0.89	0.22	79,99,108,113	0
6	CA	F	606	1/1	0.89	0.14	110,110,110,110	0
5	MPD	G	605	8/8	0.89	0.29	114,117,141,153	0
5	MPD	B	604	8/8	0.90	0.20	52,80,90,92	0
5	MPD	F	604	8/8	0.90	0.22	119,124,125,130	0
6	CA	E	605	1/1	0.91	0.11	108,108,108,108	0
5	MPD	D	604	8/8	0.91	0.17	95,110,115,123	0
6	CA	A	610	1/1	0.91	0.13	129,129,129,129	0
5	MPD	B	607	8/8	0.91	0.21	92,108,124,126	0
5	MPD	B	605	8/8	0.92	0.23	89,107,112,123	0
5	MPD	A	608	8/8	0.92	0.26	103,110,120,123	0
6	CA	G	607	1/1	0.93	0.14	114,114,114,114	0
5	MPD	A	605	8/8	0.93	0.17	90,96,105,107	0
5	MPD	A	606	8/8	0.94	0.23	98,111,115,115	0
6	CA	D	607	1/1	0.95	0.11	118,118,118,118	0
4	K	E	603	1/1	0.95	0.09	89,89,89,89	0
6	CA	G	606	1/1	0.96	0.12	88,88,88,88	0
6	CA	A	611	1/1	0.96	0.27	107,107,107,107	0
6	CA	E	606	1/1	0.96	0.06	111,111,111,111	0
2	ADP	B	601	27/27	0.97	0.08	30,48,62,127	0
2	ADP	E	601	27/27	0.97	0.09	57,70,80,250	0
4	K	C	603	1/1	0.97	0.11	79,79,79,79	0
2	ADP	G	601	27/27	0.98	0.07	41,50,65,94	0
2	ADP	C	601	27/27	0.98	0.07	43,55,64,66	0
2	ADP	D	601	27/27	0.98	0.09	36,57,70,80	0
2	ADP	A	601	27/27	0.98	0.07	39,56,64,75	0
2	ADP	F	601	27/27	0.98	0.09	38,62,74,86	0
4	K	D	603	1/1	0.99	0.06	64,64,64,64	0
4	K	A	603	1/1	0.99	0.08	58,58,58,58	0
4	K	F	603	1/1	0.99	0.10	60,60,60,60	0
4	K	B	603	1/1	0.99	0.09	62,62,62,62	0
4	K	G	603	1/1	0.99	0.06	65,65,65,65	0
3	MG	B	602	1/1	0.99	0.06	29,29,29,29	0
3	MG	E	602	1/1	1.00	0.01	38,38,38,38	0
3	MG	F	602	1/1	1.00	0.02	28,28,28,28	0
3	MG	G	602	1/1	1.00	0.04	25,25,25,25	0
3	MG	A	602	1/1	1.00	0.06	33,33,33,33	0
3	MG	C	602	1/1	1.00	0.03	34,34,34,34	0
3	MG	D	602	1/1	1.00	0.05	30,30,30,30	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.

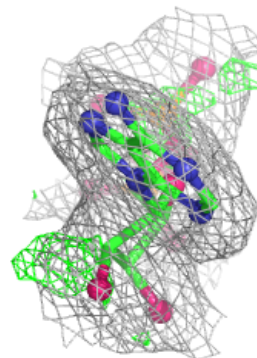
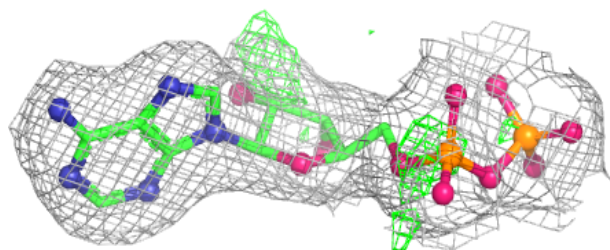
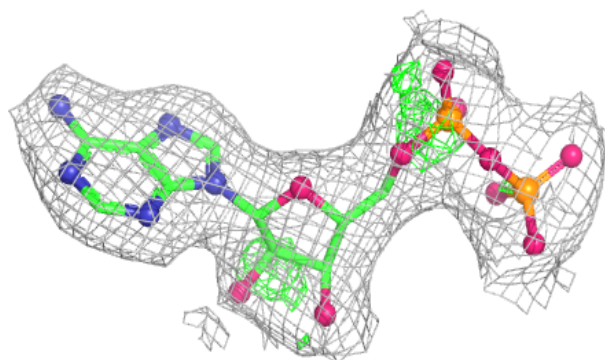


Electron density around ADP E 601:

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

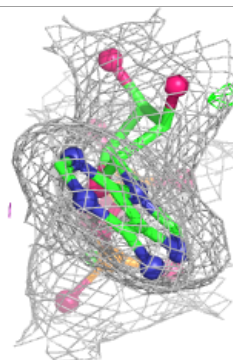
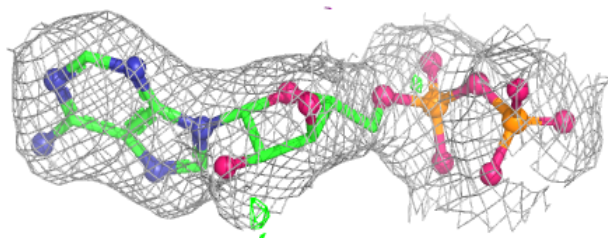
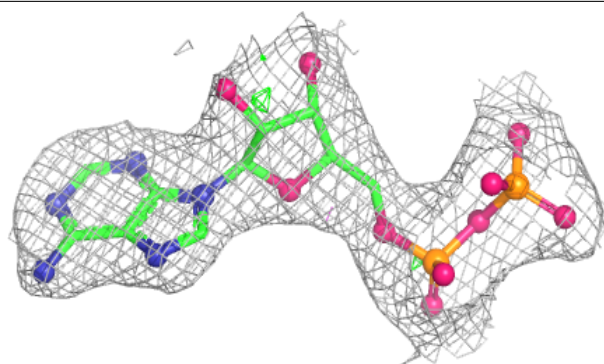
**Electron density around ADP G 601:**

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

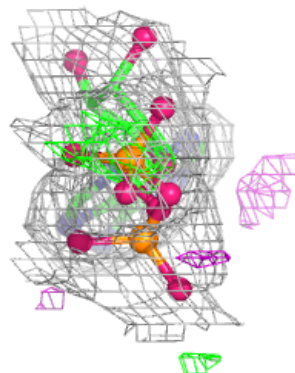
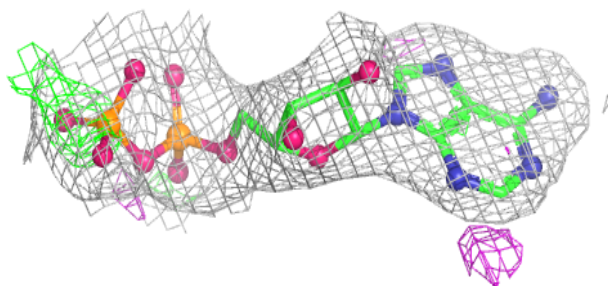
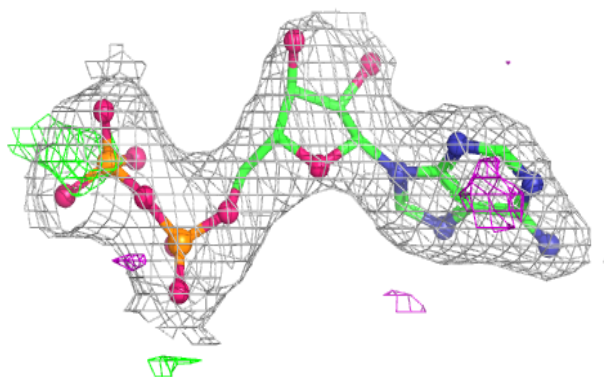


Electron density around ADP C 601:

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

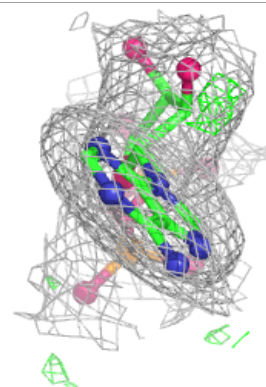
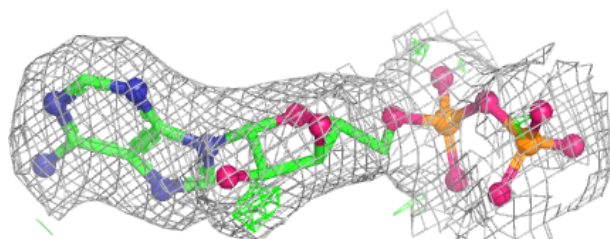
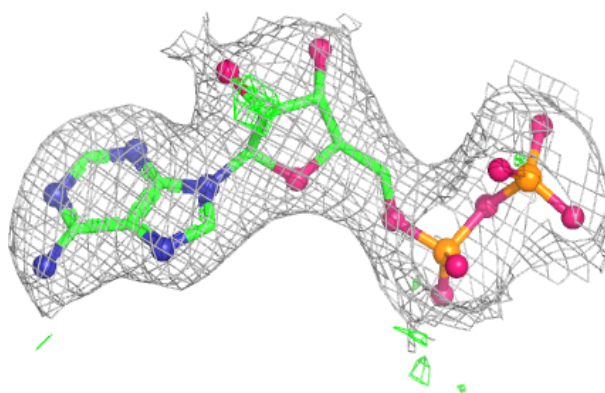
**Electron density around ADP D 601:**

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

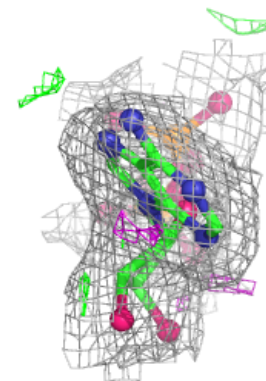
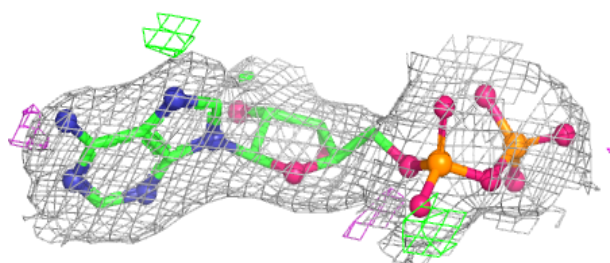
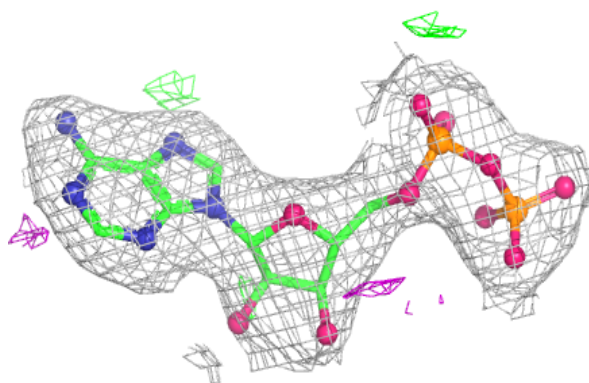


Electron density around ADP A 601:

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

**Electron density around ADP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.