



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 PM UTC

PDB ID : 2P1N / pdb_00002p1n
Title : Mechanism of Auxin Perception by the TIR1 Ubiquitin Ligase
Authors : Tan, X.; Calderon-Villalobos, L.I.A.; Sharon, M.; Robinson, C.V.; Estelle, M.;
Zheng, C.; Zheng, N.
Deposited on : 2007-03-06
Resolution : 2.50 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:

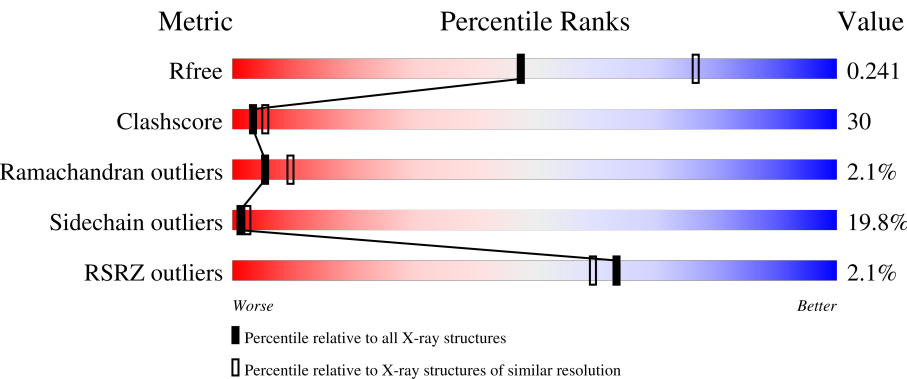
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	160	2% 30% 31% 17% • 21%
1	D	160	% 34% 26% 17% • 21%
2	B	594	2% 46% 35% 12% • •
2	E	594	2% 43% 36% 13% • •
3	C	13	15% 15% 31% 46% 8%

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Mol	Chain	Length	Quality of chain
3	F	13	46% 8% 38% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11872 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1009	638	165	201	5			
1	D	127	Total	C	N	O	S	0	0	0
			1023	649	167	202	5			

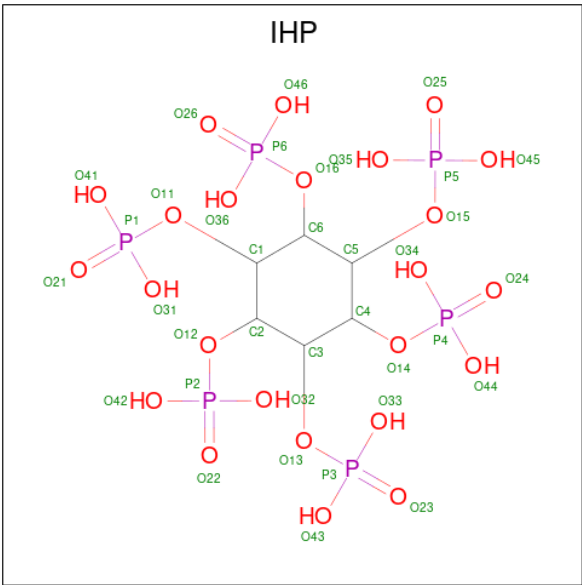
- Molecule 2 is a protein called TRANSPORT INHIBITOR RESPONSE 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	571	Total	C	N	O	S	0	0	0
			4495	2871	759	828	37			
2	E	571	Total	C	N	O	S	0	0	0
			4495	2871	759	828	37			

- Molecule 3 is a protein called Auxin-responsive protein IAA7.

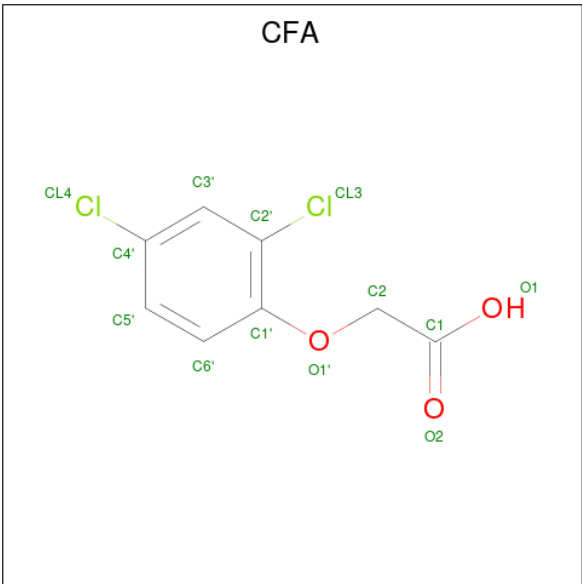
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			114	74	23	17			
3	F	13	Total	C	N	O	0	0	0
			114	74	23	17			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			36	6	24	6		
4	E	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 5 is (2,4-DICHLOROPHENOXY)ACETIC ACID (CCD ID: CFA) (formula: C₈H₆Cl₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	O	0	0
			13	8	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	Cl	O	0	0
			13	8	2	3		

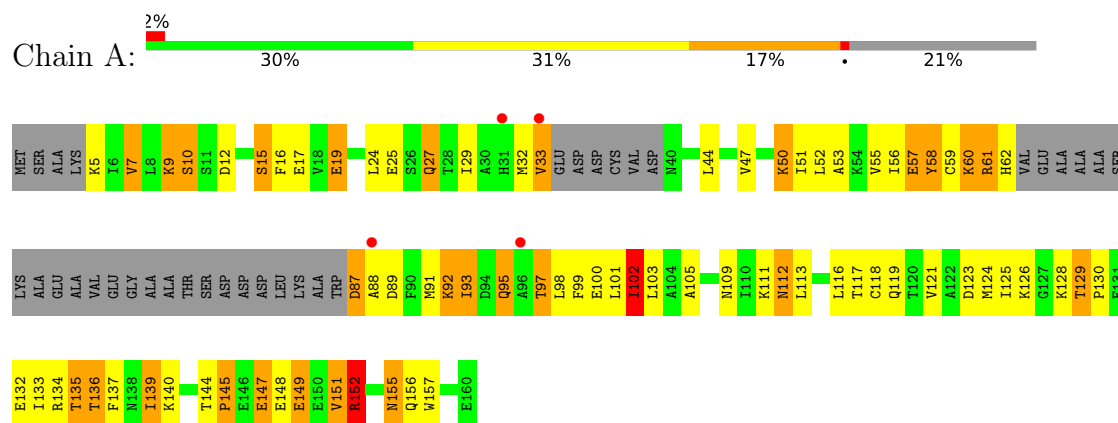
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	217	Total	O	0	0
			217	217		
6	C	6	Total	O	0	0
			6	6		
6	D	32	Total	O	0	0
			32	32		
6	E	240	Total	O	0	0
			240	240		
6	F	4	Total	O	0	0
			4	4		

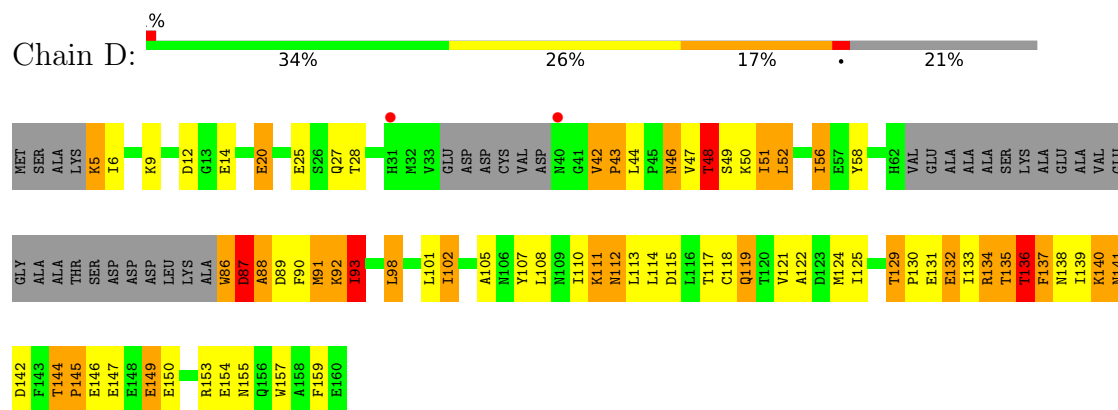
3 Residue-property plots

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

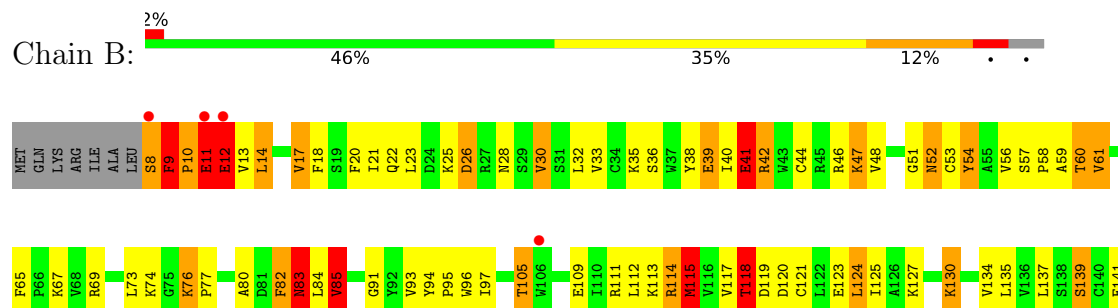
• Molecule 1: SKP1-like protein 1A

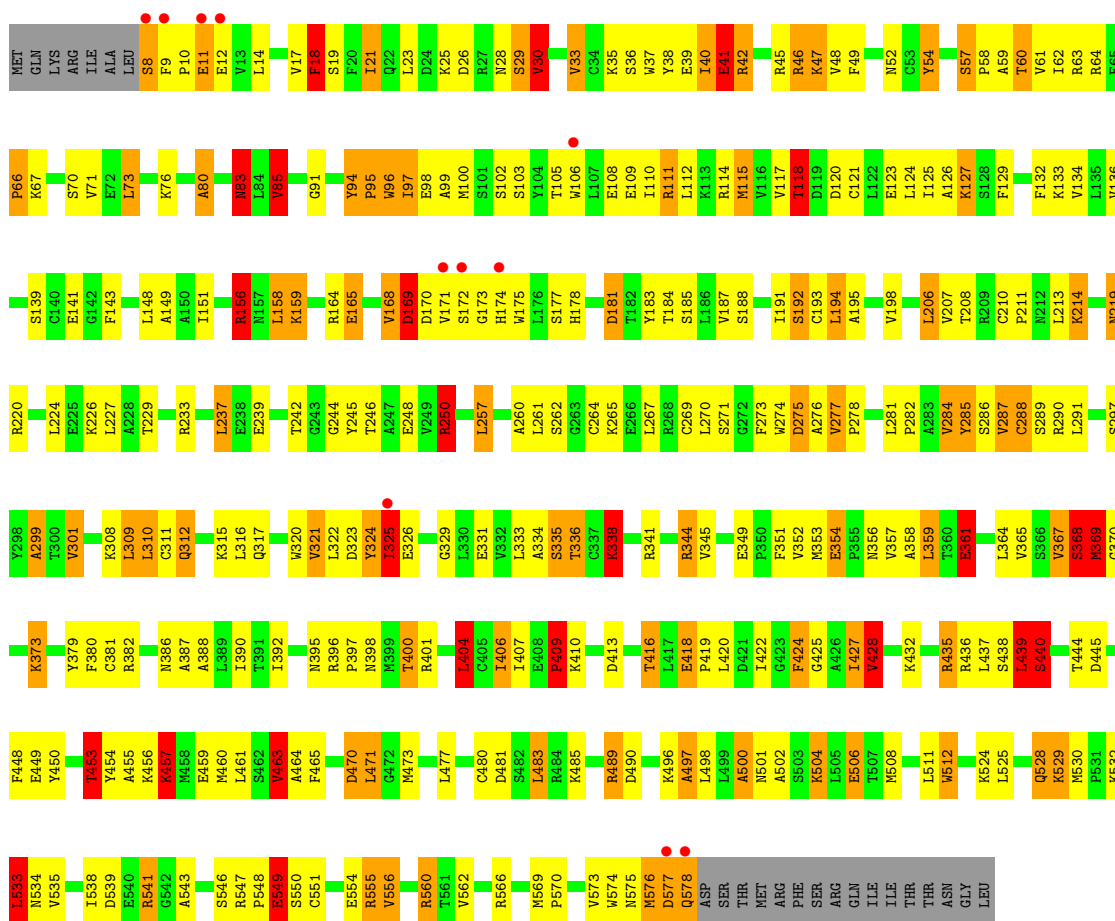


• Molecule 1: SKP1-like protein 1A

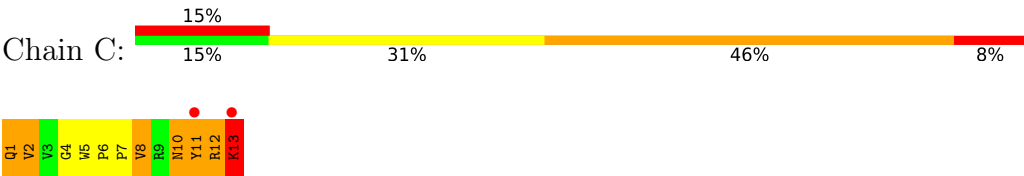


• Molecule 2: TRANSPORT INHIBITOR RESPONSE 1 protein

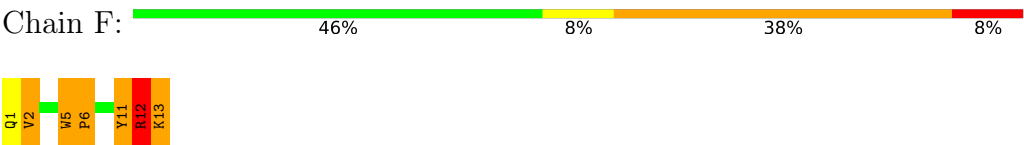




● Molecule 3: Auxin-responsive protein IAA7



● Molecule 3: Auxin-responsive protein IAA7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.67Å 82.75Å 125.79Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.50) 90.5 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.274 0.236 , 0.241	Depositor DCC
R_{free} test set	3305 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.177	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9529e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IHP, CFA

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	1.22	5/1022 (0.5%)	1.44	14/1377 (1.0%)
1	D	1.18	1/1038 (0.1%)	1.46	14/1400 (1.0%)
2	B	1.65	53/4593 (1.2%)	1.74	99/6226 (1.6%)
2	E	1.60	45/4593 (1.0%)	1.73	102/6226 (1.6%)
3	C	3.93	1/118 (0.8%)	1.30	0/159
3	F	1.23	1/118 (0.8%)	1.35	2/159 (1.3%)
All	All	1.59	106/11482 (0.9%)	1.68	231/15547 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	3
1	D	0	4
2	B	2	14
2	E	3	7
3	F	0	3
All	All	8	31

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	LYS	C-OXT	-39.90	0.43	1.23
2	B	56	VAL	CA-CB	9.98	1.66	1.55
2	B	85	VAL	CA-CB	8.58	1.62	1.53
2	E	461	LEU	CA-C	8.45	1.62	1.52
2	E	250	ARG	N-CA	8.44	1.55	1.45
2	B	550	SER	C-N	-8.27	1.22	1.33
2	B	85	VAL	CA-C	8.02	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	371	CYS	C-O	-8.01	1.15	1.24
2	B	270	LEU	CA-C	7.99	1.62	1.52
2	E	85	VAL	CA-CB	7.78	1.61	1.53
2	E	502	ALA	C-O	7.68	1.32	1.24
2	E	464	ALA	C-O	-7.62	1.15	1.23
2	B	191	ILE	CA-CB	7.52	1.64	1.54
2	B	54	TYR	N-CA	7.49	1.55	1.46
2	B	17	VAL	CA-C	7.42	1.61	1.52
2	E	85	VAL	CA-C	7.36	1.59	1.53
2	B	485	LYS	C-O	7.25	1.32	1.24
2	B	117	VAL	CA-CB	7.11	1.63	1.54
2	E	71	VAL	CA-CB	6.88	1.62	1.54
2	B	73	LEU	N-CA	6.83	1.54	1.46
2	B	513	MET	N-CA	6.81	1.54	1.46
2	E	480	CYS	CA-C	-6.80	1.45	1.53
2	B	463	VAL	CA-C	6.77	1.60	1.52
2	E	369	MET	C-O	-6.70	1.15	1.24
2	B	492	PRO	CA-CB	6.48	1.58	1.53
2	B	437	LEU	C-O	6.46	1.31	1.24
2	E	387	ALA	C-O	-6.43	1.16	1.24
2	B	347	PRO	CA-C	6.43	1.58	1.52
2	B	125	ILE	CA-CB	6.42	1.62	1.54
2	E	534	ASN	CA-C	6.41	1.61	1.52
2	B	277	VAL	CA-C	6.38	1.58	1.53
2	E	504	LYS	N-CA	6.33	1.54	1.46
2	E	427	ILE	N-CA	-6.19	1.39	1.46
2	B	51	GLY	C-O	-6.18	1.15	1.24
2	E	335	SER	N-CA	-6.18	1.38	1.46
2	E	316	LEU	C-O	-6.16	1.16	1.23
2	B	391	THR	CA-CB	6.16	1.63	1.53
2	E	66	PRO	N-CA	-6.10	1.39	1.47
2	B	488	ILE	CA-CB	-6.05	1.46	1.54
2	B	301	VAL	CA-C	6.05	1.59	1.53
2	E	562	VAL	CA-CB	6.04	1.62	1.54
2	B	383	GLN	N-CA	6.00	1.53	1.45
2	E	409	PRO	C-O	5.95	1.31	1.24
2	E	195	ALA	CA-CB	5.94	1.63	1.53
2	E	477	LEU	C-O	-5.94	1.17	1.24
2	E	535	VAL	CA-CB	-5.94	1.46	1.53
2	B	514	SER	CA-C	5.87	1.59	1.52
2	B	515	SER	CA-C	-5.86	1.45	1.53
2	B	313	CYS	N-CA	-5.83	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	457	LYS	CA-C	-5.79	1.45	1.52
1	A	156	GLN	C-O	-5.76	1.17	1.24
2	B	268	ARG	CA-C	5.75	1.59	1.52
2	E	284	VAL	CA-C	5.72	1.58	1.52
2	E	380	PHE	N-CA	5.71	1.53	1.46
2	E	437	LEU	CA-C	5.70	1.59	1.52
2	B	403	ARG	C-O	5.66	1.30	1.24
2	E	38	TYR	N-CA	-5.63	1.39	1.46
2	B	428	VAL	CA-C	5.58	1.60	1.52
2	E	54	TYR	C-O	5.57	1.31	1.24
2	E	480	CYS	N-CA	-5.57	1.39	1.46
2	B	331	GLU	N-CA	-5.56	1.39	1.46
2	B	458	MET	C-O	5.55	1.30	1.24
2	E	194	LEU	N-CA	-5.51	1.39	1.46
2	B	558	ILE	CA-CB	-5.49	1.47	1.54
2	E	453	THR	C-O	-5.49	1.16	1.24
2	B	390	ILE	C-O	-5.48	1.17	1.24
2	B	464	ALA	N-CA	5.47	1.52	1.46
2	B	232	GLN	CA-C	5.44	1.59	1.52
2	B	105	THR	CA-CB	5.42	1.62	1.53
2	B	44	CYS	CA-C	5.40	1.60	1.52
2	B	114	ARG	C-O	5.38	1.29	1.23
2	B	404	LEU	CG-CD1	-5.37	1.34	1.52
2	E	502	ALA	CA-C	5.36	1.59	1.52
2	B	135	LEU	N-CA	5.36	1.52	1.46
2	B	358	ALA	CA-C	5.34	1.59	1.53
3	F	5	TRP	CA-C	-5.33	1.46	1.52
2	E	381	CYS	CA-C	5.32	1.59	1.52
2	B	459	GLU	C-O	5.31	1.31	1.23
2	B	507	THR	CA-C	-5.31	1.45	1.52
2	E	379	TYR	CA-C	5.30	1.58	1.52
2	E	168	VAL	CA-CB	-5.29	1.48	1.54
2	E	438	SER	N-CA	5.29	1.52	1.46
2	E	440	SER	CB-OG	-5.23	1.31	1.42
1	A	151	VAL	CA-CB	5.21	1.61	1.54
1	A	55	VAL	CA-CB	5.21	1.60	1.54
2	B	382	ARG	CA-C	-5.21	1.45	1.52
2	B	182	THR	CA-CB	5.20	1.62	1.53
1	A	102	ILE	CA-CB	5.20	1.61	1.54
2	B	365	VAL	CA-CB	5.18	1.60	1.54
1	A	58	TYR	CA-C	-5.18	1.46	1.52
2	B	436	ARG	C-O	5.17	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	480	CYS	N-CA	-5.16	1.40	1.46
1	D	14	GLU	CA-C	-5.11	1.46	1.52
2	E	345	VAL	N-CA	5.11	1.52	1.46
2	E	512	TRP	N-CA	5.09	1.52	1.46
2	E	310	LEU	N-CA	-5.09	1.40	1.46
2	B	446	LYS	CA-C	5.08	1.59	1.52
2	E	344	ARG	C-O	5.08	1.29	1.24
2	B	491	CYS	CA-C	-5.07	1.47	1.52
2	E	336	THR	CB-CG2	5.07	1.69	1.52
2	B	493	PHE	N-CA	5.06	1.52	1.46
2	E	435	ARG	CA-C	5.06	1.58	1.52
2	E	470	ASP	CA-C	5.05	1.59	1.52
2	B	252	ASP	C-O	-5.03	1.18	1.24
2	E	193	CYS	C-O	-5.03	1.17	1.24
2	E	464	ALA	CA-CB	-5.01	1.45	1.53

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	220	ARG	N-CA-CB	-20.01	80.88	110.49
2	B	478	SER	N-CA-C	14.83	128.90	111.11
2	E	102	SER	N-CA-C	13.21	125.20	111.07
2	E	61	VAL	N-CA-C	-12.47	98.36	111.58
1	D	144	THR	C-N-CD	-11.70	77.03	125.00
2	E	126	ALA	N-CA-C	-11.69	98.62	111.36
2	E	424	PHE	N-CA-C	-11.46	97.89	112.90
2	E	261	LEU	N-CA-C	-10.47	99.03	112.23
2	B	125	ILE	N-CA-C	-10.47	100.15	110.72
2	B	409	PRO	CA-C-N	-10.21	103.83	123.13
2	B	409	PRO	C-N-CA	-10.21	103.83	123.13
2	E	94	TYR	CA-C-N	-9.96	108.33	119.28
2	E	94	TYR	C-N-CA	-9.96	108.33	119.28
2	B	427	ILE	N-CA-C	-9.81	100.81	110.72
2	B	543	ALA	CA-C-N	9.73	129.98	119.28
2	B	543	ALA	C-N-CA	9.73	129.98	119.28
2	B	477	LEU	N-CA-C	-9.60	100.68	111.82
2	E	257	LEU	N-CA-C	-9.01	101.54	111.36
2	E	277	VAL	N-CA-C	8.92	117.61	107.89
1	A	29	ILE	N-CA-C	8.84	118.90	110.42
2	E	528	GLN	N-CA-C	-8.78	100.25	112.45
2	B	222	VAL	CB-CA-C	-8.74	100.72	111.04
2	B	85	VAL	N-CA-C	8.63	116.83	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	425	GLY	N-CA-C	-8.62	102.21	112.64
2	E	473	MET	N-CA-C	-8.60	102.23	112.89
2	E	409	PRO	N-CA-C	8.49	129.96	112.47
1	D	93	ILE	N-CA-C	-8.43	96.18	108.23
1	D	42	VAL	CA-C-N	-8.39	111.52	120.66
1	D	42	VAL	C-N-CA	-8.39	111.52	120.66
2	E	260	ALA	N-CA-C	-8.30	102.03	112.90
1	D	129	THR	CA-C-N	8.28	130.19	119.84
1	D	129	THR	C-N-CA	8.28	130.19	119.84
2	E	321	VAL	CB-CA-C	-8.18	96.46	111.18
2	B	447	VAL	N-CA-CB	8.17	120.69	110.47
2	B	321	VAL	CB-CA-C	-8.16	95.80	110.48
1	A	118	CYS	N-CA-C	8.07	119.71	111.07
2	B	447	VAL	CB-CA-C	-8.01	101.55	112.04
2	E	33	VAL	N-CA-C	7.96	118.54	110.82
2	E	418	GLU	N-CA-C	7.93	121.63	110.20
2	E	168	VAL	N-CA-C	7.88	119.50	107.99
2	E	457	LYS	N-CA-C	-7.88	101.80	113.61
2	B	191	ILE	CA-CB-CG2	7.67	123.54	110.50
2	E	83	ASN	N-CA-C	7.65	121.71	111.30
2	B	277	VAL	N-CA-C	7.64	115.48	107.76
2	B	409	PRO	N-CA-C	7.59	128.11	112.47
2	E	334	ALA	N-CA-C	-7.56	103.05	111.82
2	B	550	SER	CB-CA-C	-7.53	95.43	110.42
1	A	155	ASN	N-CA-C	-7.53	103.01	111.14
2	E	501	ASN	N-CA-C	-7.51	101.23	110.61
2	B	191	ILE	CB-CG1-CD1	-7.48	98.08	113.80
2	B	451	ILE	N-CA-C	-7.48	103.16	110.72
2	E	338	LYS	N-CA-C	-7.38	104.28	113.28
2	B	146	ASP	N-CA-C	-7.37	102.62	111.69
2	E	309	LEU	N-CA-C	-7.33	102.45	111.40
2	B	191	ILE	CB-CA-C	7.32	121.14	111.85
2	B	301	VAL	N-CA-C	7.31	118.02	110.05
2	E	132	PHE	N-CA-C	7.30	120.53	110.24
2	E	369	MET	N-CA-C	-7.25	104.58	113.50
2	B	61	VAL	N-CA-C	-7.20	103.15	111.00
2	E	448	PHE	N-CA-C	-7.18	102.86	111.69
2	E	244	GLY	N-CA-C	-7.17	102.89	112.14
2	E	556	VAL	CB-CA-C	-7.11	100.00	110.81
2	E	57	SER	CA-C-N	-7.11	111.46	119.28
2	E	57	SER	C-N-CA	-7.11	111.46	119.28
2	B	26	ASP	N-CA-C	-7.07	103.51	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	124	LEU	N-CA-C	-6.96	103.77	111.36
2	B	60	THR	N-CA-C	6.92	118.82	111.28
2	E	395	ASN	N-CA-C	6.90	119.65	111.71
2	B	39	GLU	N-CA-C	6.88	118.78	111.28
2	E	59	ALA	N-CA-C	-6.84	103.75	111.14
2	B	502	ALA	N-CA-C	-6.80	103.94	111.36
2	B	76	LYS	CA-C-N	6.80	127.20	119.92
2	B	76	LYS	C-N-CA	6.80	127.20	119.92
2	B	139	SER	CB-CA-C	-6.78	102.27	111.89
2	E	33	VAL	N-CA-CB	6.75	120.23	110.52
1	D	141	ASN	N-CA-C	6.73	119.11	108.67
1	A	112	ASN	N-CA-C	6.71	125.09	110.80
2	E	195	ALA	CA-C-N	-6.69	110.62	122.07
2	E	195	ALA	C-N-CA	-6.69	110.62	122.07
2	B	312	GLN	N-CA-C	6.66	121.26	111.87
2	E	534	ASN	N-CA-C	6.66	119.28	108.63
2	E	373	LYS	N-CA-C	6.63	121.44	112.88
2	B	41	GLU	N-CA-C	6.57	119.42	111.40
2	B	473	MET	N-CA-C	-6.56	104.21	111.36
2	B	20	PHE	N-CA-C	-6.52	104.96	113.17
2	E	576	MET	N-CA-C	6.52	124.68	110.80
2	E	285	TYR	N-CA-C	6.51	118.25	111.03
2	E	331	GLU	N-CA-C	-6.49	104.30	111.82
1	D	20	GLU	N-CA-C	6.47	120.03	111.75
3	F	6	PRO	CA-C-N	-6.46	111.77	119.84
3	F	6	PRO	C-N-CA	-6.46	111.77	119.84
1	D	46	ASN	N-CA-C	6.46	121.96	113.30
2	E	368	SER	CB-CA-C	-6.42	100.13	110.79
2	B	60	THR	CB-CA-C	6.41	121.43	110.79
2	E	549	GLU	N-CA-C	-6.36	104.07	112.34
2	E	480	CYS	N-CA-C	6.35	119.15	109.62
2	B	191	ILE	CA-CB-CG1	-6.32	99.66	110.40
2	B	96	TRP	N-CA-C	-6.29	103.72	111.40
1	A	12	ASP	N-CA-C	-6.27	105.67	113.38
2	E	397	PRO	N-CA-C	-6.27	106.51	114.35
2	B	311	CYS	CA-CB-SG	-6.25	100.03	114.40
2	B	446	LYS	N-CA-C	6.23	118.15	111.36
2	E	275	ASP	N-CA-C	-6.23	104.98	112.58
2	B	550	SER	N-CA-C	6.18	123.97	110.80
1	A	27	GLN	N-CA-C	-6.18	104.65	111.82
2	B	556	VAL	CB-CA-C	-6.18	101.42	110.81
2	E	19	SER	N-CA-C	6.16	120.35	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	178	HIS	N-CA-C	6.14	118.94	111.82
2	B	407	ILE	N-CA-CB	-6.11	101.42	110.58
2	B	257	LEU	N-CA-C	-6.09	103.96	111.33
2	E	169	ASP	CB-CA-C	6.06	119.88	110.67
2	E	498	LEU	N-CA-C	-6.05	104.02	111.40
2	B	462	SER	CA-C-N	-6.05	114.59	122.51
2	B	462	SER	C-N-CA	-6.05	114.59	122.51
2	E	345	VAL	N-CA-C	6.01	116.27	107.37
2	E	547	ARG	CA-C-N	6.00	125.91	119.85
2	E	547	ARG	C-N-CA	6.00	125.91	119.85
2	B	550	SER	O-C-N	-6.00	114.61	122.59
2	E	419	PRO	CB-CA-C	-5.96	103.14	110.95
2	B	512	TRP	N-CA-C	5.93	118.39	108.96
2	E	329	GLY	N-CA-C	-5.92	105.19	112.77
2	B	409	PRO	O-C-N	-5.91	114.66	122.64
2	E	435	ARG	NE-CZ-NH2	-5.90	113.89	119.20
2	B	463	VAL	N-CA-C	5.88	117.56	108.44
2	E	356	ASN	N-CA-C	-5.87	105.97	113.02
2	E	156	ARG	N-CA-C	5.86	119.53	112.38
2	E	463	VAL	N-CA-C	5.86	116.79	108.42
2	E	80	ALA	N-CA-C	-5.84	104.99	111.71
2	E	271	SER	CA-C-N	-5.83	116.90	121.86
2	E	271	SER	C-N-CA	-5.83	116.90	121.86
2	E	207	VAL	N-CA-C	-5.82	103.81	111.09
2	B	60	THR	N-CA-CB	5.81	118.66	110.12
2	B	544	PRO	N-CA-C	5.80	121.47	113.65
2	E	428	VAL	N-CA-C	-5.80	104.18	112.35
2	B	259	VAL	N-CA-C	-5.79	104.71	110.62
2	B	391	THR	N-CA-C	-5.76	105.35	112.90
2	B	21	ILE	CB-CA-C	-5.73	103.29	111.31
2	E	192	SER	N-CA-C	-5.72	106.28	113.20
2	B	57	SER	CA-C-N	-5.70	113.04	118.97
2	B	57	SER	C-N-CA	-5.70	113.04	118.97
1	D	132	GLU	N-CA-C	-5.69	104.69	111.69
2	B	401	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	109	ASN	CA-C-N	-5.66	115.18	123.10
1	A	109	ASN	C-N-CA	-5.66	115.18	123.10
2	E	299	ALA	CA-C-N	-5.63	113.65	122.49
2	E	299	ALA	C-N-CA	-5.63	113.65	122.49
2	B	115	MET	CG-SD-CE	5.61	113.25	100.90
1	D	118	CYS	N-CA-C	5.61	117.19	111.14
2	E	481	ASP	CA-C-N	-5.57	113.81	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	481	ASP	C-N-CA	-5.57	113.81	122.67
2	E	529	LYS	N-CA-CB	5.57	118.30	110.12
2	E	535	VAL	N-CA-CB	-5.57	104.92	111.60
1	A	58	TYR	CA-C-N	-5.56	111.70	120.60
1	A	58	TYR	C-N-CA	-5.56	111.70	120.60
2	E	497	ALA	N-CA-C	-5.56	105.37	111.82
2	B	193	CYS	N-CA-C	5.53	119.65	113.01
2	B	401	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	D	43	PRO	CA-C-N	-5.51	116.78	122.85
1	D	43	PRO	C-N-CA	-5.51	116.78	122.85
2	E	406	ILE	CB-CA-C	-5.49	104.32	110.96
2	E	73	LEU	N-CA-C	5.48	118.02	108.76
2	E	30	VAL	N-CA-C	5.46	116.10	110.36
2	B	382	ARG	N-CA-C	5.45	120.04	113.17
2	B	277	VAL	CA-C-O	5.45	122.36	119.15
2	E	248	GLU	N-CA-C	-5.43	102.58	110.24
2	E	46	ARG	N-CA-C	-5.43	106.79	113.41
1	A	44	LEU	CA-C-N	5.43	125.09	119.56
1	A	44	LEU	C-N-CA	5.43	125.09	119.56
2	B	253	VAL	CB-CA-C	-5.43	104.73	112.22
2	B	340	LEU	N-CA-C	5.41	118.41	110.30
2	E	97	ILE	CG1-CB-CG2	-5.41	94.48	110.70
2	B	85	VAL	CB-CA-C	5.39	117.37	111.18
1	D	42	VAL	N-CA-C	5.38	120.51	108.88
2	B	531	PRO	CA-C-N	-5.38	114.04	122.65
2	B	531	PRO	C-N-CA	-5.38	114.04	122.65
2	B	17	VAL	N-CA-C	5.37	115.51	110.30
2	E	301	VAL	N-CA-C	5.37	120.51	109.34
2	B	262	SER	N-CA-C	-5.33	106.62	113.23
2	E	118	THR	N-CA-CB	-5.33	102.65	110.85
2	E	511	LEU	N-CA-C	-5.32	99.74	108.41
2	B	153	ALA	N-CA-C	-5.30	105.55	112.23
2	B	321	VAL	CG1-CB-CG2	5.29	122.45	110.80
2	B	118	THR	N-CA-CB	-5.28	102.64	111.20
2	E	95	PRO	N-CA-C	-5.28	106.52	113.65
2	B	130	LYS	N-CA-C	-5.28	105.58	112.23
1	A	19	GLU	N-CA-C	5.26	117.48	110.53
2	B	354	GLU	CA-C-N	5.24	125.54	119.93
2	B	354	GLU	C-N-CA	5.24	125.54	119.93
2	B	276	ALA	CA-C-N	5.24	126.36	122.59
2	B	276	ALA	C-N-CA	5.24	126.36	122.59
2	B	481	ASP	CA-C-N	-5.24	114.27	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	481	ASP	C-N-CA	-5.24	114.27	122.65
2	B	400	THR	CB-CA-C	5.24	118.45	109.65
2	E	158	LEU	N-CA-C	5.23	117.62	110.24
2	E	369	MET	N-CA-CB	5.23	118.21	110.53
2	E	407	ILE	CB-CA-C	-5.23	104.06	112.16
2	E	506	GLU	N-CA-C	5.22	121.91	110.80
2	B	495	ASP	N-CA-C	-5.21	105.28	111.69
2	E	404	LEU	CA-C-N	-5.20	115.47	123.07
2	E	404	LEU	C-N-CA	-5.20	115.47	123.07
2	B	428	VAL	CB-CA-C	5.19	118.48	111.94
2	E	45	ARG	N-CA-C	5.18	117.86	110.24
2	E	450	TYR	N-CA-C	-5.17	105.56	111.14
2	E	547	ARG	N-CA-C	-5.15	101.17	109.82
2	E	560	ARG	N-CA-C	-5.15	103.24	110.50
2	B	381	CYS	CA-C-N	-5.15	114.05	122.54
2	B	381	CYS	C-N-CA	-5.15	114.05	122.54
2	E	533	LEU	N-CA-C	-5.14	101.33	109.76
2	E	96	TRP	N-CA-C	-5.13	105.60	111.14
2	E	361	GLU	N-CA-CB	5.13	119.16	110.49
2	B	65	PHE	CA-C-N	-5.12	114.70	120.89
2	B	65	PHE	C-N-CA	-5.12	114.70	120.89
2	B	551	CYS	N-CA-CB	5.10	119.26	110.23
2	E	459	GLU	N-CA-C	5.10	119.49	113.12
2	E	359	LEU	CB-CG-CD2	5.09	125.97	110.70
2	E	500	ALA	N-CA-C	-5.08	107.03	113.18
2	E	151	ILE	N-CA-C	5.08	115.69	110.36
2	B	111	ARG	CG-CD-NE	-5.07	100.84	112.00
2	B	182	THR	N-CA-C	-5.07	107.10	113.28
2	B	473	MET	CA-CB-CG	-5.06	103.99	114.10
2	E	49	PHE	CA-C-N	-5.06	116.81	122.93
2	E	49	PHE	C-N-CA	-5.06	116.81	122.93
2	B	33	VAL	N-CA-C	5.05	115.48	110.23
2	B	307	VAL	N-CA-C	-5.04	105.58	110.42
2	B	556	VAL	CA-CB-CG1	5.04	118.97	110.40
2	E	481	ASP	O-C-N	-5.03	115.90	122.59
2	B	281	LEU	CA-C-N	-5.02	114.49	119.56
2	B	281	LEU	C-N-CA	-5.02	114.49	119.56
2	B	73	LEU	N-CA-C	5.01	117.61	109.24
2	E	535	VAL	CB-CA-C	-5.01	104.94	111.81
1	A	148	GLU	N-CA-C	-5.00	106.02	111.82

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	PHE	CA
1	A	112	ASN	CA
1	A	153	ARG	CA
2	B	60	THR	CA
2	B	478	SER	CA
2	E	41	GLU	CA
2	E	60	THR	CA
2	E	390	ILE	CB

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide
1	A	87	ASP	Peptide
1	A	97	THR	Peptide
2	B	10	PRO	Peptide
2	B	11	GLU	Peptide
2	B	170	ASP	Peptide
2	B	171	VAL	Peptide
2	B	191	ILE	Peptide
2	B	218	LEU	Peptide
2	B	262	SER	Peptide
2	B	287	VAL	Peptide
2	B	41	GLU	Peptide
2	B	415	LEU	Peptide
2	B	549	GLU	Peptide
2	B	577	ASP	Peptide
2	B	82	PHE	Peptide
2	B	9	PHE	Peptide
1	D	136	THR	Peptide
1	D	86	TRP	Peptide
1	D	87	ASP	Peptide
1	D	88	ALA	Peptide
2	E	169	ASP	Peptide
2	E	17	VAL	Peptide
2	E	262	SER	Peptide
2	E	324	TYR	Peptide
2	E	40	ILE	Peptide
2	E	439	LEU	Peptide
2	E	533	LEU	Peptide
3	F	1	GLN	Peptide
3	F	11	TYR	Peptide
3	F	12	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1009	0	1003	75	3
1	D	1023	0	1013	116	0
2	B	4495	0	4529	237	0
2	E	4495	0	4529	239	0
3	C	114	0	118	24	3
3	F	114	0	118	17	0
4	B	36	0	6	1	0
4	E	36	0	6	2	0
5	B	13	0	5	1	0
5	E	13	0	5	0	0
6	A	25	0	0	3	0
6	B	217	0	0	22	0
6	C	6	0	0	1	0
6	D	32	0	0	6	0
6	E	240	0	0	22	0
6	F	4	0	0	1	0
All	All	11872	0	11332	685	3

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 30.

All (685) 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)
2:B:351:PHE:CD2	3:C:13:LYS:HD2	1.56	1.40
1:D:144:THR:CB	1:D:145:PRO:CD	2.02	1.32
1:A:129:THR:HG23	1:A:132:GLU:OE1	1.14	1.31
1:D:144:THR:CB	1:D:145:PRO:HD2	1.40	1.26
2:B:11:GLU:N	2:B:12:GLU:HG3	1.55	1.21
2:B:145:THR:OG1	2:B:171:VAL:O	1.59	1.20
1:D:93:ILE:HD11	1:D:98:LEU:HB2	1.23	1.20
2:B:453:THR:HG21	6:B:815:HOH:O	1.39	1.20
3:F:13:LYS:HB2	6:F:292:HOH:O	1.40	1.20
1:D:144:THR:HB	1:D:145:PRO:CD	1.63	1.19
2:B:373:LYS:HE3	6:B:810:HOH:O	1.44	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TRP:CZ2	6:D:189:HOH:O	1.98	1.13
1:A:62:HIS:HE1	1:A:87:ASP:OD1	1.32	1.12
1:A:62:HIS:CE1	1:A:87:ASP:OD1	2.02	1.12
1:D:86:TRP:CE2	6:D:189:HOH:O	1.99	1.11
1:D:91:MET:HA	1:D:91:MET:HE3	1.23	1.10
2:B:530:MET:HB3	2:B:533:LEU:HD22	1.34	1.07
2:E:569:MET:HE2	2:E:573:VAL:HG12	1.33	1.07
1:A:89:ASP:HA	1:A:92:LYS:CG	1.86	1.06
2:E:569:MET:CE	2:E:573:VAL:HG12	1.85	1.05
1:A:32:MET:O	1:A:33:VAL:HG23	1.58	1.04
2:E:352:VAL:O	2:E:382:ARG:NH2	1.90	1.04
2:B:400:THR:HG22	2:B:401:ARG:HE	1.19	1.03
2:B:11:GLU:C	2:B:12:GLU:CG	2.30	1.03
1:A:129:THR:CG2	1:A:132:GLU:OE1	2.06	1.03
2:B:156:ARG:HG2	2:B:156:ARG:HH11	1.24	1.01
2:E:156:ARG:HG2	2:E:156:ARG:HH11	0.88	1.01
2:E:549:GLU:HB3	6:E:838:HOH:O	1.58	1.01
2:B:11:GLU:H	2:B:12:GLU:HG3	1.06	1.00
1:D:140:LYS:HZ2	1:D:140:LYS:HB2	1.23	1.00
1:A:89:ASP:HA	1:A:92:LYS:HG2	1.41	1.00
1:D:48:THR:HG21	1:D:50:LYS:HB3	1.42	1.00
2:B:369:MET:HG2	2:B:395:ASN:ND2	1.75	1.00
2:B:400:THR:CG2	2:B:401:ARG:HE	1.74	0.99
2:B:11:GLU:C	2:B:12:GLU:HG2	1.85	0.98
2:B:13:VAL:O	2:B:17:VAL:HG23	1.64	0.98
3:F:12:ARG:O	3:F:12:ARG:HD3	1.61	0.98
2:E:156:ARG:HH11	2:E:156:ARG:CG	1.76	0.98
1:D:134:ARG:HD3	1:D:141:ASN:HB2	1.43	0.96
2:B:351:PHE:HD2	3:C:13:LYS:HD2	1.21	0.95
2:E:569:MET:HE1	2:E:575:ASN:N	1.81	0.95
1:D:91:MET:HE1	1:D:93:ILE:HD12	1.46	0.95
2:B:354:GLU:N	2:B:354:GLU:OE2	2.00	0.94
1:A:91:MET:HE1	1:A:117:THR:HG22	1.46	0.94
2:B:351:PHE:CD2	3:C:13:LYS:CD	2.50	0.94
1:D:144:THR:HB	1:D:145:PRO:HD3	1.45	0.94
2:E:354:GLU:CD	2:E:354:GLU:H	1.75	0.94
2:E:181:ASP:OD1	2:E:181:ASP:N	1.97	0.93
2:E:436:ARG:CD	2:E:460:MET:HE3	1.99	0.93
2:B:11:GLU:O	2:B:12:GLU:HG2	1.68	0.92
3:F:13:LYS:O	3:F:13:LYS:HD3	1.70	0.92
1:A:89:ASP:HB2	1:A:92:LYS:HG3	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:353:MET:HB3	2:E:354:GLU:OE2	1.69	0.92
1:A:128:LYS:NZ	1:A:136:THR:HG21	1.83	0.92
2:B:575:ASN:HD22	2:B:577:ASP:H	1.18	0.91
2:E:156:ARG:HG2	2:E:156:ARG:NH1	1.60	0.91
1:A:149:GLU:HB2	6:A:183:HOH:O	1.69	0.91
1:D:91:MET:HE3	1:D:91:MET:CA	2.01	0.91
1:D:140:LYS:HB2	1:D:140:LYS:NZ	1.86	0.90
1:D:58:TYR:OH	1:D:112:ASN:HB2	1.72	0.90
2:E:529:LYS:HG2	2:E:530:MET:CE	2.01	0.90
1:A:89:ASP:CB	1:A:92:LYS:HG3	2.01	0.89
1:A:89:ASP:CA	1:A:92:LYS:HG3	2.03	0.89
2:B:569:MET:HE1	2:B:575:ASN:HB2	1.52	0.89
1:D:48:THR:HG22	1:D:51:ILE:H	1.35	0.89
2:E:529:LYS:HG2	2:E:530:MET:HE2	1.52	0.89
2:E:326:GLU:HB3	2:E:358:ALA:O	1.71	0.89
1:D:144:THR:OG1	1:D:145:PRO:HD2	1.72	0.88
2:B:118:THR:HG22	2:B:121:CYS:H	1.39	0.88
1:A:129:THR:OG1	1:A:132:GLU:HG3	1.74	0.88
2:E:299:ALA:O	2:E:322:LEU:HD12	1.74	0.87
2:B:285:TYR:O	2:B:288:CYS:HB2	1.73	0.87
2:E:410:LYS:N	6:E:809:HOH:O	1.79	0.87
2:E:436:ARG:HD2	2:E:460:MET:HE3	1.53	0.87
2:B:11:GLU:H	2:B:12:GLU:CG	1.87	0.87
1:D:153:ARG:HD3	6:D:177:HOH:O	1.74	0.86
1:D:86:TRP:N	1:D:89:ASP:H	1.72	0.86
1:D:129:THR:N	1:D:132:GLU:OE2	2.06	0.86
1:A:91:MET:CE	1:A:117:THR:HG22	2.05	0.86
2:E:354:GLU:CD	2:E:354:GLU:N	2.30	0.86
1:D:91:MET:CE	1:D:93:ILE:HD12	2.05	0.86
1:D:91:MET:HA	1:D:91:MET:CE	2.05	0.85
2:E:436:ARG:NE	2:E:460:MET:HE3	1.92	0.85
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.57	0.84
2:B:530:MET:CB	2:B:533:LEU:HD22	2.08	0.84
1:D:140:LYS:NZ	1:D:140:LYS:CB	2.37	0.83
2:B:541:ARG:HD2	2:B:554:GLU:OE1	1.78	0.83
2:B:156:ARG:HH11	2:B:156:ARG:CG	1.92	0.82
6:B:818:HOH:O	3:C:2:VAL:HG11	1.80	0.82
2:B:156:ARG:HG2	2:B:156:ARG:NH1	1.87	0.81
2:E:83:ASN:HA	6:E:693:HOH:O	1.79	0.81
1:A:89:ASP:HA	1:A:92:LYS:HG3	1.59	0.81
1:D:48:THR:CG2	1:D:50:LYS:N	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:LYS:CG	2:B:530:MET:HE3	2.11	0.81
1:A:128:LYS:HZ3	1:A:136:THR:HG21	1.45	0.80
2:E:353:MET:CB	2:E:354:GLU:OE2	2.30	0.80
3:F:13:LYS:O	3:F:13:LYS:CG	2.30	0.80
2:B:529:LYS:HG2	2:B:530:MET:HE3	1.63	0.79
1:A:89:ASP:O	1:A:92:LYS:HB2	1.81	0.79
3:C:13:LYS:CG	3:C:13:LYS:O	2.30	0.79
3:F:13:LYS:O	3:F:13:LYS:CD	2.30	0.78
2:B:320:TRP:CE2	2:B:344:ARG:HD2	2.18	0.78
1:D:48:THR:HG22	1:D:50:LYS:N	1.99	0.78
2:B:569:MET:HE1	2:B:575:ASN:N	1.98	0.78
2:B:76:LYS:NZ	2:B:141:GLU:OE2	2.12	0.77
2:B:145:THR:HG1	2:B:171:VAL:C	1.86	0.77
2:E:325:ILE:CG2	2:E:325:ILE:O	2.31	0.77
2:E:416:THR:HG21	6:E:737:HOH:O	1.83	0.77
1:D:48:THR:HG21	1:D:50:LYS:CB	2.14	0.76
1:D:133:ILE:C	1:D:135:THR:H	1.93	0.76
3:F:12:ARG:O	3:F:12:ARG:CD	2.32	0.76
1:D:93:ILE:CD1	1:D:98:LEU:HB2	2.12	0.76
3:C:8:VAL:HG13	3:C:10:ASN:OD1	1.85	0.75
2:E:413:ASP:HB3	2:E:416:THR:HG22	1.66	0.75
3:F:11:TYR:O	3:F:12:ARG:HG3	1.86	0.75
1:A:103:LEU:HD21	2:B:9:PHE:CB	2.17	0.75
1:D:137:PHE:H	1:D:137:PHE:HD2	1.33	0.74
2:E:575:ASN:HD22	2:E:577:ASP:H	1.35	0.74
2:B:351:PHE:HD2	3:C:13:LYS:CD	1.94	0.74
2:B:575:ASN:ND2	2:B:577:ASP:H	1.85	0.74
3:C:12:ARG:O	3:C:13:LYS:HB3	1.84	0.74
2:E:432:LYS:HG2	6:E:842:HOH:O	1.88	0.74
2:E:118:THR:HG23	6:E:675:HOH:O	1.85	0.74
2:E:489:ARG:HD3	2:E:490:ASP:OD2	1.88	0.74
2:B:489:ARG:HD3	2:B:490:ASP:OD2	1.88	0.73
2:B:287:VAL:O	2:B:290:ARG:HG2	1.88	0.73
2:B:529:LYS:HG2	2:B:530:MET:CE	2.18	0.73
2:E:416:THR:CG2	2:E:418:GLU:H	2.01	0.73
2:B:529:LYS:CD	2:B:530:MET:HE3	2.19	0.72
2:E:118:THR:CG2	2:E:120:ASP:HB2	2.18	0.72
2:B:77:PRO:HG3	2:B:557:PHE:CZ	2.25	0.72
1:D:121:VAL:O	1:D:124:MET:HB2	1.89	0.72
1:D:91:MET:HE1	1:D:93:ILE:CD1	2.18	0.72
1:D:93:ILE:HD11	1:D:98:LEU:CB	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:CA	1:A:92:LYS:CG	2.60	0.72
2:B:41:GLU:OE1	6:B:733:HOH:O	2.08	0.72
2:B:578:GLN:HA	6:B:795:HOH:O	1.88	0.71
2:B:569:MET:HE1	2:B:575:ASN:CB	2.19	0.71
1:D:131:GLU:O	1:D:135:THR:HB	1.90	0.71
2:E:18:PHE:H	2:E:18:PHE:HD2	1.38	0.71
2:E:428:VAL:HG13	2:E:454:TYR:HB2	1.72	0.71
2:B:164:ARG:C	2:B:165:GLU:HG2	2.15	0.71
1:D:5:LYS:O	1:D:6:ILE:HD13	1.90	0.71
2:E:569:MET:HE3	2:E:573:VAL:HG12	1.70	0.71
2:B:11:GLU:N	2:B:12:GLU:CG	2.46	0.70
2:B:400:THR:CG2	2:B:401:ARG:NE	2.53	0.70
1:D:132:GLU:O	1:D:136:THR:OG1	2.08	0.70
3:C:13:LYS:CD	3:C:13:LYS:O	2.39	0.70
2:B:35:LYS:HE3	6:B:808:HOH:O	1.91	0.70
2:E:282:PRO:HA	2:E:285:TYR:CE1	2.26	0.69
2:B:404:LEU:HD23	2:B:424:PHE:HZ	1.57	0.69
1:D:144:THR:HB	1:D:145:PRO:HD2	1.35	0.69
2:E:416:THR:HG22	2:E:418:GLU:H	1.57	0.69
2:E:435:ARG:HD2	6:E:679:HOH:O	1.90	0.69
2:E:118:THR:HG22	2:E:121:CYS:H	1.58	0.69
1:A:105:ALA:HB2	1:A:113:LEU:CD2	2.21	0.69
3:C:5:TRP:CG	3:C:6:PRO:HA	2.27	0.69
2:E:524:LYS:HE2	2:E:549:GLU:OE1	1.93	0.69
2:E:233:ARG:HD3	6:E:714:HOH:O	1.92	0.68
1:A:103:LEU:HD21	2:B:9:PHE:HB3	1.74	0.68
1:D:155:ASN:HD22	2:E:28:ASN:HB3	1.58	0.68
2:B:9:PHE:HD1	2:B:9:PHE:O	1.75	0.68
2:B:9:PHE:CD1	2:B:9:PHE:N	2.52	0.68
2:E:325:ILE:O	2:E:325:ILE:HG22	1.92	0.68
3:C:13:LYS:O	3:C:13:LYS:HG2	1.91	0.68
1:A:155:ASN:HB3	2:B:28:ASN:ND2	2.08	0.67
2:E:210:CYS:HB3	6:E:661:HOH:O	1.93	0.67
3:F:13:LYS:O	3:F:13:LYS:HG2	1.93	0.67
2:B:11:GLU:CA	2:B:12:GLU:HG3	2.23	0.67
2:E:351:PHE:CD2	3:F:13:LYS:HD2	2.30	0.67
2:E:400:THR:HG22	2:E:401:ARG:HG3	1.75	0.67
2:E:164:ARG:C	2:E:165:GLU:HG2	2.17	0.67
2:B:25:LYS:HG2	6:B:647:HOH:O	1.94	0.67
2:E:171:VAL:O	2:E:172:SER:HB3	1.92	0.67
1:A:32:MET:O	1:A:33:VAL:CG2	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:320:TRP:CE2	2:E:344:ARG:HD2	2.30	0.67
1:D:129:THR:HB	1:D:130:PRO:HD2	1.77	0.67
2:B:369:MET:HB3	6:B:686:HOH:O	1.95	0.66
1:D:131:GLU:HG3	1:D:134:ARG:HH21	1.60	0.66
2:E:436:ARG:CZ	2:E:460:MET:HE3	2.25	0.66
3:C:13:LYS:O	3:C:13:LYS:HD3	1.95	0.66
2:E:422:ILE:O	6:E:717:HOH:O	2.13	0.66
2:E:91:GLY:O	2:E:115:MET:HE3	1.95	0.66
1:D:48:THR:CG2	1:D:50:LYS:HB3	2.20	0.66
2:B:529:LYS:O	2:B:530:MET:HE2	1.95	0.66
2:E:409:PRO:CA	6:E:809:HOH:O	2.44	0.66
1:A:105:ALA:CB	1:A:113:LEU:HD23	2.25	0.66
1:D:48:THR:CG2	1:D:50:LYS:CB	2.73	0.66
2:E:118:THR:HG21	2:E:120:ASP:HB2	1.77	0.65
2:E:245:TYR:HB3	2:E:276:ALA:HA	1.79	0.65
1:D:154:GLU:HG2	1:D:159:PHE:HE1	1.60	0.65
2:E:264:CYS:HB2	2:E:267:LEU:HD12	1.79	0.65
2:E:354:GLU:OE2	2:E:354:GLU:N	2.29	0.65
2:E:76:LYS:NZ	2:E:141:GLU:OE2	2.30	0.65
2:E:281:LEU:N	2:E:282:PRO:CD	2.59	0.65
2:E:575:ASN:ND2	2:E:577:ASP:H	1.93	0.65
2:B:160:GLU:HG2	2:B:188:SER:HB3	1.76	0.65
2:B:139:SER:HA	2:B:165:GLU:O	1.97	0.64
1:D:155:ASN:ND2	2:E:28:ASN:HB3	2.12	0.64
2:B:191:ILE:HD12	2:B:191:ILE:C	1.97	0.64
2:B:300:THR:HG22	2:B:324:TYR:CE1	2.32	0.64
2:B:529:LYS:HD3	2:B:530:MET:HE3	1.79	0.64
2:E:436:ARG:HD2	2:E:460:MET:CE	2.25	0.64
2:B:220:ARG:NH2	2:B:275:ASP:OD2	2.31	0.64
1:D:91:MET:CA	1:D:91:MET:CE	2.71	0.64
2:E:250:ARG:HG2	2:E:250:ARG:HH11	1.63	0.64
2:B:578:GLN:O	6:B:623:HOH:O	2.14	0.64
3:C:12:ARG:O	3:C:13:LYS:CB	2.45	0.64
1:D:119:GLN:HB3	6:D:170:HOH:O	1.97	0.64
2:B:52:ASN:HD22	2:B:52:ASN:C	2.06	0.64
2:B:109:GLU:HG2	2:B:134:VAL:HB	1.80	0.64
2:E:220:ARG:HH21	2:E:275:ASP:CG	2.05	0.64
2:E:288:CYS:O	2:E:312:GLN:O	2.16	0.64
2:B:344:ARG:HG2	2:B:378:LEU:HB3	1.80	0.64
2:B:489:ARG:NH1	2:B:490:ASP:OD2	2.25	0.63
2:B:83:ASN:HA	6:B:672:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:PHE:CE2	3:C:13:LYS:HD2	2.27	0.63
1:D:140:LYS:CB	1:D:140:LYS:HZ3	2.11	0.63
2:E:400:THR:HG22	2:E:401:ARG:HE	1.62	0.63
1:D:86:TRP:C	1:D:88:ALA:N	2.57	0.63
2:E:42:ARG:HB3	2:E:64:ARG:O	1.98	0.63
1:D:155:ASN:HB3	2:E:28:ASN:ND2	2.13	0.62
1:D:86:TRP:CG	1:D:87:ASP:H	2.17	0.62
2:E:428:VAL:HG22	2:E:455:ALA:HB2	1.80	0.62
3:C:1:GLN:HB3	3:C:13:LYS:HE2	1.81	0.62
1:A:125:ILE:O	1:A:128:LYS:HB2	2.00	0.62
2:B:369:MET:HE2	6:B:686:HOH:O	1.99	0.62
1:D:46:ASN:HB2	1:D:107:TYR:CE2	2.35	0.62
3:F:5:TRP:CG	3:F:6:PRO:HA	2.35	0.62
1:A:103:LEU:HD21	2:B:9:PHE:HB2	1.80	0.62
1:A:135:THR:O	1:A:137:PHE:N	2.33	0.62
2:B:282:PRO:HA	2:B:285:TYR:CE1	2.35	0.62
1:A:135:THR:C	1:A:137:PHE:H	2.07	0.61
2:B:209:ARG:HD3	6:B:804:HOH:O	1.98	0.61
1:D:130:PRO:O	1:D:134:ARG:HB2	2.00	0.61
1:D:142:ASP:OD1	1:D:142:ASP:N	2.27	0.61
1:D:135:THR:C	1:D:137:PHE:O	2.43	0.61
2:B:277:VAL:HG21	2:B:280:TYR:HD1	1.64	0.61
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.01	0.61
2:E:80:ALA:HA	2:E:85:VAL:HG13	1.80	0.61
2:E:439:LEU:HD12	2:E:439:LEU:H	1.65	0.61
2:E:529:LYS:HG2	2:E:530:MET:HE3	1.83	0.61
2:B:145:THR:CB	2:B:171:VAL:O	2.49	0.60
2:B:349:GLU:HG3	2:B:356:ASN:ND2	2.15	0.60
2:B:364:LEU:HD13	2:B:392:ILE:HD13	1.83	0.60
2:E:18:PHE:HD2	2:E:18:PHE:N	1.99	0.60
2:B:9:PHE:HD1	2:B:9:PHE:H	1.49	0.60
1:D:86:TRP:C	1:D:88:ALA:H	2.09	0.60
1:A:56:ILE:HG22	1:A:60:LYS:HE3	1.82	0.60
1:D:48:THR:HG22	1:D:51:ILE:N	2.12	0.60
2:E:416:THR:HG23	2:E:418:GLU:HB2	1.84	0.60
1:D:144:THR:CB	1:D:145:PRO:HD3	1.90	0.60
2:B:385:THR:HG21	2:B:415:LEU:HD12	1.82	0.60
2:E:21:ILE:O	2:E:21:ILE:HG22	2.00	0.60
1:D:42:VAL:O	1:D:42:VAL:HG12	2.02	0.60
2:E:281:LEU:N	2:E:282:PRO:HD3	2.17	0.60
2:E:129:PHE:HB3	6:E:701:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:GLU:O	2:B:453:THR:HG23	2.02	0.59
1:A:102:ILE:HD11	1:A:121:VAL:HG21	1.84	0.59
2:E:109:GLU:HG2	2:E:134:VAL:HB	1.84	0.59
1:D:133:ILE:O	1:D:135:THR:N	2.35	0.59
2:B:83:ASN:CA	6:B:672:HOH:O	2.50	0.59
2:E:577:ASP:O	2:E:578:GLN:OE1	2.20	0.59
2:B:118:THR:HG23	2:B:120:ASP:H	1.67	0.59
1:D:86:TRP:HB3	1:D:88:ALA:HB3	1.83	0.59
1:D:134:ARG:HD3	1:D:141:ASN:CB	2.25	0.59
2:E:569:MET:HE1	2:E:574:TRP:C	2.26	0.59
1:D:86:TRP:N	1:D:89:ASP:HB3	2.18	0.59
2:B:299:ALA:O	2:B:322:LEU:HD12	2.03	0.58
1:A:125:ILE:N	1:A:125:ILE:HD13	2.18	0.58
2:B:22:GLN:HE22	2:B:46:ARG:HD2	1.69	0.58
2:B:300:THR:HG22	2:B:324:TYR:HE1	1.66	0.58
2:E:436:ARG:CZ	2:E:460:MET:CE	2.81	0.58
2:B:361:GLU:N	2:B:361:GLU:OE2	2.35	0.58
2:E:127:LYS:CG	2:E:127:LYS:O	2.50	0.58
2:E:529:LYS:CD	2:E:530:MET:HE3	2.34	0.58
1:A:102:ILE:HG21	2:B:13:VAL:HG11	1.85	0.58
2:B:335:SER:HA	2:B:338:LYS:HZ1	1.69	0.58
2:B:529:LYS:C	2:B:530:MET:HE2	2.29	0.58
2:B:569:MET:CE	2:B:573:VAL:HG12	2.34	0.58
1:D:48:THR:HG23	1:D:50:LYS:H	1.69	0.58
2:B:14:LEU:HD12	2:B:40:ILE:HG13	1.86	0.58
2:B:428:VAL:HG13	2:B:454:TYR:HB2	1.86	0.57
2:B:464:ALA:HA	2:B:489:ARG:O	2.03	0.57
2:E:351:PHE:CD2	3:F:13:LYS:CD	2.87	0.57
2:E:156:ARG:CG	2:E:156:ARG:NH1	2.44	0.57
2:B:439:LEU:CD1	2:B:463:VAL:HG23	2.34	0.57
1:D:43:PRO:O	1:D:44:LEU:HD23	2.05	0.57
2:B:569:MET:HG2	2:B:573:VAL:CG1	2.33	0.57
2:E:96:TRP:O	2:E:100:MET:HG3	2.04	0.57
1:A:7:VAL:HG12	1:A:17:GLU:HG3	1.86	0.57
1:A:134:ARG:HB2	1:A:139:ILE:HB	1.86	0.57
1:A:144:THR:OG1	1:A:147:GLU:HG3	2.04	0.57
2:E:58:PRO:O	2:E:62:ILE:HD12	2.03	0.57
2:B:416:THR:O	2:B:417:LEU:HB2	2.05	0.57
1:A:91:MET:O	1:A:93:ILE:N	2.30	0.56
2:E:219:ASN:HD22	2:E:219:ASN:H	1.52	0.56
2:B:384:MET:HE3	2:B:404:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ALA:HB2	2:B:427:ILE:HD13	1.87	0.56
1:D:102:ILE:HG12	1:D:117:THR:HB	1.86	0.56
2:E:485:LYS:NZ	4:E:601:IHP:O36	2.38	0.56
2:B:533:LEU:N	2:B:533:LEU:HD13	2.21	0.56
2:E:239:GLU:HA	2:E:269:CYS:HB2	1.86	0.56
1:A:50:LYS:O	1:A:53:ALA:HB3	2.05	0.56
2:B:58:PRO:O	2:B:59:ALA:C	2.48	0.56
2:E:541:ARG:HD2	2:E:554:GLU:OE1	2.06	0.56
2:E:106:TRP:HB2	6:E:726:HOH:O	2.06	0.56
2:E:127:LYS:O	2:E:127:LYS:HG3	2.04	0.56
2:E:400:THR:CG2	2:E:401:ARG:HE	2.18	0.56
2:B:281:LEU:N	2:B:282:PRO:HD3	2.20	0.56
3:C:5:TRP:CD2	3:C:6:PRO:HA	2.41	0.56
1:D:134:ARG:CD	1:D:141:ASN:HB2	2.28	0.55
2:E:60:THR:HB	2:E:63:ARG:HH12	1.71	0.55
2:E:569:MET:HE1	2:E:575:ASN:H	1.66	0.55
2:E:483:LEU:HD13	2:E:508:MET:HE3	1.88	0.55
2:B:338:LYS:HE3	2:B:370:GLY:O	2.07	0.55
1:A:52:LEU:O	1:A:52:LEU:HD23	2.07	0.55
2:B:578:GLN:C	2:B:578:GLN:OE1	2.49	0.55
2:E:18:PHE:N	2:E:18:PHE:CD2	2.68	0.55
2:B:11:GLU:CA	2:B:12:GLU:CG	2.82	0.55
1:D:137:PHE:N	1:D:137:PHE:CD2	2.67	0.55
2:E:219:ASN:HD22	2:E:219:ASN:N	2.05	0.55
1:D:133:ILE:C	1:D:135:THR:N	2.58	0.54
2:B:416:THR:HG22	2:B:418:GLU:H	1.73	0.54
1:D:86:TRP:N	1:D:89:ASP:N	2.48	0.54
2:B:543:ALA:O	2:B:546:SER:HB2	2.06	0.54
1:D:135:THR:O	1:D:137:PHE:O	2.26	0.54
2:E:413:ASP:CG	2:E:416:THR:HB	2.32	0.54
1:A:151:VAL:HG12	2:B:32:LEU:HD21	1.88	0.54
1:D:91:MET:CE	1:D:93:ILE:CD1	2.81	0.54
1:D:48:THR:HG23	1:D:50:LYS:N	2.21	0.54
2:B:52:ASN:ND2	2:B:54:TYR:H	2.06	0.54
2:B:416:THR:HG23	2:B:418:GLU:HG3	1.90	0.54
1:D:86:TRP:N	1:D:89:ASP:CB	2.71	0.54
2:B:277:VAL:CG2	2:B:280:TYR:HD1	2.21	0.54
1:D:52:LEU:HD22	1:D:56:ILE:HD11	1.90	0.54
2:B:539:ASP:OD2	2:B:541:ARG:HD3	2.07	0.54
2:E:117:VAL:O	2:E:143:PHE:HB3	2.08	0.54
2:B:11:GLU:C	2:B:12:GLU:HG3	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ASP:O	2:B:30:VAL:HG13	2.08	0.53
2:B:52:ASN:C	2:B:52:ASN:ND2	2.66	0.53
2:B:118:THR:HG21	6:B:718:HOH:O	2.07	0.53
2:B:190:ASN:OD1	2:B:190:ASN:C	2.51	0.53
1:D:49:SER:O	1:D:50:LYS:C	2.51	0.53
2:E:365:VAL:O	2:E:368:SER:HB2	2.07	0.53
2:B:578:GLN:C	2:B:578:GLN:CD	2.76	0.53
2:E:63:ARG:NH2	6:E:667:HOH:O	2.33	0.53
2:E:158:LEU:C	2:E:159:LYS:HG2	2.31	0.53
2:E:8:SER:O	2:E:9:PHE:CD2	2.62	0.53
2:E:439:LEU:CD1	2:E:463:VAL:HG23	2.39	0.53
2:B:281:LEU:N	2:B:282:PRO:CD	2.72	0.53
2:B:569:MET:CE	2:B:575:ASN:HB2	2.33	0.53
2:E:80:ALA:CA	2:E:85:VAL:HG13	2.39	0.53
2:E:416:THR:CG2	2:E:418:GLU:HB2	2.39	0.53
1:A:151:VAL:HG12	2:B:32:LEU:CD2	2.40	0.52
2:B:320:TRP:NE1	2:B:344:ARG:HD2	2.24	0.52
2:E:529:LYS:HE3	2:E:530:MET:CE	2.39	0.52
1:D:134:ARG:NH1	1:D:141:ASN:HB2	2.25	0.52
3:C:1:GLN:CB	3:C:13:LYS:HE2	2.38	0.52
2:E:52:ASN:C	2:E:52:ASN:HD22	2.17	0.52
1:A:89:ASP:O	1:A:92:LYS:CB	2.54	0.52
1:D:52:LEU:O	1:D:56:ILE:HG12	2.09	0.52
1:D:131:GLU:HG3	6:D:168:HOH:O	2.09	0.52
2:E:351:PHE:HD2	3:F:13:LYS:HD2	1.73	0.52
2:B:9:PHE:O	2:B:9:PHE:CD1	2.62	0.52
2:B:569:MET:HE1	2:B:575:ASN:CA	2.39	0.52
3:C:1:GLN:OE1	3:C:13:LYS:HG3	2.10	0.51
1:A:133:ILE:O	1:A:137:PHE:HB2	2.10	0.51
2:B:410:LYS:O	2:B:442:LEU:HB2	2.10	0.51
1:D:88:ALA:N	1:D:90:PHE:H	2.08	0.51
2:E:94:TYR:O	2:E:95:PRO:C	2.51	0.51
2:E:449:GLU:O	2:E:453:THR:HG23	2.10	0.51
1:D:115:ASP:O	1:D:119:GLN:HG3	2.10	0.51
1:D:134:ARG:HH11	1:D:141:ASN:HB2	1.74	0.51
1:A:95:GLN:C	1:A:97:THR:H	2.18	0.51
2:B:119:ASP:O	2:B:123:GLU:HG3	2.09	0.51
2:B:160:GLU:CG	2:B:188:SER:HB3	2.41	0.51
1:D:122:ALA:O	1:D:125:ILE:N	2.33	0.51
2:E:539:ASP:OD2	2:E:541:ARG:HD3	2.11	0.51
2:B:404:LEU:HD23	2:B:424:PHE:CZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ALA:C	1:D:124:MET:N	2.66	0.51
2:B:214:LYS:HG3	6:B:799:HOH:O	2.11	0.51
2:B:569:MET:CE	2:B:575:ASN:N	2.72	0.51
2:E:538:ILE:O	2:E:555:ARG:HG2	2.11	0.51
2:B:400:THR:HG22	2:B:401:ARG:NE	2.05	0.50
2:E:569:MET:CE	2:E:573:VAL:CG1	2.75	0.50
1:A:87:ASP:O	1:A:87:ASP:OD2	2.30	0.50
2:B:147:GLY:O	2:B:150:ALA:HB3	2.11	0.50
2:B:348:SER:C	2:B:349:GLU:HG2	2.35	0.50
2:B:444:THR:C	2:B:446:LYS:N	2.65	0.50
2:B:310:LEU:C	2:B:312:GLN:N	2.68	0.50
2:B:439:LEU:HD13	2:B:463:VAL:HG23	1.92	0.50
2:B:442:LEU:HA	6:B:689:HOH:O	2.10	0.50
2:B:444:THR:C	2:B:446:LYS:H	2.19	0.50
1:D:28:THR:HB	1:D:108:LEU:HA	1.93	0.50
1:D:138:ASN:O	1:D:138:ASN:OD1	2.30	0.50
1:D:154:GLU:HG2	1:D:159:PHE:CE1	2.44	0.50
2:E:73:LEU:HB2	2:E:112:LEU:CD2	2.41	0.50
2:E:416:THR:HG23	2:E:418:GLU:H	1.74	0.50
2:E:338:LYS:NZ	2:E:370:GLY:O	2.45	0.50
1:A:135:THR:C	1:A:137:PHE:N	2.67	0.50
2:E:324:TYR:O	2:E:326:GLU:HG3	2.12	0.50
2:E:10:PRO:O	2:E:11:GLU:C	2.54	0.49
2:E:364:LEU:HG	2:E:392:ILE:HD13	1.94	0.49
2:B:288:CYS:C	2:B:290:ARG:H	2.20	0.49
2:B:9:PHE:CD1	2:B:9:PHE:C	2.90	0.49
4:B:601:IHP:O44	4:B:601:IHP:O33	2.31	0.49
2:B:310:LEU:O	2:B:312:GLN:N	2.46	0.49
1:A:152:ARG:O	1:A:155:ASN:HB2	2.12	0.49
2:E:229:THR:HA	6:E:819:HOH:O	2.13	0.49
1:D:48:THR:CG2	1:D:50:LYS:CA	2.91	0.49
1:D:48:THR:CG2	1:D:51:ILE:H	2.15	0.49
1:D:86:TRP:CG	1:D:87:ASP:N	2.80	0.49
3:F:11:TYR:C	3:F:12:ARG:HG3	2.38	0.49
1:A:56:ILE:CG2	1:A:60:LYS:HE3	2.43	0.49
2:B:9:PHE:HB2	2:B:10:PRO:HD2	1.94	0.49
2:E:118:THR:HG22	2:E:120:ASP:N	2.28	0.49
2:E:164:ARG:O	2:E:165:GLU:HG2	2.12	0.49
2:E:52:ASN:C	2:E:52:ASN:ND2	2.68	0.49
2:B:38:TYR:CD1	2:B:38:TYR:C	2.91	0.48
2:B:8:SER:HB3	6:B:813:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:SER:CB	2:B:462:SER:HB2	2.43	0.48
2:E:529:LYS:CG	2:E:530:MET:HE3	2.42	0.48
1:D:122:ALA:C	1:D:124:MET:H	2.20	0.48
2:E:206:LEU:C	2:E:206:LEU:CD2	2.86	0.48
2:E:548:PRO:C	2:E:550:SER:N	2.69	0.48
2:E:97:ILE:HG22	2:E:124:LEU:HD23	1.94	0.48
2:E:548:PRO:C	2:E:550:SER:H	2.20	0.48
1:A:91:MET:C	1:A:93:ILE:N	2.72	0.48
2:B:91:GLY:O	2:B:115:MET:HB3	2.14	0.48
2:B:118:THR:HB	2:B:121:CYS:SG	2.53	0.48
1:A:135:THR:HG22	1:A:136:THR:N	2.28	0.48
1:A:103:LEU:CD2	2:B:9:PHE:HB2	2.43	0.48
1:A:157:TRP:N	1:A:157:TRP:CD1	2.80	0.48
2:E:404:LEU:O	2:E:440:SER:HB2	2.14	0.48
2:B:404:LEU:CD2	2:B:424:PHE:HZ	2.26	0.48
1:D:88:ALA:H	1:D:90:PHE:H	1.60	0.48
2:B:438:SER:HB3	2:B:462:SER:HB2	1.95	0.47
2:E:325:ILE:O	2:E:325:ILE:HG23	2.12	0.47
1:D:144:THR:HB	1:D:145:PRO:CG	2.39	0.47
2:E:118:THR:HG21	6:E:759:HOH:O	2.14	0.47
1:A:9:LYS:O	1:A:10:SER:O	2.33	0.47
2:B:220:ARG:HB2	6:B:755:HOH:O	2.14	0.47
1:D:141:ASN:OD1	1:D:141:ASN:C	2.54	0.47
1:A:7:VAL:HA	1:A:16:PHE:O	2.15	0.47
2:B:118:THR:CG2	2:B:120:ASP:HB2	2.43	0.47
2:B:239:GLU:HG2	2:B:269:CYS:HB2	1.96	0.47
2:E:323:ASP:O	2:E:325:ILE:O	2.32	0.47
2:B:93:VAL:HG13	2:B:97:ILE:HD12	1.97	0.47
2:E:37:TRP:CD1	2:E:37:TRP:N	2.79	0.47
2:E:439:LEU:HD13	2:E:463:VAL:HG23	1.95	0.47
2:B:47:LYS:HE3	6:B:698:HOH:O	2.15	0.47
2:E:64:ARG:O	2:E:66:PRO:HD3	2.15	0.47
2:E:191:ILE:O	2:E:219:ASN:HB3	2.15	0.47
2:B:118:THR:CG2	2:B:120:ASP:N	2.78	0.46
1:D:131:GLU:CG	1:D:134:ARG:HH21	2.28	0.46
1:D:147:GLU:C	1:D:149:GLU:N	2.71	0.46
2:E:317:GLN:HB3	2:E:341:ARG:HG2	1.96	0.46
2:E:388:ALA:O	2:E:392:ILE:HG13	2.16	0.46
2:E:444:THR:O	2:E:445:ASP:C	2.58	0.46
2:E:538:ILE:HB	2:E:555:ARG:HG3	1.96	0.46
2:E:539:ASP:OD1	2:E:541:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:578:GLN:HB2	6:E:710:HOH:O	2.15	0.46
2:B:18:PHE:N	2:B:18:PHE:CD2	2.80	0.46
2:B:569:MET:HE2	2:B:573:VAL:HG12	1.97	0.46
1:D:140:LYS:HZ3	1:D:140:LYS:HB3	1.80	0.46
1:D:145:PRO:HG2	1:D:146:GLU:OE1	2.15	0.46
2:E:159:LYS:HB3	2:E:187:VAL:HG23	1.98	0.46
2:E:369:MET:HE3	2:E:369:MET:HB3	1.83	0.46
2:E:569:MET:HE3	2:E:573:VAL:CG1	2.42	0.46
1:A:144:THR:O	1:A:145:PRO:C	2.59	0.46
2:E:108:GLU:O	2:E:133:LYS:N	2.49	0.46
2:E:118:THR:CG2	2:E:120:ASP:N	2.79	0.46
1:A:51:ILE:HG13	1:A:100:GLU:HB3	1.96	0.46
2:B:219:ASN:HB3	2:B:222:VAL:HG23	1.97	0.46
2:B:543:ALA:HA	2:B:544:PRO:HD3	1.61	0.46
2:E:213:LEU:O	2:E:214:LYS:HD3	2.16	0.46
2:B:41:GLU:O	2:B:42:ARG:C	2.58	0.46
2:E:80:ALA:CB	2:E:85:VAL:HG13	2.46	0.46
2:E:285:TYR:O	2:E:288:CYS:HB2	2.16	0.46
2:B:577:ASP:CG	2:B:578:GLN:N	2.73	0.46
1:D:150:GLU:HG2	6:D:162:HOH:O	2.15	0.46
2:E:206:LEU:C	2:E:206:LEU:HD22	2.41	0.46
2:B:164:ARG:O	2:B:164:ARG:HG3	2.15	0.46
2:E:471:LEU:C	2:E:471:LEU:HD22	2.41	0.46
2:B:94:TYR:HB3	2:B:95:PRO:HD3	1.98	0.45
1:D:105:ALA:HB2	1:D:113:LEU:HD23	1.98	0.45
2:E:57:SER:OG	2:E:60:THR:HG23	2.16	0.45
2:B:569:MET:HE3	2:B:573:VAL:HG12	1.98	0.45
2:B:303:SER:HB2	2:B:324:TYR:O	2.16	0.45
2:B:361:GLU:HG3	2:B:384:MET:HA	1.98	0.45
2:B:365:VAL:O	2:B:368:SER:HB2	2.16	0.45
2:B:367:VAL:HG12	2:B:374:LEU:HD22	1.97	0.45
2:B:369:MET:HG2	2:B:395:ASN:HD21	1.70	0.45
2:E:118:THR:HG22	2:E:121:CYS:N	2.29	0.45
2:E:242:THR:HG1	2:E:273:PHE:H	1.58	0.45
2:E:282:PRO:HA	2:E:285:TYR:CD1	2.51	0.45
2:B:38:TYR:CE1	2:B:42:ARG:HD2	2.52	0.45
2:B:94:TYR:O	2:B:95:PRO:C	2.59	0.45
2:B:112:LEU:HD12	2:B:137:LEU:CD2	2.46	0.45
2:B:212:ASN:HB2	6:B:627:HOH:O	2.15	0.45
2:B:288:CYS:C	2:B:290:ARG:N	2.73	0.45
2:E:73:LEU:HB2	2:E:112:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:THR:CG2	2:B:171:VAL:O	2.64	0.45
2:E:192:SER:HB2	2:E:274:TRP:HH2	1.82	0.45
2:B:38:TYR:O	2:B:42:ARG:HG3	2.16	0.45
2:B:529:LYS:HE2	2:E:500:ALA:O	2.17	0.45
2:B:354:GLU:N	2:B:354:GLU:CD	2.75	0.45
1:D:115:ASP:O	1:D:119:GLN:CG	2.65	0.45
2:E:183:TYR:C	2:E:184:THR:CG2	2.90	0.45
2:B:82:PHE:CZ	3:C:7:PRO:HB2	2.52	0.44
2:B:457:LYS:HA	2:B:457:LYS:HD3	1.80	0.44
2:E:47:LYS:HB2	2:E:70:SER:HB3	1.97	0.44
1:A:91:MET:HE3	1:A:117:THR:HG22	1.94	0.44
2:B:118:THR:CG2	2:B:120:ASP:H	2.30	0.44
2:B:395:ASN:C	2:B:396:ARG:HG2	2.41	0.44
2:E:35:LYS:O	2:E:39:GLU:HG2	2.17	0.44
2:E:310:LEU:C	2:E:312:GLN:H	2.24	0.44
2:E:333:LEU:HD23	2:E:367:VAL:HG21	1.98	0.44
2:B:9:PHE:HB2	2:B:10:PRO:CD	2.47	0.44
2:B:39:GLU:O	2:B:42:ARG:HB2	2.16	0.44
2:B:310:LEU:C	2:B:312:GLN:H	2.24	0.44
2:B:368:SER:HB3	2:B:395:ASN:HD22	1.82	0.44
2:B:395:ASN:O	2:B:396:ARG:CZ	2.66	0.44
2:E:36:SER:O	2:E:40:ILE:HG13	2.18	0.44
2:E:42:ARG:H	2:E:42:ARG:HG3	1.50	0.44
2:E:67:LYS:HA	2:E:67:LYS:HD2	1.71	0.44
2:E:148:LEU:O	2:E:149:ALA:C	2.61	0.44
2:E:400:THR:HG22	2:E:401:ARG:NE	2.30	0.44
2:B:416:THR:CG2	2:B:418:GLU:HG3	2.48	0.44
1:D:48:THR:HG22	1:D:49:SER:C	2.42	0.44
2:E:111:ARG:HB3	2:E:136:VAL:HB	2.00	0.44
2:E:471:LEU:HA	2:E:471:LEU:HD23	1.22	0.44
1:A:123:ASP:HA	1:A:126:LYS:HG3	2.00	0.44
1:A:124:MET:O	1:A:128:LYS:HE3	2.17	0.44
1:A:149:GLU:HA	6:A:183:HOH:O	2.18	0.44
2:B:569:MET:CE	2:B:574:TRP:C	2.91	0.44
3:C:4:GLY:HA2	6:C:509:HOH:O	2.17	0.44
1:D:46:ASN:HB2	1:D:107:TYR:CD2	2.52	0.44
2:E:114:ARG:HA	2:E:139:SER:O	2.18	0.44
1:A:95:GLN:C	1:A:97:THR:N	2.73	0.44
2:B:91:GLY:O	2:B:115:MET:HE3	2.18	0.44
2:E:80:ALA:HB2	2:E:85:VAL:HG13	2.00	0.44
2:E:112:LEU:HB3	2:E:115:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:129:PHE:CA	6:E:701:HOH:O	2.66	0.44
2:E:400:THR:HG22	2:E:401:ARG:CG	2.43	0.44
1:A:102:ILE:CG2	2:B:13:VAL:HG11	2.46	0.44
2:B:245:TYR:O	2:B:276:ALA:HA	2.18	0.44
2:B:307:VAL:O	2:B:308:LYS:C	2.59	0.44
2:B:535:VAL:HG13	2:B:558:ILE:HG12	1.99	0.44
2:B:569:MET:HG2	2:B:573:VAL:HG12	2.00	0.44
2:E:353:MET:CA	2:E:354:GLU:OE2	2.66	0.44
2:E:386:ASN:OD1	2:E:420:LEU:HA	2.18	0.44
2:B:224:LEU:HA	2:B:224:LEU:HD12	1.66	0.43
2:B:416:THR:HG22	2:B:417:LEU:N	2.33	0.43
2:E:428:VAL:CG2	2:E:455:ALA:HB2	2.45	0.43
2:E:285:TYR:O	2:E:286:SER:C	2.60	0.43
2:E:424:PHE:O	2:E:425:GLY:C	2.59	0.43
1:A:132:GLU:O	1:A:136:THR:OG1	2.33	0.43
2:B:82:PHE:O	2:B:84:LEU:HG	2.19	0.43
2:B:118:THR:HG22	2:B:121:CYS:N	2.19	0.43
2:B:191:ILE:HD12	2:B:191:ILE:O	2.17	0.43
2:B:282:PRO:HA	2:B:285:TYR:CD1	2.54	0.43
5:B:602:CFA:H6'	5:B:602:CFA:C1	2.48	0.43
2:E:465:PHE:HZ	3:F:2:VAL:HG11	1.83	0.43
3:C:10:ASN:OD1	3:C:10:ASN:N	2.50	0.43
2:E:270:LEU:HD23	2:E:270:LEU:HA	1.30	0.43
1:A:116:LEU:O	1:A:116:LEU:HG	2.19	0.43
2:B:256:GLY:O	2:B:257:LEU:C	2.61	0.43
3:C:8:VAL:CG1	3:C:10:ASN:H	2.32	0.43
2:B:9:PHE:HD1	2:B:9:PHE:C	2.24	0.43
2:B:47:LYS:CE	6:B:698:HOH:O	2.66	0.43
2:B:191:ILE:HA	2:B:191:ILE:HD13	0.99	0.43
2:B:416:THR:HG23	2:B:418:GLU:CG	2.48	0.43
2:E:26:ASP:O	2:E:29:SER:HB2	2.19	0.43
2:E:396:ARG:C	2:E:398:ASN:N	2.76	0.43
2:B:420:LEU:O	2:B:421:ASP:C	2.60	0.43
1:D:125:ILE:HG23	1:D:133:ILE:HD13	2.01	0.43
2:E:143:PHE:CZ	2:E:168:VAL:HG22	2.53	0.43
2:E:471:LEU:C	2:E:471:LEU:CD2	2.85	0.43
1:D:157:TRP:CD2	2:E:560:ARG:HD2	2.54	0.43
2:E:177:SER:HA	6:E:636:HOH:O	2.18	0.43
2:E:110:ILE:HD13	2:E:125:ILE:CD1	2.49	0.43
2:E:183:TYR:C	2:E:184:THR:HG23	2.43	0.43
2:E:361:GLU:OE2	2:E:361:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:396:ARG:HA	2:E:396:ARG:NE	2.34	0.43
2:E:400:THR:CG2	2:E:401:ARG:NE	2.82	0.43
2:E:470:ASP:HB3	2:E:497:ALA:HB2	2.01	0.43
2:B:58:PRO:O	2:B:61:VAL:N	2.52	0.42
1:D:86:TRP:CE3	1:D:87:ASP:HB2	2.54	0.42
2:E:273:PHE:O	2:E:274:TRP:C	2.59	0.42
2:E:274:TRP:O	2:E:275:ASP:HB2	2.20	0.42
1:A:95:GLN:HG3	1:A:99:PHE:CE2	2.54	0.42
1:A:128:LYS:HZ2	1:A:136:THR:HG21	1.76	0.42
1:D:48:THR:HG22	1:D:50:LYS:CA	2.48	0.42
2:E:30:VAL:CG2	2:E:41:GLU:HG2	2.49	0.42
2:E:250:ARG:HH11	2:E:250:ARG:CG	2.29	0.42
1:D:140:LYS:O	1:D:140:LYS:HG3	2.11	0.42
2:E:512:TRP:CD1	2:E:512:TRP:C	2.97	0.42
2:E:529:LYS:HE3	6:E:692:HOH:O	2.19	0.42
2:E:287:VAL:O	2:E:287:VAL:CG1	2.67	0.42
2:E:569:MET:HE2	2:E:573:VAL:C	2.44	0.42
1:A:119:GLN:HB3	6:A:164:HOH:O	2.20	0.42
2:B:250:ARG:HG2	2:B:250:ARG:HH11	1.84	0.42
2:B:274:TRP:NE1	2:B:298:TYR:CD1	2.87	0.42
2:B:47:LYS:HZ2	2:B:47:LYS:HG2	1.77	0.42
2:B:220:ARG:HG3	2:B:274:TRP:CD2	2.55	0.42
1:D:155:ASN:HB3	2:E:28:ASN:HD22	1.83	0.42
2:E:270:LEU:HD13	2:E:273:PHE:HZ	1.84	0.42
2:B:272:GLY:O	2:B:273:PHE:HB2	2.20	0.42
1:D:111:LYS:HZ2	1:D:111:LYS:HG2	1.34	0.42
1:D:147:GLU:C	1:D:149:GLU:H	2.26	0.42
1:A:61:ARG:HA	1:A:61:ARG:HD2	1.49	0.42
3:C:8:VAL:HG13	3:C:10:ASN:H	1.85	0.42
2:E:310:LEU:C	2:E:312:GLN:N	2.76	0.42
2:E:436:ARG:NH1	2:E:460:MET:HE1	2.34	0.42
2:E:533:LEU:HD23	2:E:560:ARG:HA	2.01	0.42
1:D:153:ARG:HG3	1:D:157:TRP:CE2	2.55	0.42
2:B:36:SER:O	2:B:40:ILE:HG12	2.20	0.42
2:E:277:VAL:O	2:E:278:PRO:C	2.62	0.42
2:E:529:LYS:CE	2:E:530:MET:HE3	2.50	0.42
1:A:56:ILE:O	1:A:57:GLU:C	2.63	0.41
2:B:365:VAL:O	2:B:366:SER:C	2.63	0.41
2:E:52:ASN:ND2	2:E:54:TYR:H	2.18	0.41
2:E:210:CYS:HA	2:E:211:PRO:HD2	1.89	0.41
2:B:435:ARG:HA	2:B:458:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:ILE:CD1	2:E:99:ALA:HB1	2.50	0.41
2:E:237:LEU:HA	2:E:237:LEU:HD12	1.70	0.41
1:A:98:LEU:O	1:A:99:PHE:C	2.62	0.41
2:B:80:ALA:HA	2:B:85:VAL:HG13	2.01	0.41
2:B:342:GLU:HA	2:B:376:SER:O	2.20	0.41
1:D:105:ALA:HB2	1:D:113:LEU:CD2	2.50	0.41
1:D:52:LEU:O	1:D:56:ILE:CG1	2.67	0.41
2:E:173:GLY:C	2:E:175:TRP:N	2.76	0.41
2:E:191:ILE:HB	2:E:194:LEU:HD12	2.01	0.41
2:B:483:LEU:HD13	2:B:508:MET:HE3	2.01	0.41
1:D:5:LYS:HB3	1:D:5:LYS:HE2	1.53	0.41
1:D:145:PRO:CG	1:D:146:GLU:H	2.34	0.41
2:E:250:ARG:HG2	2:E:250:ARG:NH1	2.34	0.41
2:E:351:PHE:CD2	3:F:13:LYS:HD3	2.56	0.41
2:E:439:LEU:HD12	2:E:439:LEU:N	2.32	0.41
2:E:570:PRO:HD2	2:E:573:VAL:CG2	2.50	0.41
4:E:601:IHP:O44	4:E:601:IHP:O33	2.39	0.41
2:B:74:LYS:HG2	2:B:113:LYS:HB3	2.03	0.41
2:E:9:PHE:HA	2:E:10:PRO:HD2	1.82	0.41
2:E:62:ILE:HD13	2:E:99:ALA:HB1	2.01	0.41
1:A:129:THR:HB	1:A:130:PRO:HD2	2.03	0.41
2:B:268:ARG:HA	2:B:268:ARG:HD3	1.78	0.41
2:B:300:THR:CG2	2:B:324:TYR:HE1	2.32	0.41
2:B:566:ARG:NH1	2:B:568:ASP:OD1	2.52	0.41
6:B:818:HOH:O	3:C:2:VAL:CG1	2.51	0.41
2:E:264:CYS:CB	2:E:267:LEU:HD12	2.50	0.41
1:A:58:TYR:O	1:A:59:CYS:C	2.61	0.41
2:B:39:GLU:OE2	2:B:42:ARG:HD3	2.21	0.41
2:B:277:VAL:O	2:B:278:PRO:C	2.62	0.41
2:B:319:LEU:HG	2:B:321:VAL:HG22	2.03	0.41
2:B:354:GLU:HA	2:B:355:PRO:HD3	1.76	0.41
2:E:282:PRO:HA	2:E:285:TYR:CZ	2.55	0.41
2:E:291:LEU:HD23	2:E:291:LEU:HA	1.93	0.41
2:E:322:LEU:HD23	2:E:322:LEU:HA	1.80	0.41
2:E:406:ILE:HD11	2:E:420:LEU:HD11	2.03	0.41
2:E:413:ASP:OD1	2:E:416:THR:HB	2.21	0.41
2:E:543:ALA:O	2:E:546:SER:HB2	2.21	0.41
1:A:52:LEU:HD21	1:A:56:ILE:HD11	2.02	0.40
2:B:76:LYS:HA	2:B:77:PRO:HD3	1.90	0.40
2:B:501:ASN:O	2:B:502:ALA:C	2.64	0.40
2:B:439:LEU:CD1	2:B:463:VAL:CG2	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:325:ILE:O	2:E:359:LEU:HD13	2.21	0.40
2:E:457:LYS:HD2	2:E:457:LYS:HA	1.94	0.40
3:F:5:TRP:CD2	3:F:6:PRO:HA	2.55	0.40
2:B:543:ALA:O	2:B:546:SER:CB	2.69	0.40
1:D:154:GLU:O	1:D:155:ASN:C	2.62	0.40
2:E:174:HIS:HD2	6:E:742:HOH:O	2.02	0.40
2:E:224:LEU:HD12	2:E:224:LEU:HA	1.52	0.40
2:B:114:ARG:HA	2:B:139:SER:O	2.20	0.40
2:B:360:THR:O	2:B:361:GLU:C	2.63	0.40
2:E:416:THR:HG22	2:E:418:GLU:N	2.32	0.40
2:E:496:LYS:HB2	2:E:496:LYS:HE2	1.92	0.40
1:A:9:LYS:C	1:A:10:SER:O	2.64	0.40
2:B:237:LEU:HD12	2:B:237:LEU:HA	1.89	0.40
2:B:270:LEU:HD11	2:B:284:VAL:HG22	2.03	0.40
2:B:278:PRO:HD3	2:B:301:VAL:HG12	2.04	0.40
2:E:413:ASP:CB	2:E:416:THR:HG22	2.45	0.40
2:E:566:ARG:HG2	6:E:657:HOH:O	2.21	0.40
3:F:5:TRP:CD1	3:F:6:PRO:HA	2.57	0.40

All (3) 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:A:15:SER:O	3:C:11:TYR:O[1_545]	0.76	1.44
1:A:15:SER:O	3:C:11:TYR:C[1_545]	1.98	0.22
1:A:15:SER:C	3:C:11:TYR:O[1_545]	1.98	0.22

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	120/160 (75%)	98 (82%)	15 (12%)	7 (6%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	121/160 (76%)	98 (81%)	18 (15%)	5 (4%)	2	3
2	B	569/594 (96%)	520 (91%)	41 (7%)	8 (1%)	9	17
2	E	569/594 (96%)	510 (90%)	50 (9%)	9 (2%)	7	14
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
3	F	11/13 (85%)	8 (73%)	2 (18%)	1 (9%)	0	0
All	All	1401/1534 (91%)	1244 (89%)	127 (9%)	30 (2%)	5	9

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	92	LYS
2	B	42	ARG
2	B	83	ASN
2	B	219	ASN
2	B	550	SER
1	D	48	THR
1	D	87	ASP
1	D	145	PRO
2	E	11	GLU
2	E	18	PHE
2	E	41	GLU
1	A	88	ALA
2	B	12	GLU
2	B	289	SER
1	D	92	LYS
1	D	134	ARG
2	E	297	SER
2	E	325	ILE
2	E	506	GLU
1	A	25	GLU
1	A	145	PRO
1	A	152	ARG
2	B	53	CYS
2	B	172	SER
3	F	12	ARG
2	E	301	VAL
2	E	311	CYS
1	A	102	ILE
2	E	409	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/137 (82%)	87 (77%)	26 (23%)	1	1
1	D	114/137 (83%)	85 (75%)	29 (25%)	0	1
2	B	504/525 (96%)	415 (82%)	89 (18%)	2	3
2	E	504/525 (96%)	409 (81%)	95 (19%)	1	3
3	C	12/12 (100%)	5 (42%)	7 (58%)	0	0
3	F	12/12 (100%)	9 (75%)	3 (25%)	0	1
All	All	1259/1348 (93%)	1010 (80%)	249 (20%)	1	2

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	7	VAL
1	A	9	LYS
1	A	15	SER
1	A	19	GLU
1	A	24	LEU
1	A	27	GLN
1	A	33	VAL
1	A	47	VAL
1	A	50	LYS
1	A	57	GLU
1	A	60	LYS
1	A	61	ARG
1	A	93	ILE
1	A	95	GLN
1	A	101	LEU
1	A	102	ILE
1	A	111	LYS
1	A	112	ASN
1	A	129	THR
1	A	135	THR
1	A	136	THR

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Mol	Chain	Res	Type
1	A	139	ILE
1	A	140	LYS
1	A	147	GLU
1	A	149	GLU
2	B	8	SER
2	B	9	PHE
2	B	11	GLU
2	B	12	GLU
2	B	14	LEU
2	B	23	LEU
2	B	30	VAL
2	B	41	GLU
2	B	47	LYS
2	B	48	VAL
2	B	52	ASN
2	B	60	THR
2	B	67	LYS
2	B	69	ARG
2	B	83	ASN
2	B	85	VAL
2	B	105	THR
2	B	115	MET
2	B	118	THR
2	B	124	LEU
2	B	127	LYS
2	B	130	LYS
2	B	156	ARG
2	B	159	LYS
2	B	164	ARG
2	B	165	GLU
2	B	170	ASP
2	B	171	VAL
2	B	177	SER
2	B	185	SER
2	B	191	ILE
2	B	198	VAL
2	B	206	LEU
2	B	208	THR
2	B	214	LYS
2	B	227	LEU
2	B	237	LEU
2	B	257	LEU

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Mol	Chain	Res	Type
2	B	258	SER
2	B	270	LEU
2	B	284	VAL
2	B	287	VAL
2	B	288	CYS
2	B	300	THR
2	B	302	GLN
2	B	321	VAL
2	B	325	ILE
2	B	335	SER
2	B	338	LYS
2	B	340	LEU
2	B	357	VAL
2	B	359	LEU
2	B	361	GLU
2	B	362	GLN
2	B	364	LEU
2	B	394	ARG
2	B	400	THR
2	B	404	LEU
2	B	407	ILE
2	B	416	THR
2	B	418	GLU
2	B	422	ILE
2	B	427	ILE
2	B	428	VAL
2	B	432	LYS
2	B	439	LEU
2	B	446	LYS
2	B	447	VAL
2	B	453	THR
2	B	456	LYS
2	B	458	MET
2	B	471	LEU
2	B	478	SER
2	B	482	SER
2	B	483	LEU
2	B	489	ARG
2	B	504	LYS
2	B	517	SER
2	B	525	LEU
2	B	533	LEU

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Mol	Chain	Res	Type
2	B	541	ARG
2	B	545	ASP
2	B	556	VAL
2	B	561	THR
2	B	569	MET
2	B	575	ASN
2	B	576	MET
2	B	577	ASP
2	B	578	GLN
3	C	1	GLN
3	C	2	VAL
3	C	8	VAL
3	C	10	ASN
3	C	11	TYR
3	C	12	ARG
3	C	13	LYS
1	D	5	LYS
1	D	9	LYS
1	D	12	ASP
1	D	20	GLU
1	D	25	GLU
1	D	27	GLN
1	D	47	VAL
1	D	48	THR
1	D	51	ILE
1	D	52	LEU
1	D	56	ILE
1	D	87	ASP
1	D	91	MET
1	D	92	LYS
1	D	93	ILE
1	D	98	LEU
1	D	101	LEU
1	D	102	ILE
1	D	110	ILE
1	D	111	LYS
1	D	112	ASN
1	D	114	LEU
1	D	119	GLN
1	D	135	THR
1	D	136	THR
1	D	137	PHE

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Mol	Chain	Res	Type
1	D	139	ILE
1	D	140	LYS
1	D	149	GLU
2	E	8	SER
2	E	12	GLU
2	E	14	LEU
2	E	18	PHE
2	E	21	ILE
2	E	23	LEU
2	E	25	LYS
2	E	29	SER
2	E	30	VAL
2	E	33	VAL
2	E	41	GLU
2	E	42	ARG
2	E	46	ARG
2	E	47	LYS
2	E	48	VAL
2	E	60	THR
2	E	83	ASN
2	E	85	VAL
2	E	98	GLU
2	E	103	SER
2	E	105	THR
2	E	111	ARG
2	E	115	MET
2	E	118	THR
2	E	123	GLU
2	E	127	LYS
2	E	156	ARG
2	E	159	LYS
2	E	165	GLU
2	E	169	ASP
2	E	170	ASP
2	E	181	ASP
2	E	185	SER
2	E	188	SER
2	E	198	VAL
2	E	206	LEU
2	E	208	THR
2	E	214	LYS
2	E	219	ASN

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Mol	Chain	Res	Type
2	E	226	LYS
2	E	227	LEU
2	E	237	LEU
2	E	246	THR
2	E	250	ARG
2	E	257	LEU
2	E	265	LYS
2	E	284	VAL
2	E	287	VAL
2	E	288	CYS
2	E	289	SER
2	E	290	ARG
2	E	308	LYS
2	E	309	LEU
2	E	312	GLN
2	E	315	LYS
2	E	321	VAL
2	E	325	ILE
2	E	335	SER
2	E	336	THR
2	E	338	LYS
2	E	349	GLU
2	E	354	GLU
2	E	357	VAL
2	E	361	GLU
2	E	367	VAL
2	E	368	SER
2	E	369	MET
2	E	373	LYS
2	E	390	ILE
2	E	400	THR
2	E	404	LEU
2	E	416	THR
2	E	427	ILE
2	E	428	VAL
2	E	439	LEU
2	E	440	SER
2	E	453	THR
2	E	456	LYS
2	E	457	LYS
2	E	463	VAL
2	E	471	LEU

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Mol	Chain	Res	Type
2	E	483	LEU
2	E	489	ARG
2	E	504	LYS
2	E	525	LEU
2	E	528	GLN
2	E	532	LYS
2	E	541	ARG
2	E	549	GLU
2	E	551	CYS
2	E	555	ARG
2	E	556	VAL
2	E	576	MET
2	E	577	ASP
2	E	578	GLN
3	F	2	VAL
3	F	12	ARG
3	F	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	95	GLN
1	A	112	ASN
2	B	22	GLN
2	B	52	ASN
2	B	174	HIS
2	B	232	GLN
2	B	383	GLN
2	B	395	ASN
2	B	575	ASN
1	D	31	HIS
1	D	62	HIS
2	E	16	HIS
2	E	52	ASN
2	E	83	ASN
2	E	174	HIS
2	E	219	ASN
2	E	312	GLN
2	E	317	GLN
2	E	383	GLN
2	E	575	ASN

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Mol	Chain	Res	Type
2	E	578	GLN

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	IHP	B	601	-	36,36,36	2.80	11 (30%)	60,60,60	2.16	21 (35%)
4	IHP	E	601	-	36,36,36	3.17	14 (38%)	60,60,60	2.06	23 (38%)
5	CFA	E	602	-	13,13,13	1.77	3 (23%)	17,17,17	2.44	7 (41%)
5	CFA	B	602	-	13,13,13	1.40	2 (15%)	17,17,17	1.45	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IHP	B	601	-	-	5/30/54/54	0/1/1/1
4	IHP	E	601	-	-	4/30/54/54	0/1/1/1
5	CFA	E	602	-	-	0/5/5/5	0/1/1/1
5	CFA	B	602	-	-	0/5/5/5	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	601	IHP	P2-O42	7.97	1.84	1.54
4	B	601	IHP	P3-O13	7.82	1.73	1.59
4	B	601	IHP	P5-O15	7.05	1.71	1.59
4	E	601	IHP	P3-O43	6.93	1.80	1.54
4	E	601	IHP	P2-O12	6.45	1.70	1.59
4	B	601	IHP	P2-O32	6.37	1.78	1.54
4	E	601	IHP	P5-O15	5.87	1.69	1.59
4	E	601	IHP	P1-O11	5.50	1.69	1.59
4	B	601	IHP	P3-O43	5.41	1.74	1.54
4	E	601	IHP	P2-O32	5.32	1.74	1.54
4	E	601	IHP	P1-O41	4.79	1.72	1.54
4	E	601	IHP	P3-O13	4.66	1.67	1.59
4	B	601	IHP	P2-O12	4.28	1.67	1.59
4	E	601	IHP	P6-O16	4.16	1.66	1.59
4	B	601	IHP	P2-O42	3.91	1.69	1.54
4	B	601	IHP	P1-O41	3.82	1.69	1.54
4	B	601	IHP	P3-O33	3.60	1.68	1.54
4	E	601	IHP	P4-O14	3.59	1.65	1.59
5	E	602	CFA	O1'-C1'	-3.18	1.31	1.37
4	B	601	IHP	O16-C6	-2.66	1.35	1.44
4	E	601	IHP	C4-C3	2.54	1.57	1.52
5	B	602	CFA	C2-C1	2.50	1.58	1.50
5	E	602	CFA	C4'-CL4	-2.45	1.68	1.74
4	E	601	IHP	P1-O31	2.26	1.63	1.54
4	E	601	IHP	P4-O24	2.21	1.57	1.50
5	E	602	CFA	C2-C1	2.20	1.57	1.50
4	E	601	IHP	P4-O44	2.12	1.62	1.54
4	B	601	IHP	P6-O46	2.06	1.62	1.54
5	B	602	CFA	C5'-C4'	2.05	1.41	1.38
4	B	601	IHP	C4-C3	2.03	1.56	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	IHP	P3-O13-C3	-6.57	105.87	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	IHP	O41-P1-O31	-5.52	87.11	107.80
4	E	601	IHP	O41-P1-O31	5.37	127.95	107.80
5	E	602	CFA	C1'-C2'-CL3	-5.31	113.36	119.44
4	B	601	IHP	O12-C2-C3	-4.72	98.72	108.76
5	E	602	CFA	C2'-C3'-C4'	-4.71	113.40	118.72
4	E	601	IHP	P3-O13-C3	-4.53	111.33	123.43
4	E	601	IHP	P6-O16-C6	-4.03	112.66	123.43
4	B	601	IHP	O14-C4-C5	-4.01	100.22	108.76
4	E	601	IHP	O14-C4-C5	-3.49	101.34	108.76
4	E	601	IHP	O12-P2-O22	-3.44	97.07	109.33
4	B	601	IHP	O32-P2-O22	3.40	124.10	110.83
4	B	601	IHP	O12-C2-C1	-3.38	101.58	108.76
4	E	601	IHP	C5-C6-C1	3.32	117.71	110.43
4	E	601	IHP	C6-C5-C4	3.31	117.70	110.43
5	B	602	CFA	C3'-C4'-CL4	-3.27	115.07	119.17
4	E	601	IHP	O45-P5-O15	-3.21	93.36	105.85
4	E	601	IHP	P1-O11-C1	-3.20	114.88	123.43
4	B	601	IHP	O45-P5-O15	-3.10	93.79	105.85
5	E	602	CFA	C3'-C2'-CL3	3.05	123.44	118.45
5	E	602	CFA	C6'-C1'-C2'	2.88	123.13	118.87
4	B	601	IHP	O13-P3-O23	-2.88	99.07	109.33
4	B	601	IHP	O11-C1-C6	-2.86	102.69	108.76
5	E	602	CFA	C6'-C5'-C4'	2.84	122.10	119.24
4	E	601	IHP	C6-C1-C2	2.80	116.58	110.43
4	E	601	IHP	O12-C2-C1	-2.78	102.84	108.76
4	B	601	IHP	O15-C5-C6	2.78	114.68	108.76
4	B	601	IHP	O31-P1-O21	2.77	121.65	110.83
4	E	601	IHP	O13-C3-C4	2.71	114.52	108.76
5	E	602	CFA	C5'-C6'-C1'	-2.70	114.94	120.06
4	B	601	IHP	O36-P6-O26	2.69	121.33	110.83
4	B	601	IHP	P5-O15-C5	-2.66	116.33	123.43
5	B	602	CFA	C5'-C6'-C1'	-2.47	115.38	120.06
4	B	601	IHP	O44-P4-O34	2.44	116.95	107.80
5	E	602	CFA	C5'-C4'-CL4	-2.44	115.76	119.36
4	E	601	IHP	O12-C2-C3	-2.39	103.68	108.76
4	B	601	IHP	O45-P5-O35	2.36	116.66	107.80
4	B	601	IHP	O41-P1-O21	2.33	119.92	110.83
5	B	602	CFA	C5'-C4'-CL4	2.33	122.79	119.36
4	B	601	IHP	O36-P6-O16	-2.32	96.83	105.85
4	E	601	IHP	O11-P1-O21	2.31	117.56	109.33
4	B	601	IHP	O15-P5-O25	2.30	117.52	109.33
4	E	601	IHP	O14-P4-O24	2.25	117.35	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	IHP	O16-C6-C1	-2.24	103.99	108.76
4	E	601	IHP	P5-O15-C5	-2.22	117.50	123.43
4	E	601	IHP	O36-P6-O16	-2.20	97.29	105.85
4	E	601	IHP	O31-P1-O21	-2.18	102.36	110.83
4	E	601	IHP	P4-O14-C4	-2.16	117.67	123.43
4	B	601	IHP	O13-C3-C4	2.14	113.31	108.76
4	B	601	IHP	O41-P1-O11	2.13	114.14	105.85
4	E	601	IHP	O41-P1-O11	-2.12	97.61	105.85
4	E	601	IHP	O45-P5-O35	2.07	115.57	107.80
4	E	601	IHP	O44-P4-O14	-2.03	97.93	105.85
4	E	601	IHP	O35-P5-O25	2.03	118.73	110.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	IHP	C2-O12-P2-O22
4	E	601	IHP	C2-O12-P2-O22
4	B	601	IHP	C1-O11-P1-O21
4	B	601	IHP	C3-O13-P3-O23
4	E	601	IHP	C4-O14-P4-O24
4	B	601	IHP	C5-O15-P5-O35
4	E	601	IHP	C3-O13-P3-O33
4	B	601	IHP	C6-O16-P6-O26
4	E	601	IHP	C6-O16-P6-O26

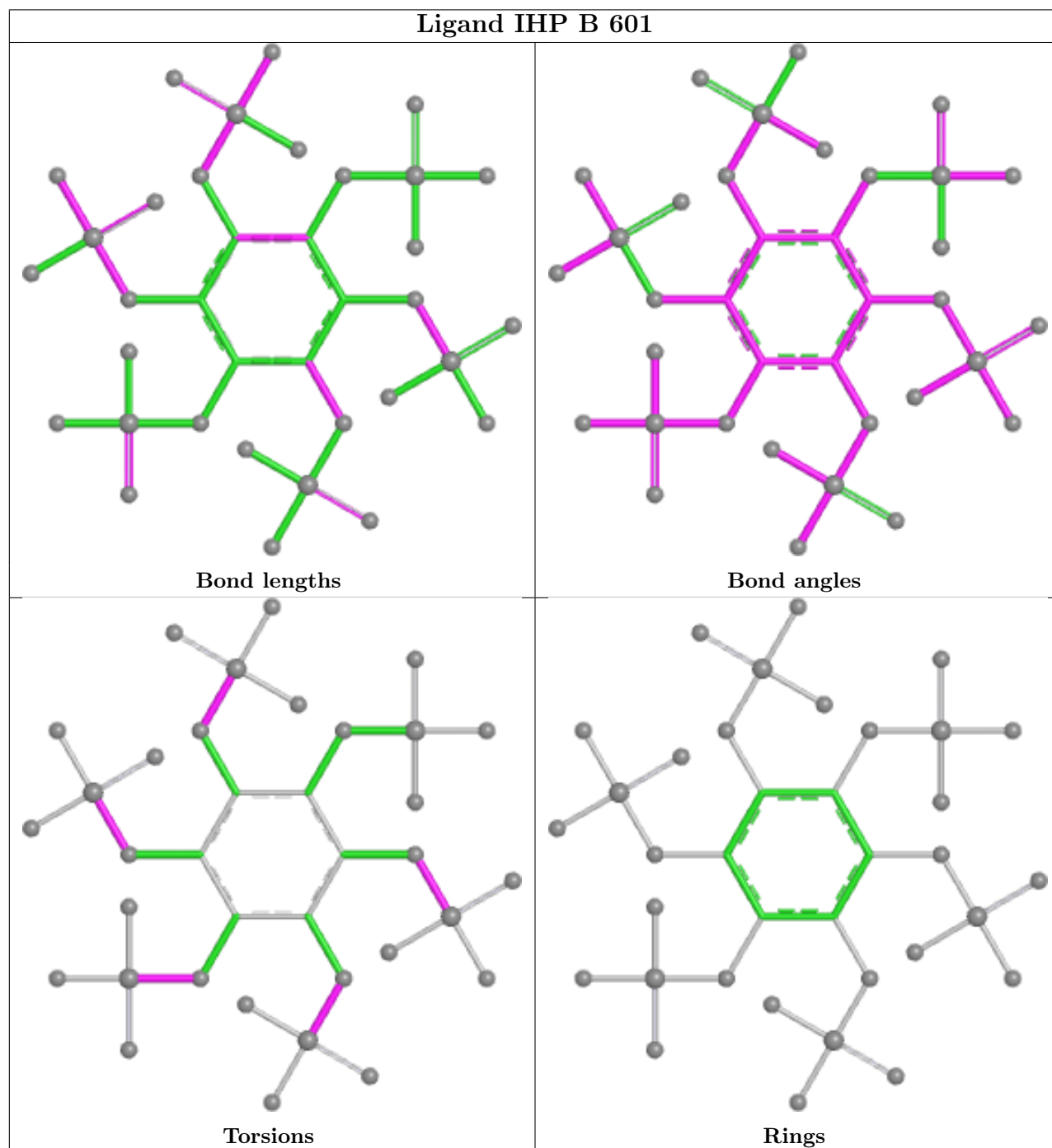
There are no ring outliers.

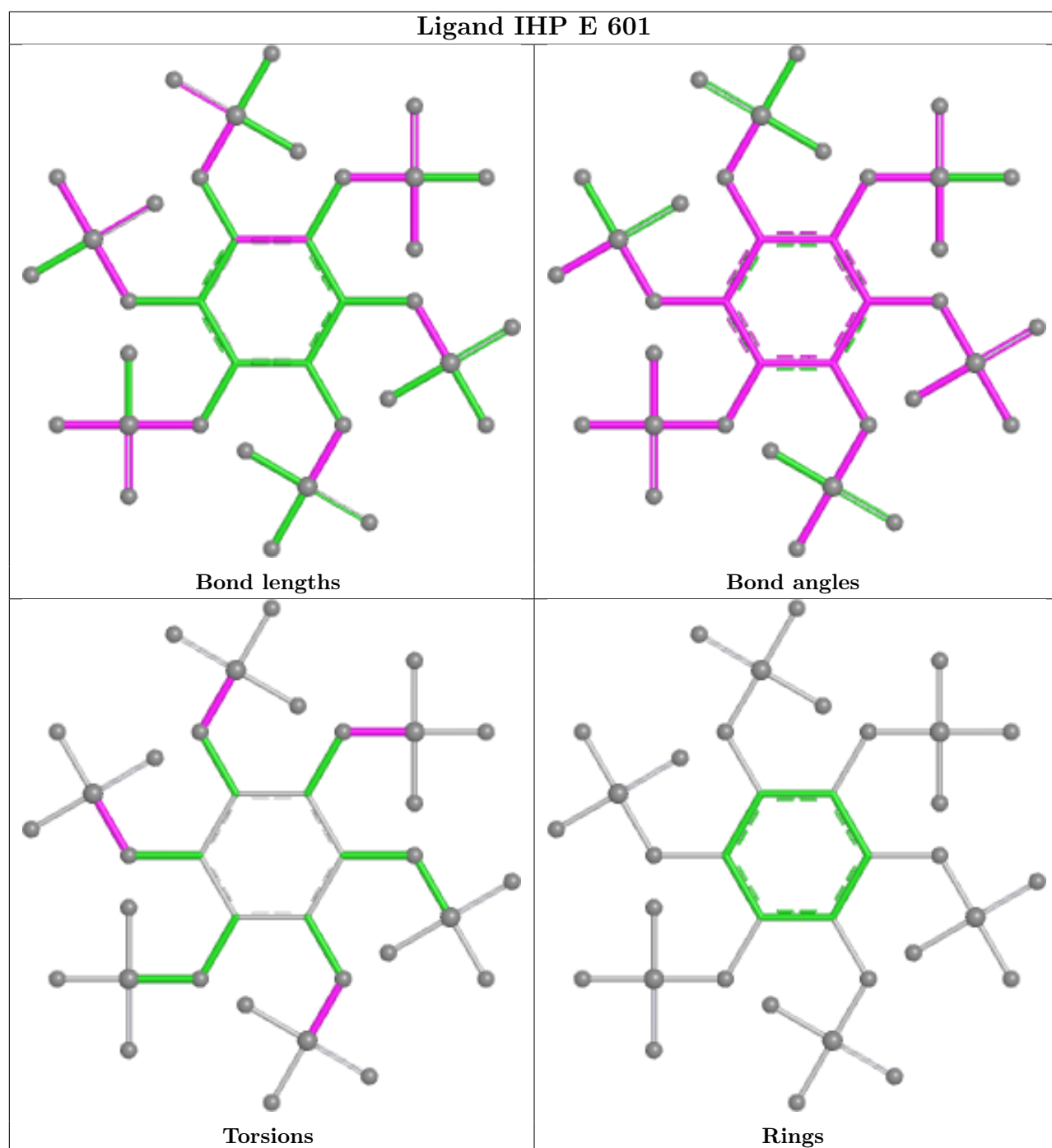
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	IHP	1	0
4	E	601	IHP	2	0
5	B	602	CFA	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	126/160 (78%)	0.34	4 (3%) 50 46	2, 6, 13, 22	0
1	D	127/160 (79%)	0.19	2 (1%) 70 67	2, 6, 13, 22	0
2	B	571/594 (96%)	-0.23	11 (1%) 66 62	2, 6, 18, 41	0
2	E	571/594 (96%)	-0.14	11 (1%) 66 62	2, 6, 16, 32	0
3	C	13/13 (100%)	0.74	2 (15%) 5 4	5, 8, 13, 16	0
3	F	13/13 (100%)	0.47	0 100 100	2, 7, 11, 12	0
All	All	1421/1534 (92%)	-0.09	30 (2%) 63 59	2, 6, 16, 41	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	325	ILE	5.3
2	B	12	GLU	3.8
2	B	174	HIS	3.7
2	E	172	SER	3.6
2	B	577	ASP	3.4
2	B	171	VAL	3.4
2	E	174	HIS	3.4
2	E	11	GLU	3.4
2	B	578	GLN	3.2
2	E	8	SER	3.2
2	B	11	GLU	3.1
2	B	550	SER	3.1
2	E	106	TRP	3.0
2	E	578	GLN	3.0
2	E	171	VAL	2.9
2	B	106	TRP	2.7
1	A	31	HIS	2.7
2	B	8	SER	2.6
2	E	12	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	172	SER	2.4
1	A	33	VAL	2.3
2	B	354	GLU	2.3
1	D	31	HIS	2.3
1	D	40	ASN	2.3
3	C	13	LYS	2.2
2	E	577	ASP	2.1
2	E	9	PHE	2.1
3	C	11	TYR	2.1
1	A	96	ALA	2.1
1	A	88	ALA	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](#)

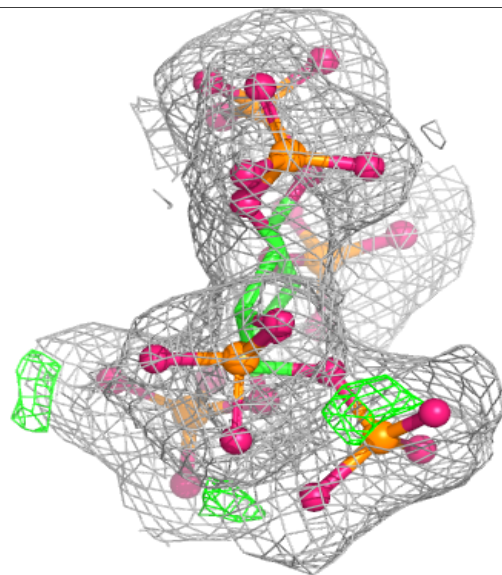
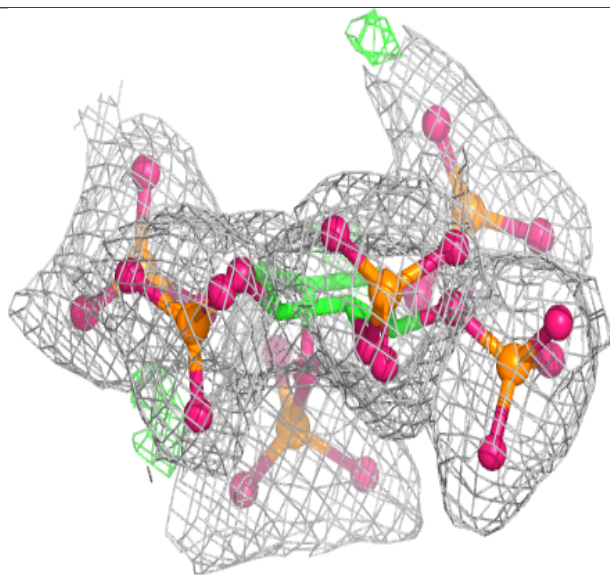
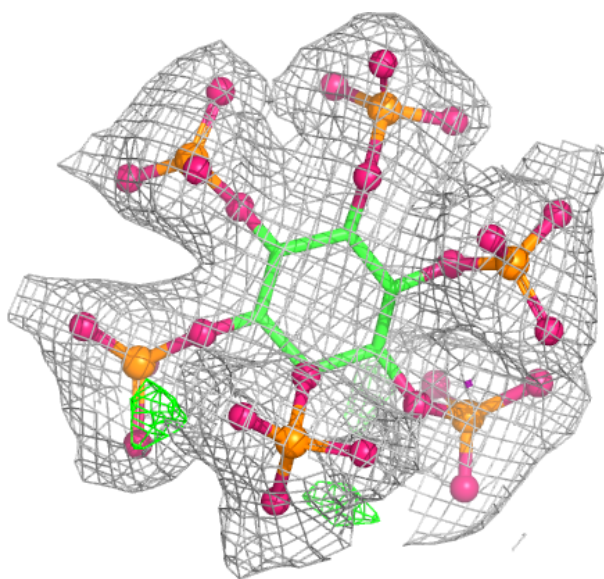
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	IHP	B	601	36/36	0.97	0.06	2,6,30,44	0
4	IHP	E	601	36/36	0.97	0.06	2,7,25,32	0
5	CFA	B	602	13/13	0.97	0.07	2,2,9,10	0
5	CFA	E	602	13/13	0.97	0.06	2,2,10,16	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.

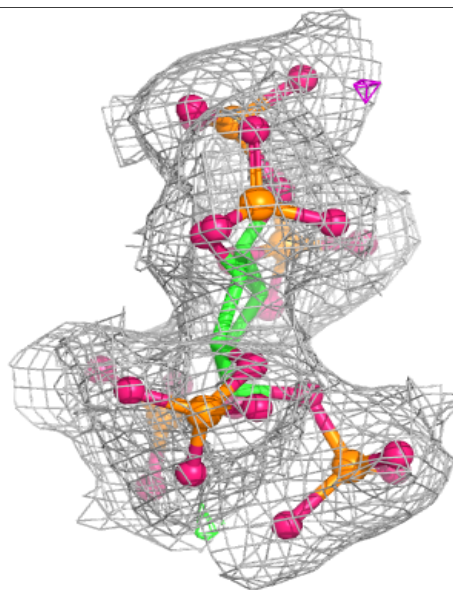
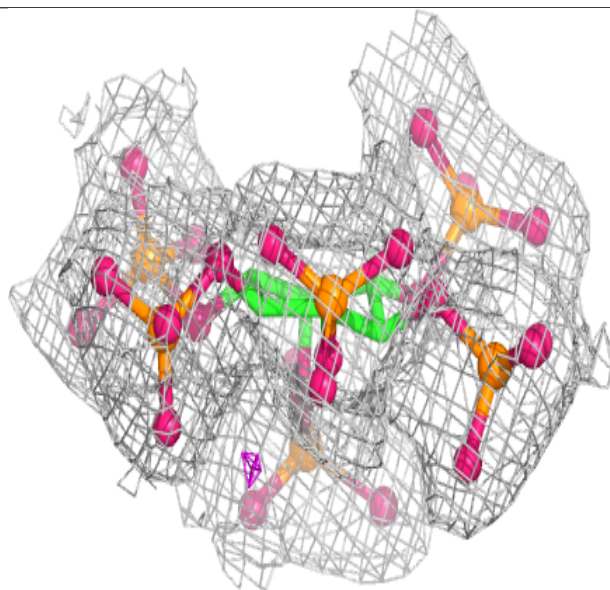
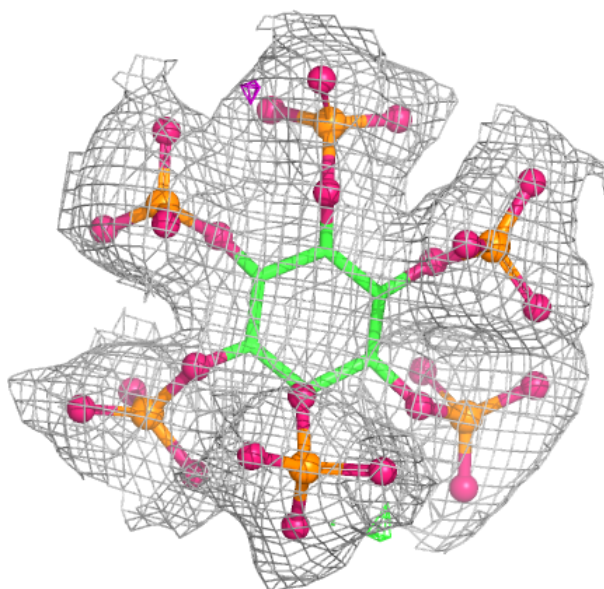
Electron density around IHP B 601:

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



Electron density around IHP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.