



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:50 PM UTC

PDB ID : 3C6N / pdb_00003c6n
Title : Small molecule agonists and antagonists of F-box protein-substrate interactions in auxin perception and signaling
Authors : Tan, X.; Zheng, N.; Hayashi, K.
Deposited on : 2008-02-04
Resolution : 2.60 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

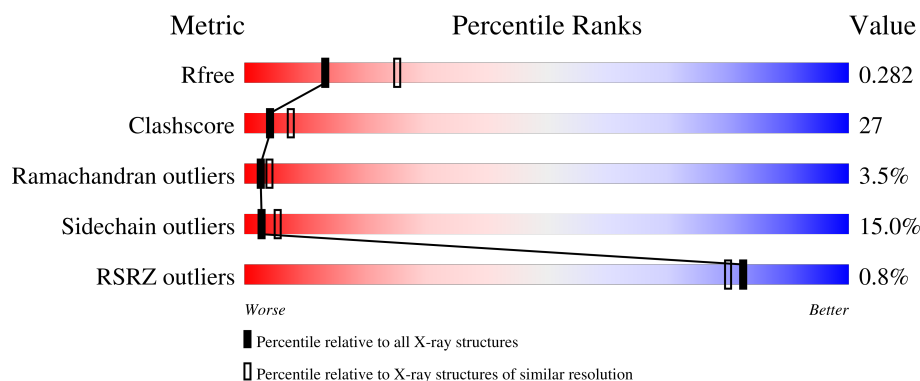
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	B	594	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5172 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.

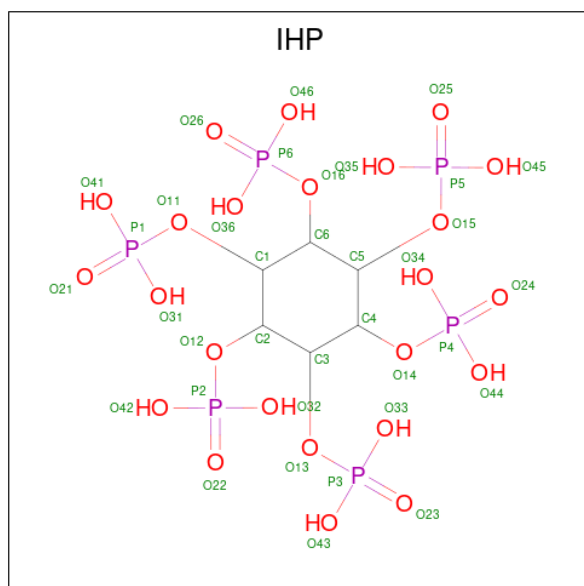
- Molecule 1 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	0	0
			471	294	79	96	2			

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

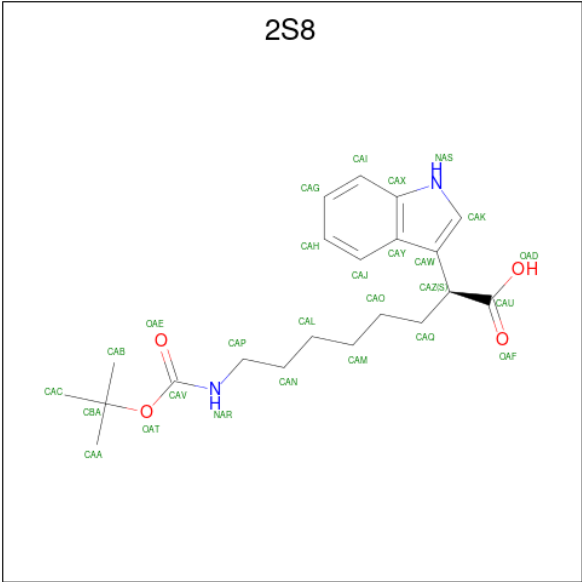
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	567	Total	C	N	O	S	0	0	0
			4461	2850	754	820	37			

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 4 is (2S)-8-[(tert-butoxycarbonyl)amino]-2-(1H-indol-3-yl)octanoic acid (CCD ID: 2S8) (formula: $C_{21}H_{30}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			27	21	2	4		

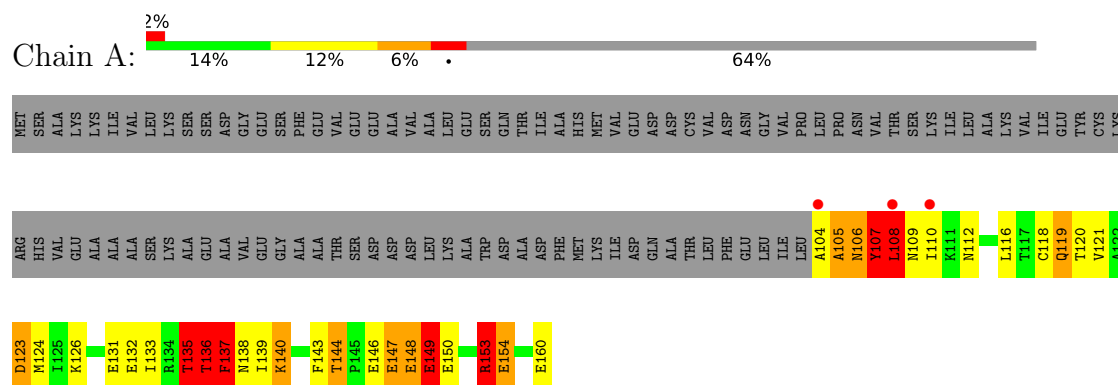
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	161	Total	O	0	0
			161	161		

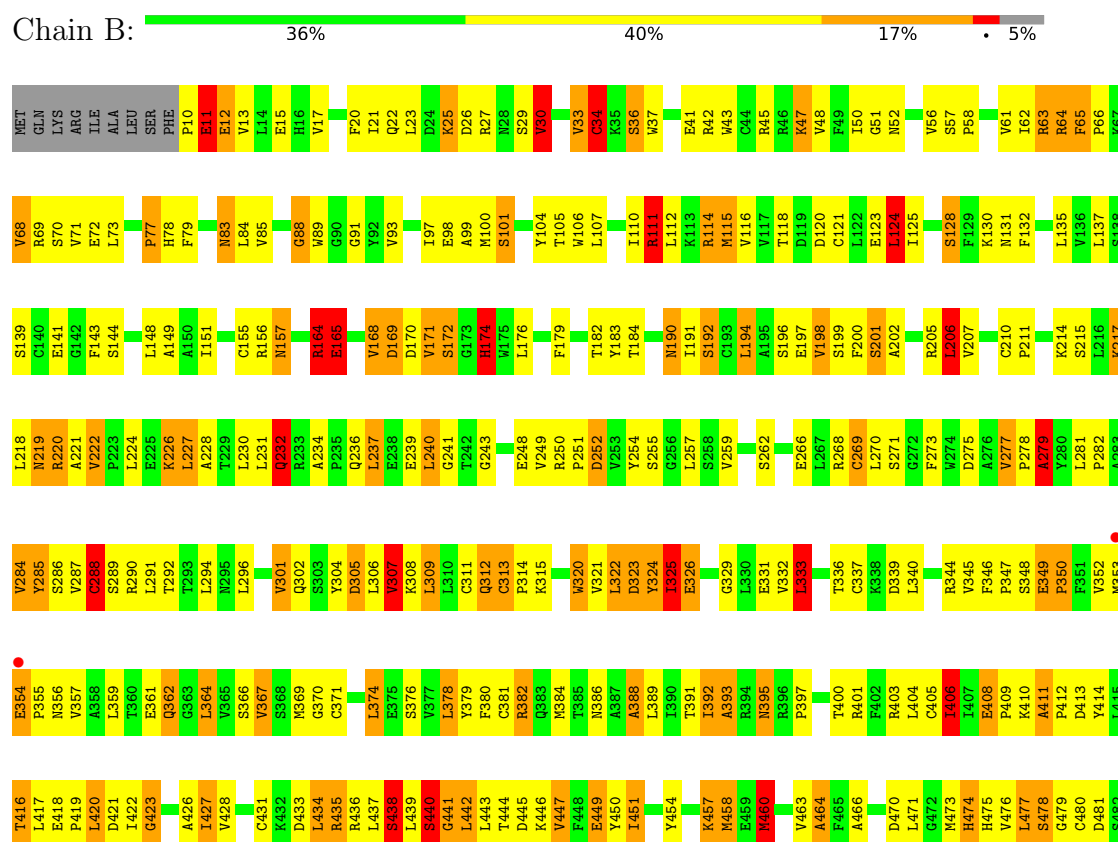
3 Residue-property plots

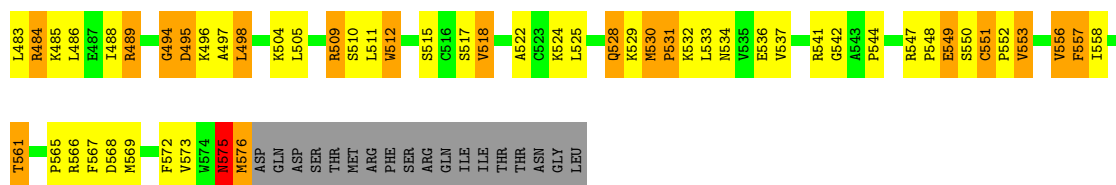
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2: TRANSPORT INHIBITOR RESPONSE 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.51Å 80.66Å 125.07Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	49.52 – 2.60 49.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.52-2.60) 91.8 (49.52-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.281 0.203 , 0.282	Depositor DCC
R_{free} test set	1440 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: 2S8, IHP

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	1.43	3/478 (0.6%)	1.60	8/646 (1.2%)
2	B	2.03	108/4558 (2.4%)	1.88	116/6178 (1.9%)
All	All	1.98	111/5036 (2.2%)	1.86	124/6824 (1.8%)

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	0	4
2	B	0	3
All	All	0	7

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	PHE	N-CA	17.98	1.59	1.46
2	B	326	GLU	N-CA	12.53	1.59	1.46
2	B	441	GLY	CA-C	10.68	1.63	1.52
2	B	553	VAL	CA-CB	-9.94	1.43	1.54
2	B	326	GLU	CA-C	-9.90	1.44	1.53
2	B	438	SER	N-CA	-9.49	1.34	1.46
2	B	476	VAL	CA-CB	9.09	1.65	1.54
2	B	65	PHE	C-O	9.04	1.28	1.23
2	B	449	GLU	C-O	8.81	1.34	1.24
2	B	376	SER	C-O	-8.66	1.14	1.24
2	B	575	ASN	CA-C	8.47	1.64	1.52
2	B	259	VAL	CA-CB	8.25	1.65	1.54
2	B	374	LEU	C-O	8.22	1.34	1.23
2	B	463	VAL	C-O	7.93	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	VAL	CA-CB	-7.62	1.44	1.53
2	B	522	ALA	CA-CB	-7.61	1.40	1.53
2	B	464	ALA	CA-CB	-7.57	1.41	1.53
2	B	420	LEU	C-O	7.54	1.34	1.24
2	B	222	VAL	N-CA	-7.46	1.40	1.46
2	B	333	LEU	N-CA	7.36	1.55	1.46
2	B	426	ALA	CA-CB	-7.26	1.42	1.53
2	B	477	LEU	N-CA	7.22	1.55	1.46
2	B	230	LEU	CA-C	-7.18	1.43	1.52
2	B	511	LEU	C-O	7.05	1.32	1.23
2	B	558	ILE	CA-CB	7.02	1.63	1.54
2	B	573	VAL	C-O	6.91	1.31	1.24
2	B	64	ARG	CZ-NH1	6.86	1.42	1.32
2	B	378	LEU	C-O	-6.73	1.16	1.23
2	B	454	TYR	N-CA	6.68	1.54	1.46
2	B	509	ARG	N-CA	-6.65	1.37	1.46
2	B	226	LYS	CA-C	-6.65	1.44	1.52
2	B	115	MET	CA-C	-6.62	1.44	1.52
2	B	29	SER	N-CA	-6.58	1.38	1.46
2	B	389	LEU	C-O	6.54	1.31	1.24
2	B	249	VAL	CA-C	6.51	1.59	1.52
2	B	404	LEU	CA-C	-6.51	1.44	1.52
2	B	52	ASN	CA-C	-6.45	1.45	1.52
2	B	573	VAL	N-CA	-6.41	1.38	1.46
2	B	405	CYS	N-CA	-6.41	1.38	1.46
2	B	494	GLY	C-O	6.40	1.29	1.24
2	B	475	HIS	N-CA	6.38	1.54	1.46
2	B	284	VAL	CA-CB	6.37	1.63	1.54
2	B	438	SER	CA-C	6.32	1.60	1.52
1	A	153	ARG	CA-C	6.28	1.60	1.52
2	B	11	GLU	N-CA	6.25	1.54	1.46
2	B	537	VAL	CA-C	-6.22	1.45	1.52
2	B	194	LEU	C-O	-6.17	1.16	1.23
2	B	434	LEU	CA-C	6.16	1.61	1.52
2	B	416	THR	CA-CB	-6.15	1.44	1.53
2	B	232	GLN	N-CA	6.05	1.53	1.46
2	B	466	ALA	CA-C	6.01	1.60	1.52
2	B	421	ASP	CA-C	6.00	1.60	1.52
2	B	240	LEU	C-O	6.00	1.30	1.23
2	B	279	ALA	CA-CB	-5.99	1.43	1.53
2	B	269	CYS	CA-C	-5.99	1.45	1.52
2	B	427	ILE	CA-CB	5.95	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	447	VAL	CA-CB	5.83	1.60	1.54
2	B	61	VAL	CA-CB	5.81	1.60	1.54
2	B	498	LEU	N-CA	-5.80	1.39	1.46
2	B	115	MET	C-O	-5.80	1.16	1.23
2	B	386	ASN	CA-CB	5.77	1.62	1.53
2	B	320	TRP	N-CA	-5.66	1.39	1.46
2	B	71	VAL	CB-CG1	-5.62	1.34	1.52
2	B	478	SER	CA-C	5.61	1.60	1.52
2	B	480	CYS	CA-C	-5.59	1.45	1.52
2	B	220	ARG	N-CA	-5.56	1.39	1.46
2	B	30	VAL	CA-CB	5.52	1.62	1.54
2	B	446	LYS	CA-C	5.49	1.59	1.52
2	B	512	TRP	CD1-NE1	5.49	1.49	1.37
2	B	50	ILE	CA-CB	-5.48	1.47	1.54
2	B	346	PHE	N-CA	-5.47	1.39	1.46
1	A	110	ILE	CA-CB	5.47	1.61	1.54
2	B	428	VAL	N-CA	5.45	1.53	1.46
2	B	307	VAL	CA-C	5.42	1.59	1.52
2	B	476	VAL	N-CA	-5.40	1.40	1.46
2	B	168	VAL	CA-CB	-5.39	1.47	1.54
2	B	288	CYS	CA-C	-5.38	1.45	1.52
2	B	405	CYS	CB-SG	5.37	1.99	1.81
2	B	304	TYR	CA-C	5.36	1.59	1.52
2	B	518	VAL	C-O	5.36	1.30	1.24
2	B	11	GLU	CA-C	5.28	1.59	1.52
2	B	556	VAL	N-CA	-5.27	1.40	1.46
2	B	77	PRO	N-CA	5.27	1.53	1.47
2	B	423	GLY	C-O	5.23	1.30	1.23
2	B	266	GLU	CA-C	5.23	1.59	1.52
2	B	169	ASP	C-O	5.21	1.29	1.24
2	B	486	LEU	CA-C	-5.21	1.46	1.52
2	B	557	PHE	CD1-CE1	5.21	1.54	1.38
2	B	406	ILE	CA-CB	-5.20	1.48	1.54
2	B	174	HIS	C-O	5.18	1.30	1.24
2	B	155	CYS	CA-C	-5.17	1.46	1.52
2	B	458	MET	N-CA	-5.17	1.39	1.46
2	B	460	MET	C-O	-5.17	1.18	1.23
2	B	112	LEU	C-O	5.15	1.30	1.24
2	B	371	CYS	CA-C	-5.14	1.47	1.52
2	B	362	GLN	C-O	-5.14	1.17	1.24
2	B	374	LEU	CA-C	5.13	1.59	1.52
2	B	388	ALA	C-O	5.11	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	292	THR	N-CA	5.11	1.52	1.46
2	B	367	VAL	CA-C	-5.11	1.46	1.52
2	B	190	ASN	CA-C	-5.08	1.47	1.53
2	B	176	LEU	CA-C	5.08	1.59	1.52
2	B	285	TYR	C-O	-5.07	1.17	1.24
2	B	406	ILE	C-O	-5.07	1.17	1.24
1	A	154	GLU	CA-C	5.05	1.59	1.52
2	B	488	ILE	CA-CB	-5.05	1.48	1.54
2	B	302	GLN	CG-CD	5.04	1.64	1.52
2	B	312	GLN	C-O	5.03	1.31	1.23
2	B	451	ILE	C-O	5.03	1.29	1.24
2	B	106	TRP	N-CA	-5.01	1.39	1.46
2	B	533	LEU	C-O	-5.00	1.17	1.23

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	243	GLY	N-CA-C	-13.26	92.77	111.20
2	B	408	GLU	CA-C-N	-12.24	107.63	120.85
2	B	408	GLU	C-N-CA	-12.24	107.63	120.85
2	B	336	THR	N-CA-C	11.28	123.55	111.03
2	B	479	GLY	N-CA-C	11.01	127.67	113.24
1	A	144	THR	CA-C-N	-9.46	109.62	120.12
1	A	144	THR	C-N-CA	-9.46	109.62	120.12
2	B	354	GLU	CA-C-N	-9.24	108.29	119.84
2	B	354	GLU	C-N-CA	-9.24	108.29	119.84
2	B	64	ARG	N-CA-C	-9.23	98.75	110.19
2	B	486	LEU	N-CA-C	-9.17	93.47	109.06
2	B	354	GLU	CB-CA-C	-8.97	101.18	110.33
2	B	325	ILE	CA-C-N	-8.88	106.34	120.81
2	B	325	ILE	C-N-CA	-8.88	106.34	120.81
2	B	532	LYS	N-CA-C	8.87	121.90	111.71
2	B	531	PRO	CA-C-N	8.58	132.63	120.28
2	B	531	PRO	C-N-CA	8.58	132.63	120.28
2	B	250	ARG	CA-C-N	-8.49	111.39	120.47
2	B	250	ARG	C-N-CA	-8.49	111.39	120.47
2	B	551	CYS	CA-C-N	8.25	128.74	119.83
2	B	551	CYS	C-N-CA	8.25	128.74	119.83
2	B	51	GLY	N-CA-C	8.17	123.47	114.40
2	B	553	VAL	CB-CA-C	-8.08	102.40	111.45
2	B	569	MET	CA-C-N	-7.99	109.85	119.84
2	B	569	MET	C-N-CA	-7.99	109.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	ALA	CA-C-N	7.99	129.37	120.66
2	B	411	ALA	C-N-CA	7.99	129.37	120.66
1	A	110	ILE	CB-CA-C	7.79	124.06	111.29
2	B	234	ALA	CA-C-N	-7.65	111.92	119.87
2	B	234	ALA	C-N-CA	-7.65	111.92	119.87
2	B	537	VAL	N-CA-C	-7.54	97.61	108.17
2	B	528	GLN	CA-C-N	-7.38	109.65	120.28
2	B	528	GLN	C-N-CA	-7.38	109.65	120.28
2	B	475	HIS	CA-C-N	-7.30	111.97	120.88
2	B	475	HIS	C-N-CA	-7.30	111.97	120.88
2	B	277	VAL	CA-C-N	-7.28	111.67	119.24
2	B	277	VAL	C-N-CA	-7.28	111.67	119.24
2	B	313	CYS	CA-C-N	-7.26	112.70	119.82
2	B	313	CYS	C-N-CA	-7.26	112.70	119.82
2	B	222	VAL	N-CA-C	-7.16	100.46	107.55
2	B	418	GLU	CA-C-N	-7.03	111.06	119.84
2	B	418	GLU	C-N-CA	-7.03	111.06	119.84
2	B	289	SER	N-CA-C	-7.03	104.36	114.12
2	B	567	PHE	N-CA-C	7.02	121.59	112.89
2	B	481	ASP	N-CA-C	7.01	119.78	111.71
2	B	427	ILE	CB-CA-C	-7.01	102.73	111.70
2	B	515	SER	N-CA-C	6.87	120.97	111.90
2	B	323	ASP	N-CA-C	-6.87	105.18	113.97
2	B	325	ILE	O-C-N	-6.79	114.08	122.57
1	A	107	TYR	N-CA-C	-6.63	96.68	110.80
2	B	349	GLU	CB-CA-C	6.61	118.78	110.98
2	B	504	LYS	N-CA-C	-6.61	104.08	111.28
1	A	150	GLU	N-CA-C	-6.55	103.98	112.23
2	B	575	ASN	N-CA-C	6.46	124.55	110.80
2	B	115	MET	CA-CB-CG	-6.42	101.26	114.10
2	B	206	LEU	N-CA-C	6.41	118.83	111.02
1	A	108	LEU	N-CA-C	-6.40	106.06	114.31
2	B	512	TRP	N-CA-C	-6.39	98.20	109.06
2	B	98	GLU	N-CA-C	6.38	118.77	111.11
2	B	395	ASN	N-CA-C	6.28	119.11	111.82
2	B	435	ARG	NE-CZ-NH2	-6.24	113.59	119.20
2	B	476	VAL	N-CA-CB	6.10	117.96	110.64
2	B	350	PRO	N-CA-C	6.04	121.49	113.57
2	B	219	ASN	N-CA-C	6.01	119.42	110.52
2	B	52	ASN	CB-CA-C	-5.86	103.44	110.94
2	B	306	LEU	N-CA-C	-5.85	104.98	111.36
2	B	47	LYS	N-CA-C	5.83	118.90	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	VAL	CA-C-N	-5.83	114.75	120.52
2	B	85	VAL	C-N-CA	-5.83	114.75	120.52
2	B	315	LYS	CA-C-N	5.83	129.38	121.05
2	B	315	LYS	C-N-CA	5.83	129.38	121.05
2	B	386	ASN	N-CA-C	-5.82	104.89	112.23
2	B	442	LEU	CB-CA-C	-5.74	102.74	109.80
2	B	151	ILE	CB-CA-C	-5.70	104.67	111.97
2	B	64	ARG	CA-C-O	-5.67	116.05	122.01
2	B	232	GLN	N-CA-CB	5.67	118.94	110.22
2	B	457	LYS	CA-C-N	-5.65	112.69	120.71
2	B	457	LYS	C-N-CA	-5.65	112.69	120.71
2	B	458	MET	CB-CG-SD	-5.63	95.80	112.70
2	B	132	PHE	N-CA-C	5.62	118.39	109.96
2	B	73	LEU	N-CA-C	5.59	118.21	108.76
2	B	111	ARG	CA-CB-CG	5.58	125.26	114.10
2	B	192	SER	CA-C-N	-5.53	112.70	122.26
2	B	192	SER	C-N-CA	-5.53	112.70	122.26
2	B	445	ASP	N-CA-C	-5.51	105.66	112.38
2	B	321	VAL	CA-C-O	-5.49	115.03	120.90
2	B	65	PHE	CA-C-N	-5.45	114.64	120.47
2	B	65	PHE	C-N-CA	-5.45	114.64	120.47
2	B	458	MET	CA-CB-CG	-5.44	103.22	114.10
2	B	400	THR	CB-CA-C	-5.43	99.90	109.02
2	B	572	PHE	N-CA-C	-5.43	105.97	112.59
2	B	191	ILE	CB-CA-C	-5.36	105.01	112.36
2	B	70	SER	CA-C-N	-5.35	115.39	122.98
2	B	70	SER	C-N-CA	-5.35	115.39	122.98
2	B	305	ASP	CA-C-N	-5.34	112.71	120.29
2	B	305	ASP	C-N-CA	-5.34	112.71	120.29
2	B	401	ARG	NE-CZ-NH1	-5.34	116.16	121.50
2	B	440	SER	CB-CA-C	-5.28	101.36	112.82
1	A	153	ARG	CB-CA-C	5.28	119.16	110.88
2	B	435	ARG	CA-C-O	5.26	125.58	119.32
1	A	149	GLU	N-CA-C	-5.23	108.16	114.75
2	B	382	ARG	CB-CA-C	-5.18	101.96	110.72
2	B	393	ALA	N-CA-C	-5.16	105.34	111.69
2	B	446	LYS	N-CA-C	5.16	116.90	111.28
2	B	361	GLU	N-CA-C	-5.13	106.87	113.23
2	B	286	SER	CA-C-N	5.13	127.48	120.46
2	B	286	SER	C-N-CA	5.13	127.48	120.46
2	B	576	MET	CB-CA-C	5.12	119.84	110.10
2	B	474	HIS	CA-C-N	-5.08	112.46	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	474	HIS	C-N-CA	-5.08	112.46	120.63
2	B	88	GLY	N-CA-C	-5.08	107.97	114.37
2	B	440	SER	N-CA-CB	5.07	119.11	111.35
2	B	326	GLU	CA-C-N	-5.06	113.71	120.54
2	B	326	GLU	C-N-CA	-5.06	113.71	120.54
2	B	542	GLY	N-CA-C	-5.05	105.23	111.70
2	B	370	GLY	CA-C-N	-5.04	116.04	123.30
2	B	370	GLY	C-N-CA	-5.04	116.04	123.30
2	B	48	VAL	N-CA-C	5.04	115.84	108.53
2	B	427	ILE	N-CA-CB	5.04	115.91	110.62
2	B	346	PHE	CA-C-N	-5.04	115.17	120.66
2	B	346	PHE	C-N-CA	-5.04	115.17	120.66
2	B	124	LEU	N-CA-C	-5.03	105.50	111.69
2	B	275	ASP	CB-CA-C	-5.01	103.79	111.66
2	B	207	VAL	CB-CA-C	-5.00	104.74	112.05

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Peptide
1	A	106	ASN	Peptide
1	A	107	TYR	Peptide
1	A	108	LEU	Peptide
2	B	164	ARG	Peptide
2	B	217	LYS	Peptide
2	B	575	ASN	Peptide

5.2 Too-close contacts [i](#)

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	471	0	453	29	0
2	B	4461	0	4504	244	0
3	B	36	0	6	3	0
4	B	27	0	29	4	0
5	A	16	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	161	0	0	24	0
All	All	5172	0	4992	272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (272) 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:352:VAL:CG1	2:B:354:GLU:HG2	1.66	1.24
2:B:232:GLN:HG3	5:B:1035:HOH:O	1.40	1.18
3:B:1000:IHP:O23	5:B:1096:HOH:O	1.67	1.12
2:B:63:ARG:HD2	5:B:1030:HOH:O	1.54	1.06
1:A:148:GLU:O	1:A:148:GLU:HG3	1.52	1.05
2:B:111:ARG:CG	2:B:111:ARG:HH11	1.70	1.04
2:B:352:VAL:HG12	2:B:354:GLU:HG2	1.05	1.03
2:B:352:VAL:HG12	2:B:354:GLU:CG	1.92	0.99
2:B:111:ARG:HH11	2:B:111:ARG:HG2	1.25	0.98
2:B:239:GLU:HB2	2:B:269:CYS:HB2	1.43	0.97
2:B:484:ARG:HG2	5:B:1069:HOH:O	1.67	0.94
1:A:132:GLU:O	1:A:136:THR:HG23	1.66	0.93
2:B:352:VAL:CG1	2:B:354:GLU:CG	2.47	0.92
2:B:352:VAL:O	2:B:382:ARG:NH2	2.02	0.92
1:A:148:GLU:O	1:A:148:GLU:CG	2.15	0.91
2:B:408:GLU:HB2	5:B:1049:HOH:O	1.71	0.91
2:B:287:VAL:HG12	2:B:291:LEU:HD13	1.53	0.89
2:B:30:VAL:O	2:B:33:VAL:CG1	2.22	0.86
2:B:354:GLU:O	2:B:355:PRO:C	2.19	0.85
1:A:140:LYS:HE3	1:A:140:LYS:HA	1.56	0.85
2:B:171:VAL:O	2:B:172:SER:HB3	1.77	0.83
2:B:422:ILE:HG12	5:B:1068:HOH:O	1.76	0.83
2:B:170:ASP:OD1	2:B:196:SER:HB3	1.80	0.82
2:B:352:VAL:HA	5:B:1151:HOH:O	1.79	0.81
2:B:403:ARG:NE	4:B:1001:2S8:OAF	2.12	0.81
2:B:309:LEU:HD23	2:B:309:LEU:O	1.80	0.80
1:A:135:THR:HG22	1:A:136:THR:N	1.97	0.78
2:B:110:ILE:HD12	2:B:125:ILE:HD13	1.66	0.78
1:A:107:TYR:HE2	5:A:174:HOH:O	1.65	0.78
2:B:111:ARG:CG	2:B:111:ARG:NH1	2.43	0.76
2:B:79:PHE:CE2	2:B:489:ARG:HG2	2.21	0.76
2:B:324:TYR:C	2:B:325:ILE:O	2.27	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:ASN:C	2:B:575:ASN:HD22	1.96	0.73
2:B:79:PHE:HE2	2:B:489:ARG:CG	2.02	0.73
1:A:144:THR:N	1:A:147:GLU:OE2	2.22	0.72
2:B:201:SER:HB2	2:B:205:ARG:HH21	1.56	0.70
2:B:33:VAL:O	2:B:33:VAL:CG2	2.40	0.70
1:A:140:LYS:HA	1:A:140:LYS:CE	2.20	0.69
2:B:239:GLU:CB	2:B:269:CYS:HB2	2.19	0.69
2:B:77:PRO:HB2	5:B:1014:HOH:O	1.92	0.69
2:B:62:ILE:CD1	2:B:99:ALA:HB1	2.23	0.69
2:B:439:LEU:O	4:B:1001:2S8:HAI	1.91	0.69
2:B:496:LYS:HE3	5:B:1050:HOH:O	1.91	0.69
2:B:79:PHE:CE2	2:B:489:ARG:CG	2.75	0.69
2:B:22:GLN:O	2:B:47:LYS:NZ	2.25	0.68
2:B:352:VAL:HG13	2:B:354:GLU:HG2	1.71	0.68
2:B:30:VAL:O	2:B:33:VAL:HG13	1.92	0.68
2:B:403:ARG:HG2	2:B:438:SER:HB3	1.76	0.67
1:A:104:ALA:HA	5:A:171:HOH:O	1.95	0.67
2:B:174:HIS:HB2	5:B:1141:HOH:O	1.94	0.67
2:B:408:GLU:HB3	2:B:411:ALA:HB2	1.77	0.66
2:B:12:GLU:OE2	2:B:12:GLU:HA	1.96	0.66
2:B:231:LEU:HD21	2:B:240:LEU:HD22	1.78	0.66
2:B:144:SER:HB3	2:B:169:ASP:HB3	1.77	0.65
1:A:135:THR:O	1:A:137:PHE:N	2.30	0.64
2:B:118:THR:O	2:B:121:CYS:HB2	1.97	0.64
2:B:548:PRO:O	2:B:550:SER:N	2.30	0.64
1:A:138:ASN:ND2	1:A:138:ASN:O	2.30	0.64
2:B:322:LEU:O	2:B:325:ILE:HG22	1.97	0.64
2:B:97:ILE:HG22	2:B:124:LEU:HD13	1.79	0.64
2:B:104:TYR:HA	5:B:1073:HOH:O	1.97	0.64
2:B:156:ARG:HG3	2:B:157:ASN:OD1	1.98	0.63
2:B:97:ILE:O	2:B:101:SER:HB3	1.97	0.63
2:B:268:ARG:NH1	2:B:290:ARG:HD3	2.15	0.62
2:B:121:CYS:O	2:B:125:ILE:HG13	2.00	0.62
2:B:435:ARG:HD2	5:B:1023:HOH:O	1.99	0.62
2:B:287:VAL:HA	2:B:290:ARG:NH2	2.14	0.62
2:B:30:VAL:O	2:B:33:VAL:HG12	1.98	0.62
1:A:105:ALA:HB2	5:A:173:HOH:O	2.00	0.62
2:B:27:ARG:HB3	2:B:45:ARG:NH2	2.16	0.61
2:B:63:ARG:C	2:B:64:ARG:O	2.41	0.61
2:B:11:GLU:OE1	2:B:11:GLU:N	2.34	0.60
2:B:544:PRO:HA	2:B:547:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLU:O	2:B:356:ASN:N	2.35	0.60
2:B:282:PRO:HB3	2:B:285:TYR:CE2	2.36	0.60
2:B:217:LYS:HE2	2:B:239:GLU:OE1	2.02	0.60
2:B:104:TYR:C	5:B:1073:HOH:O	2.44	0.60
2:B:100:MET:HG2	2:B:104:TYR:CD1	2.36	0.60
2:B:324:TYR:O	2:B:325:ILE:O	2.20	0.60
1:A:120:THR:HA	1:A:123:ASP:HB2	1.82	0.60
2:B:287:VAL:CG1	2:B:291:LEU:HD13	2.29	0.59
1:A:136:THR:O	1:A:137:PHE:HD2	1.85	0.59
2:B:57:SER:O	2:B:58:PRO:C	2.46	0.59
2:B:26:ASP:O	2:B:30:VAL:HG13	2.03	0.59
2:B:566:ARG:NH1	2:B:568:ASP:OD1	2.33	0.58
2:B:524:LYS:HE2	2:B:549:GLU:OE2	2.03	0.58
2:B:174:HIS:C	2:B:174:HIS:CD2	2.82	0.58
2:B:575:ASN:C	2:B:575:ASN:ND2	2.62	0.58
2:B:416:THR:O	2:B:417:LEU:HB2	2.04	0.58
2:B:10:PRO:C	2:B:11:GLU:OE1	2.47	0.57
2:B:83:ASN:HA	5:B:1051:HOH:O	2.04	0.57
2:B:33:VAL:O	2:B:33:VAL:HG23	2.03	0.57
2:B:512:TRP:CD1	2:B:512:TRP:C	2.83	0.57
2:B:281:LEU:O	2:B:284:VAL:HG22	2.04	0.57
2:B:323:ASP:O	2:B:325:ILE:O	2.21	0.57
1:A:104:ALA:CA	5:A:171:HOH:O	2.53	0.57
2:B:144:SER:CB	2:B:169:ASP:HB3	2.35	0.56
2:B:433:ASP:O	2:B:434:LEU:C	2.48	0.56
2:B:79:PHE:HE2	2:B:489:ARG:HG3	1.68	0.56
2:B:496:LYS:CE	5:B:1050:HOH:O	2.51	0.56
2:B:414:TYR:HB2	5:B:1081:HOH:O	2.05	0.56
2:B:464:ALA:HB2	2:B:489:ARG:HD2	1.87	0.56
2:B:268:ARG:NH1	2:B:290:ARG:CD	2.68	0.56
2:B:294:LEU:HD21	2:B:296:LEU:HD11	1.87	0.56
2:B:79:PHE:HE2	2:B:489:ARG:HG2	1.64	0.56
2:B:312:GLN:CD	5:B:1079:HOH:O	2.48	0.56
2:B:174:HIS:CG	5:B:1066:HOH:O	2.59	0.55
2:B:174:HIS:CG	5:B:1141:HOH:O	2.59	0.55
2:B:534:ASN:ND2	2:B:561:THR:HG21	2.21	0.55
2:B:33:VAL:O	2:B:34:CYS:CB	2.54	0.55
2:B:174:HIS:HD2	2:B:174:HIS:O	1.88	0.55
2:B:254:TYR:C	2:B:254:TYR:CD2	2.85	0.55
2:B:135:LEU:HD11	2:B:137:LEU:HD21	1.88	0.55
2:B:309:LEU:HD23	2:B:309:LEU:C	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:VAL:HG12	2:B:116:VAL:O	2.07	0.55
2:B:565:PRO:HB3	2:B:575:ASN:OD1	2.07	0.55
2:B:324:TYR:O	2:B:325:ILE:C	2.50	0.54
2:B:201:SER:HB2	2:B:205:ARG:NH2	2.21	0.54
2:B:325:ILE:HG13	2:B:329:GLY:HA3	1.90	0.54
2:B:325:ILE:O	2:B:326:GLU:CG	2.56	0.54
1:A:139:ILE:HG21	2:B:34:CYS:HB2	1.90	0.54
2:B:104:TYR:CA	5:B:1073:HOH:O	2.53	0.53
1:A:136:THR:O	1:A:137:PHE:CD2	2.62	0.53
2:B:518:VAL:O	2:B:552:PRO:HA	2.09	0.53
2:B:268:ARG:HH12	2:B:290:ARG:HD3	1.72	0.53
2:B:536:GLU:O	2:B:556:VAL:HA	2.09	0.53
2:B:344:ARG:HG2	2:B:378:LEU:HB3	1.90	0.53
2:B:412:PRO:O	2:B:413:ASP:C	2.52	0.52
2:B:285:TYR:HA	2:B:288:CYS:SG	2.49	0.52
2:B:393:ALA:HB2	2:B:427:ILE:HD13	1.91	0.52
2:B:41:GLU:O	2:B:42:ARG:C	2.48	0.52
2:B:218:LEU:HD13	2:B:222:VAL:HG11	1.92	0.52
2:B:434:LEU:HD21	2:B:437:LEU:HB2	1.92	0.51
2:B:444:THR:HG22	5:B:1109:HOH:O	2.09	0.51
2:B:284:VAL:O	2:B:287:VAL:HB	2.10	0.51
2:B:324:TYR:O	2:B:326:GLU:HG3	2.10	0.51
2:B:79:PHE:CE2	2:B:489:ARG:HG3	2.42	0.51
2:B:174:HIS:CB	5:B:1141:HOH:O	2.55	0.51
2:B:347:PRO:HG3	2:B:380:PHE:CD2	2.46	0.51
2:B:436:ARG:HG3	2:B:437:LEU:N	2.24	0.51
2:B:344:ARG:HD3	2:B:378:LEU:HD23	1.93	0.51
1:A:149:GLU:OE2	1:A:153:ARG:NH2	2.45	0.50
2:B:419:PRO:HB3	2:B:442:LEU:HG	1.93	0.50
3:B:1000:IHP:O25	3:B:1000:IHP:O16	2.30	0.50
2:B:43:TRP:CZ3	2:B:66:PRO:HG2	2.47	0.50
2:B:174:HIS:CD2	5:B:1066:HOH:O	2.64	0.50
2:B:510:SER:HB2	2:B:557:PHE:CE1	2.47	0.50
2:B:252:ASP:OD2	2:B:252:ASP:N	2.45	0.50
2:B:282:PRO:HA	2:B:285:TYR:CZ	2.47	0.50
2:B:42:ARG:HB2	2:B:65:PHE:H	1.75	0.49
2:B:505:LEU:N	2:B:505:LEU:HD23	2.27	0.49
2:B:34:CYS:SG	2:B:36:SER:N	2.85	0.49
2:B:79:PHE:CD2	2:B:84:LEU:HD12	2.48	0.49
2:B:309:LEU:C	2:B:309:LEU:CD2	2.85	0.49
1:A:143:PHE:HB3	1:A:148:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LEU:O	2:B:224:LEU:HD12	2.11	0.49
2:B:447:VAL:O	2:B:450:TYR:HB2	2.11	0.49
1:A:121:VAL:O	1:A:124:MET:CB	2.60	0.49
2:B:197:GLU:HG3	2:B:221:ALA:HB1	1.94	0.49
2:B:323:ASP:OD1	2:B:348:SER:HB3	2.11	0.49
2:B:288:CYS:O	2:B:313:CYS:HA	2.13	0.49
2:B:333:LEU:HD21	2:B:340:LEU:HD22	1.94	0.48
2:B:34:CYS:HG	2:B:37:TRP:CD1	2.31	0.48
2:B:111:ARG:NH1	2:B:111:ARG:HG3	2.26	0.48
2:B:190:ASN:HA	2:B:217:LYS:HB2	1.94	0.48
2:B:111:ARG:HH11	2:B:111:ARG:HG3	1.70	0.48
2:B:528:GLN:O	2:B:529:LYS:C	2.53	0.48
1:A:119:GLN:HG2	2:B:20:PHE:CD2	2.48	0.48
1:A:147:GLU:C	1:A:149:GLU:H	2.22	0.48
2:B:88:GLY:O	2:B:89:TRP:C	2.54	0.48
2:B:450:TYR:O	2:B:451:ILE:C	2.56	0.48
1:A:133:ILE:O	1:A:137:PHE:HB2	2.14	0.47
2:B:33:VAL:O	2:B:34:CYS:HB3	2.13	0.47
2:B:62:ILE:HD12	2:B:99:ALA:HB1	1.96	0.47
2:B:356:ASN:OD1	2:B:357:VAL:HG13	2.14	0.47
2:B:460:MET:CE	2:B:485:LYS:HZ2	2.28	0.47
1:A:136:THR:O	1:A:136:THR:OG1	2.30	0.47
2:B:222:VAL:O	2:B:222:VAL:HG12	2.15	0.46
2:B:384:MET:HB2	2:B:406:ILE:CD1	2.46	0.46
2:B:457:LYS:O	2:B:458:MET:C	2.55	0.46
1:A:118:CYS:HB2	2:B:20:PHE:CE1	2.51	0.46
2:B:494:GLY:CA	2:B:517:SER:O	2.64	0.46
4:B:1001:2S8:OAE	4:B:1001:2S8:CAB	2.62	0.46
1:A:118:CYS:HB2	2:B:20:PHE:HE1	1.79	0.46
1:A:160:GLU:CD	2:B:25:LYS:HD2	2.41	0.45
2:B:194:LEU:HA	2:B:194:LEU:HD23	1.63	0.45
2:B:199:SER:OG	2:B:202:ALA:HB3	2.16	0.45
2:B:441:GLY:O	2:B:443:LEU:HG	2.16	0.45
2:B:228:ALA:O	2:B:232:GLN:HG2	2.16	0.45
2:B:91:GLY:O	2:B:115:MET:HE2	2.17	0.45
2:B:277:VAL:HG12	2:B:279:ALA:HB3	1.98	0.45
2:B:287:VAL:O	2:B:290:ARG:HG2	2.16	0.45
2:B:337:CYS:C	2:B:339:ASP:H	2.25	0.45
2:B:388:ALA:C	2:B:392:ILE:HD12	2.42	0.45
2:B:413:ASP:C	2:B:413:ASP:OD1	2.59	0.45
1:A:107:TYR:CE2	5:A:174:HOH:O	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ARG:O	2:B:107:LEU:HD12	2.17	0.45
2:B:210:CYS:HA	2:B:211:PRO:HD2	1.84	0.44
2:B:326:GLU:H	2:B:329:GLY:HA3	1.81	0.44
2:B:420:LEU:HD12	2:B:441:GLY:HA3	2.00	0.44
2:B:301:VAL:HG13	2:B:305:ASP:HB2	1.99	0.44
2:B:434:LEU:HA	2:B:434:LEU:HD12	1.71	0.44
2:B:333:LEU:HD21	2:B:340:LEU:CD2	2.47	0.44
2:B:202:ALA:O	2:B:206:LEU:HB2	2.18	0.44
2:B:251:PRO:O	2:B:255:SER:HB3	2.17	0.44
2:B:277:VAL:O	2:B:278:PRO:C	2.55	0.44
2:B:353:MET:H	2:B:353:MET:HG2	1.55	0.44
2:B:124:LEU:O	2:B:128:SER:OG	2.32	0.44
2:B:174:HIS:CD2	2:B:174:HIS:O	2.69	0.44
2:B:219:ASN:O	2:B:220:ARG:C	2.60	0.44
2:B:270:LEU:HD22	2:B:273:PHE:CZ	2.52	0.44
2:B:495:ASP:N	2:B:495:ASP:OD1	2.49	0.44
2:B:33:VAL:O	2:B:33:VAL:HG22	2.17	0.44
2:B:56:VAL:HG22	2:B:57:SER:N	2.33	0.43
2:B:179:PHE:CD2	2:B:183:TYR:CD2	3.05	0.43
2:B:198:VAL:CG1	2:B:199:SER:N	2.81	0.43
2:B:198:VAL:HG13	2:B:199:SER:N	2.33	0.43
2:B:494:GLY:HA2	2:B:517:SER:O	2.19	0.43
2:B:325:ILE:O	2:B:326:GLU:HG3	2.19	0.43
2:B:347:PRO:HB2	2:B:350:PRO:HG3	1.99	0.43
2:B:366:SER:O	2:B:367:VAL:C	2.60	0.43
2:B:68:VAL:HB	2:B:104:TYR:CZ	2.53	0.43
2:B:236:GLN:O	2:B:237:LEU:C	2.61	0.43
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.57	0.43
2:B:307:VAL:HG22	2:B:332:VAL:HG11	2.01	0.43
2:B:410:LYS:O	2:B:442:LEU:HB2	2.18	0.43
2:B:440:SER:HB2	2:B:441:GLY:H	1.50	0.43
2:B:320:TRP:CD1	2:B:320:TRP:N	2.85	0.43
2:B:72:GLU:HG3	2:B:111:ARG:HB2	2.01	0.42
2:B:470:ASP:OD1	2:B:494:GLY:N	2.47	0.42
2:B:114:ARG:HA	2:B:139:SER:O	2.20	0.42
2:B:380:PHE:CD1	2:B:380:PHE:N	2.87	0.42
2:B:530:MET:O	2:B:531:PRO:C	2.62	0.42
2:B:190:ASN:CG	2:B:217:LYS:HD2	2.45	0.42
1:A:131:GLU:O	1:A:132:GLU:C	2.63	0.42
2:B:100:MET:HG2	2:B:104:TYR:HD1	1.82	0.42
2:B:471:LEU:HD23	2:B:471:LEU:HA	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:LYS:HE3	2:B:308:LYS:HB2	1.86	0.41
2:B:313:CYS:O	2:B:314:PRO:C	2.61	0.41
2:B:498:LEU:HA	2:B:498:LEU:HD12	1.66	0.41
2:B:200:PHE:CE2	2:B:226:LYS:HD2	2.55	0.41
2:B:474:HIS:O	2:B:478:SER:CB	2.68	0.41
2:B:148:LEU:O	2:B:149:ALA:C	2.63	0.41
2:B:359:LEU:HD21	2:B:379:TYR:CZ	2.55	0.41
2:B:409:PRO:C	2:B:411:ALA:H	2.28	0.41
2:B:470:ASP:HB3	2:B:497:ALA:HB2	2.02	0.41
2:B:473:MET:HE2	2:B:477:LEU:HD11	2.02	0.41
2:B:224:LEU:HD12	2:B:224:LEU:C	2.44	0.41
2:B:241:GLY:HA2	2:B:271:SER:O	2.21	0.41
2:B:391:THR:O	2:B:392:ILE:C	2.64	0.41
2:B:460:MET:CE	2:B:485:LYS:NZ	2.84	0.41
2:B:551:CYS:HA	2:B:552:PRO:HD3	1.80	0.41
2:B:395:ASN:C	2:B:397:PRO:HD2	2.45	0.41
2:B:438:SER:OG	4:B:1001:2S8:CAK	2.69	0.41
2:B:509:ARG:O	2:B:509:ARG:HG2	2.20	0.41
2:B:553:VAL:O	5:B:1147:HOH:O	2.21	0.41
2:B:143:PHE:CE1	2:B:168:VAL:HG22	2.56	0.41
2:B:164:ARG:C	2:B:165:GLU:CG	2.93	0.41
2:B:356:ASN:CG	2:B:357:VAL:HG13	2.46	0.41
2:B:364:LEU:HD23	2:B:364:LEU:HA	1.84	0.41
2:B:431:CYS:C	2:B:433:ASP:N	2.79	0.41
2:B:510:SER:HB2	2:B:557:PHE:HE1	1.85	0.41
2:B:179:PHE:CD2	2:B:183:TYR:CE2	3.08	0.41
2:B:548:PRO:O	2:B:549:GLU:C	2.64	0.41
3:B:1000:IHP:O33	3:B:1000:IHP:O44	2.38	0.41
2:B:224:LEU:O	2:B:227:LEU:HB2	2.22	0.40
2:B:13:VAL:O	2:B:17:VAL:HG23	2.20	0.40
2:B:164:ARG:C	2:B:165:GLU:HG2	2.46	0.40
2:B:215:SER:OG	2:B:239:GLU:HG2	2.21	0.40
2:B:464:ALA:HA	2:B:489:ARG:O	2.21	0.40
2:B:78:HIS:CD2	2:B:78:HIS:C	3.00	0.40
2:B:215:SER:OG	2:B:239:GLU:CG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	55/160 (34%)	42 (76%)	6 (11%)	7 (13%)	0	0
2	B	565/594 (95%)	483 (86%)	67 (12%)	15 (3%)	4	7
All	All	620/754 (82%)	525 (85%)	73 (12%)	22 (4%)	3	4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	109	ASN
1	A	137	PHE
2	B	34	CYS
2	B	549	GLU
1	A	135	THR
1	A	136	THR
2	B	172	SER
2	B	279	ALA
2	B	325	ILE
2	B	423	GLY
1	A	107	TYR
1	A	148	GLU
2	B	288	CYS
2	B	324	TYR
2	B	11	GLU
2	B	101	SER
2	B	311	CYS
2	B	114	ARG
2	B	131	ASN
2	B	165	GLU
2	B	322	LEU

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	52/137 (38%)	36 (69%)	16 (31%)	0	0
2	B	500/525 (95%)	433 (87%)	67 (13%)	4	7
All	All	552/662 (83%)	469 (85%)	83 (15%)	3	5

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	TYR
1	A	108	LEU
1	A	112	ASN
1	A	116	LEU
1	A	119	GLN
1	A	123	ASP
1	A	126	LYS
1	A	135	THR
1	A	136	THR
1	A	137	PHE
1	A	140	LYS
1	A	146	GLU
1	A	147	GLU
1	A	149	GLU
1	A	153	ARG
1	A	154	GLU
2	B	11	GLU
2	B	12	GLU
2	B	15	GLU
2	B	21	ILE
2	B	23	LEU
2	B	25	LYS
2	B	30	VAL
2	B	33	VAL
2	B	34	CYS
2	B	36	SER
2	B	63	ARG

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Mol	Chain	Res	Type
2	B	68	VAL
2	B	83	ASN
2	B	105	THR
2	B	111	ARG
2	B	120	ASP
2	B	123	GLU
2	B	124	LEU
2	B	128	SER
2	B	130	LYS
2	B	141	GLU
2	B	157	ASN
2	B	164	ARG
2	B	165	GLU
2	B	171	VAL
2	B	174	HIS
2	B	182	THR
2	B	184	THR
2	B	192	SER
2	B	198	VAL
2	B	201	SER
2	B	206	LEU
2	B	214	LYS
2	B	227	LEU
2	B	232	GLN
2	B	237	LEU
2	B	248	GLU
2	B	252	ASP
2	B	257	LEU
2	B	262	SER
2	B	301	VAL
2	B	307	VAL
2	B	309	LEU
2	B	325	ILE
2	B	331	GLU
2	B	333	LEU
2	B	349	GLU
2	B	362	GLN
2	B	364	LEU
2	B	369	MET
2	B	374	LEU
2	B	381	CYS
2	B	392	ILE

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Mol	Chain	Res	Type
2	B	406	ILE
2	B	438	SER
2	B	440	SER
2	B	449	GLU
2	B	460	MET
2	B	483	LEU
2	B	484	ARG
2	B	489	ARG
2	B	495	ASP
2	B	525	LEU
2	B	530	MET
2	B	541	ARG
2	B	561	THR
2	B	576	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	112	ASN
1	A	119	GLN
2	B	302	GLN
2	B	317	GLN
2	B	501	ASN
2	B	575	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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
3	IHP	B	1000	-	36,36,36	1.01	2 (5%)	60,60,60	0.87	2 (3%)
4	2S8	B	1001	-	28,28,28	1.41	3 (10%)	36,38,38	1.51	6 (16%)

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
3	IHP	B	1000	-	-	4/30/54/54	0/1/1/1
4	2S8	B	1001	-	-	12/23/23/23	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	2S8	OAT-CAV	3.72	1.41	1.34
4	B	1001	2S8	CAK-NAS	-3.40	1.31	1.37
4	B	1001	2S8	CAZ-CAW	3.08	1.54	1.51
3	B	1000	IHP	P6-O16	-2.77	1.54	1.59
3	B	1000	IHP	P5-O15	-2.07	1.55	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	2S8	OAT-CAV-NAR	4.26	116.05	110.00
4	B	1001	2S8	CAP-NAR-CAV	3.38	127.72	121.98
4	B	1001	2S8	CAJ-CAY-CAX	3.10	122.06	118.84
4	B	1001	2S8	CAI-CAX-CAY	-3.02	119.26	122.19
4	B	1001	2S8	CAX-CAY-CAW	-2.87	104.31	106.98
3	B	1000	IHP	P6-O16-C6	-2.65	116.34	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	IHP	P5-O15-C5	-2.52	116.70	123.43
4	B	1001	2S8	OAT-CAV-OAE	-2.33	121.50	125.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	2S8	OAE-CAV-OAT-CBA
4	B	1001	2S8	CAB-CBA-OAT-CAV
4	B	1001	2S8	CAA-CBA-OAT-CAV
4	B	1001	2S8	NAR-CAV-OAT-CBA
4	B	1001	2S8	CAC-CBA-OAT-CAV
4	B	1001	2S8	CAL-CAN-CAP-NAR
4	B	1001	2S8	CAN-CAL-CAM-CAO
4	B	1001	2S8	CAK-CAW-CAZ-CAU
4	B	1001	2S8	CAY-CAW-CAZ-CAQ
4	B	1001	2S8	CAK-CAW-CAZ-CAQ
3	B	1000	IHP	C2-O12-P2-O22
3	B	1000	IHP	C3-O13-P3-O23
4	B	1001	2S8	CAY-CAW-CAZ-CAU
4	B	1001	2S8	CAO-CAQ-CAZ-CAU
3	B	1000	IHP	C1-O11-P1-O21
3	B	1000	IHP	C2-O12-P2-O32

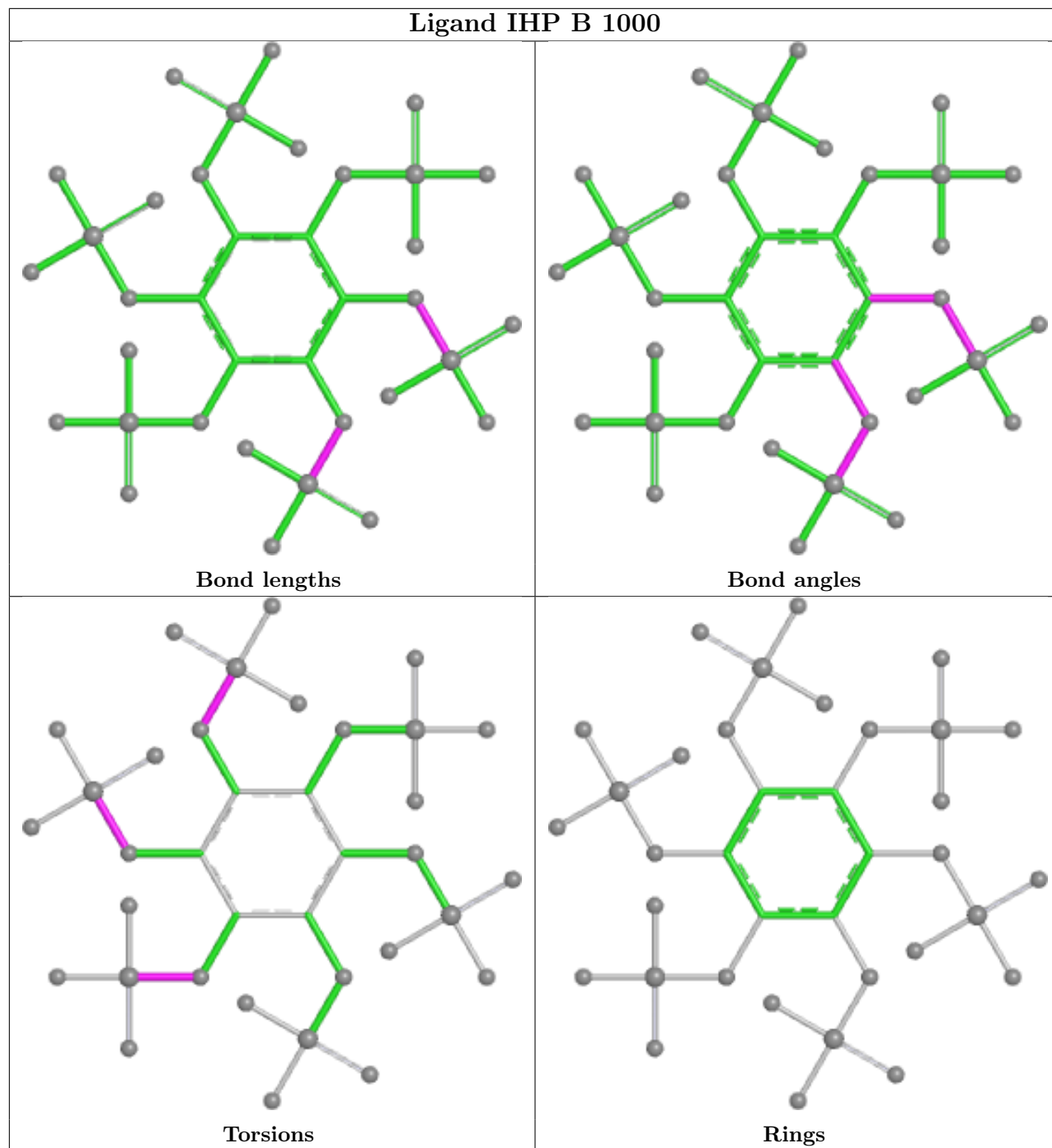
There are no ring outliers.

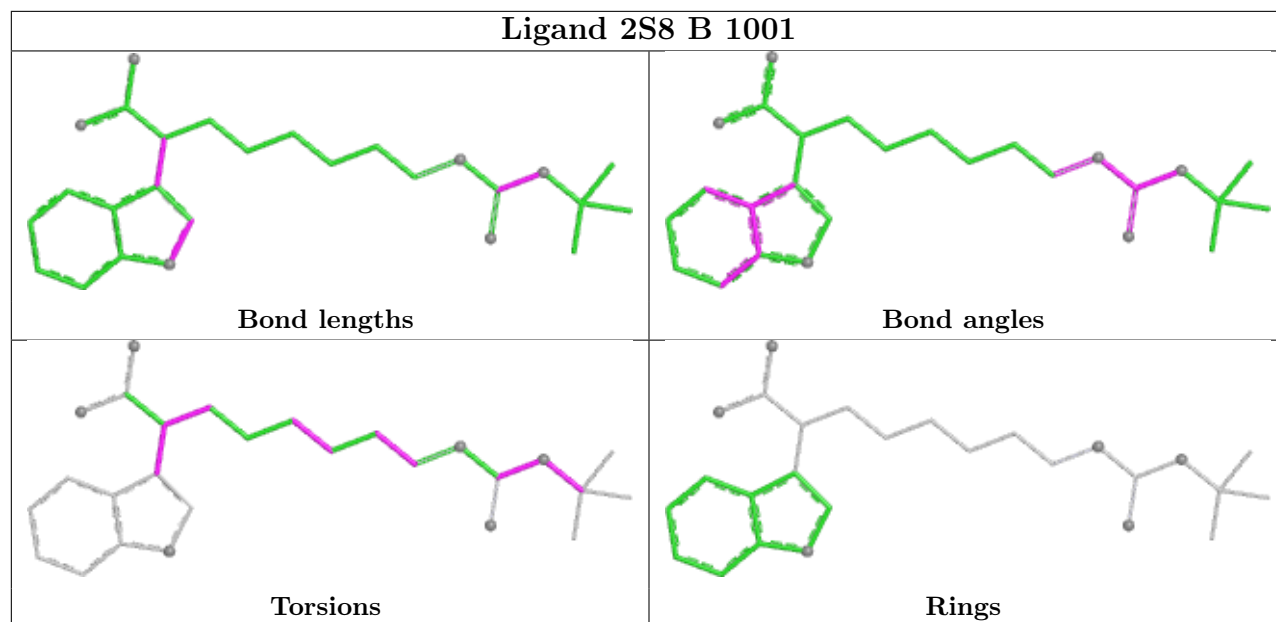
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	IHP	3	0
4	B	1001	2S8	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	57/160 (35%)	0.29	3 (5%) 32 26	26, 53, 62, 62	0
2	B	567/594 (95%)	-0.51	2 (0%) 88 86	17, 36, 51, 64	0
All	All	624/754 (82%)	-0.44	5 (0%) 82 80	17, 37, 56, 64	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	353	MET	3.6
2	B	354	GLU	2.9
1	A	108	LEU	2.6
1	A	104	ALA	2.4
1	A	110	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

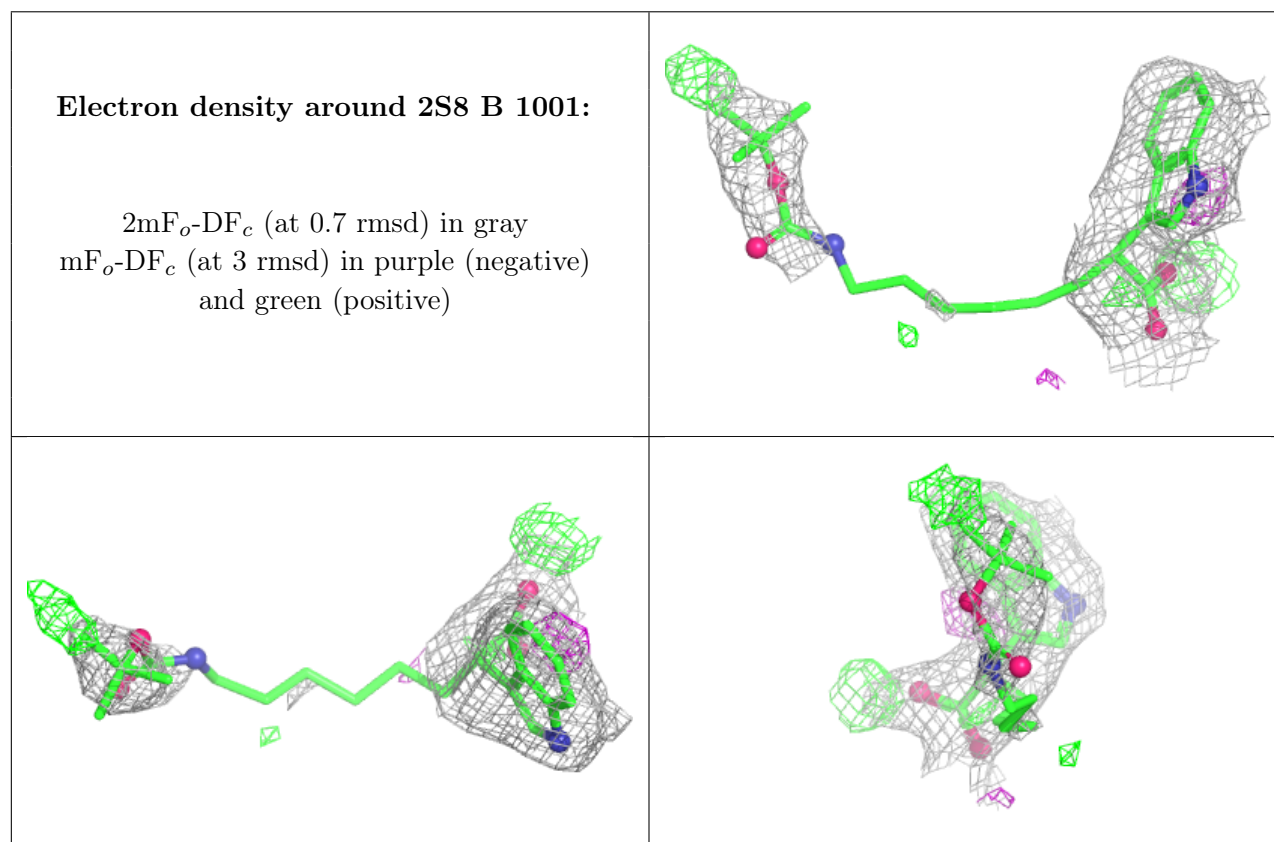
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

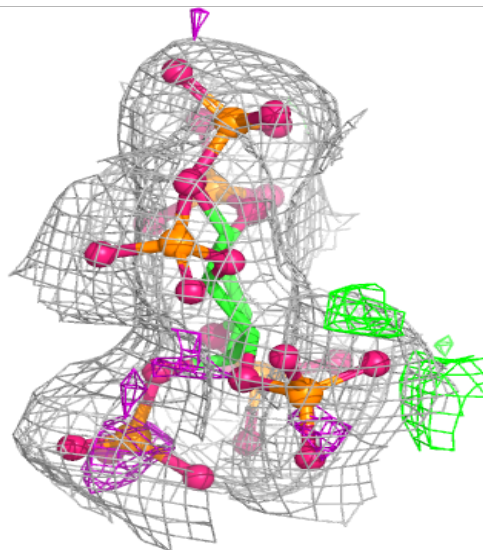
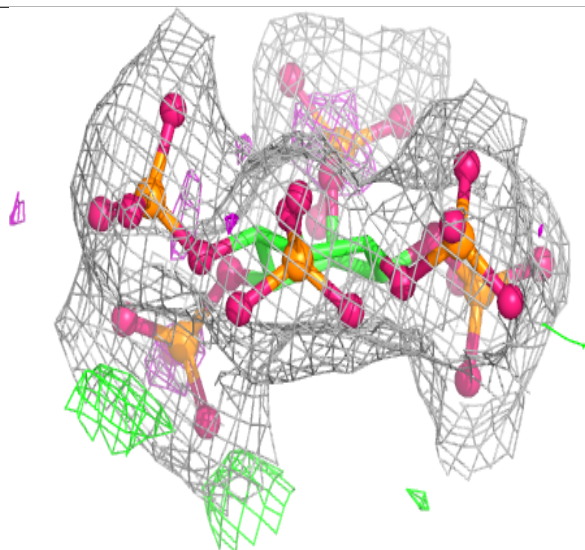
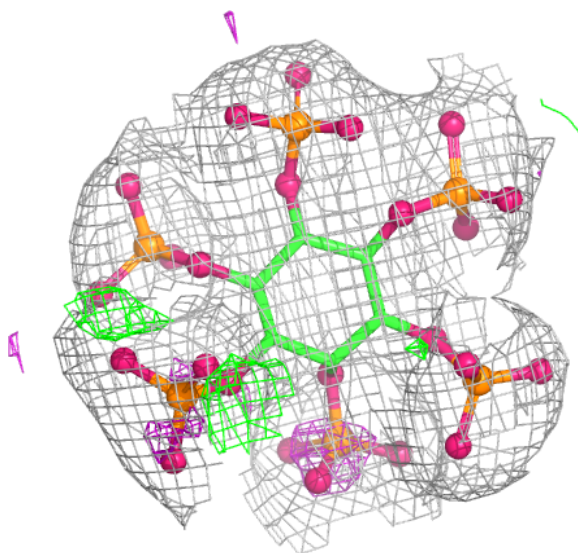
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	2S8	B	1001	27/27	0.83	0.28	70,76,124,125	0
3	IHP	B	1000	36/36	0.89	0.09	50,64,87,91	0

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 1000:

$2mF_o-DF_c$ (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.