



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:49 PM UTC

PDB ID : 3C6P / pdb_00003c6p
Title : Small molecule agonists and antagonists of F-box protein-substrate interactions in auxin perception and signaling
Authors : Tan, X.
Deposited on : 2008-02-04
Resolution : 2.70 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

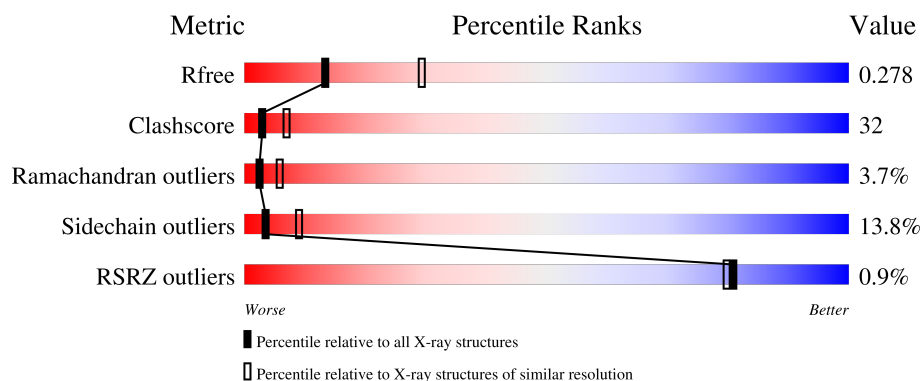
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	160	
2	B	594	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	2S3	B	1001	-	X	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5535 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.

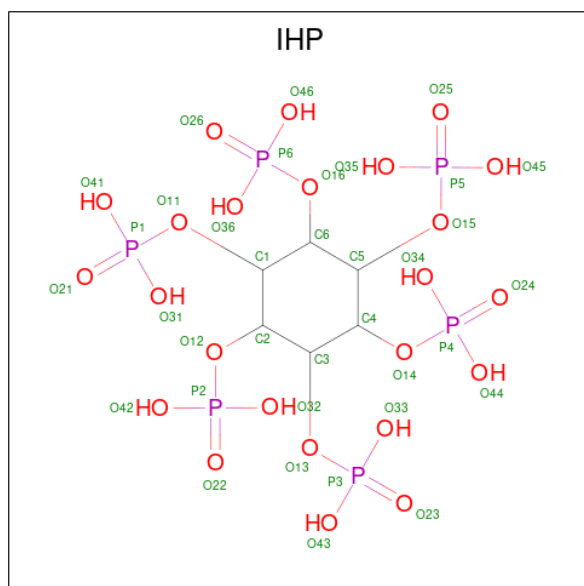
- Molecule 1 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			721	459	117	143	2			

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

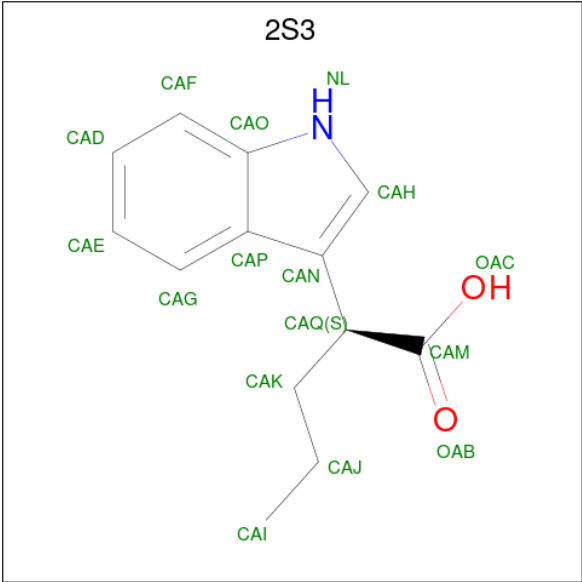
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	567	Total	C	N	O	S	0	0	0
			4461	2850	754	820	37			

- 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		

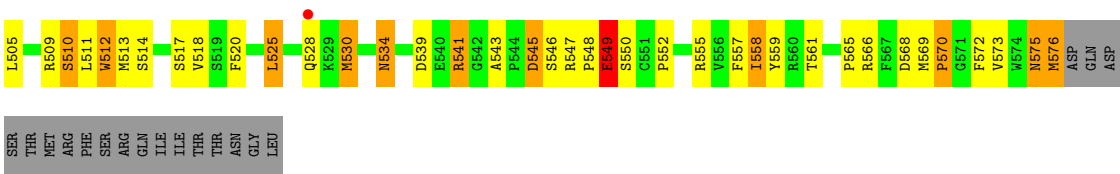
- Molecule 4 is (2S)-2-(1H-indol-3-yl)pentanoic acid (CCD ID: 2S3) (formula: $C_{13}H_{15}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	13	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	264	Total	O	0	0
			264	264		



SER
THR
MET
ARG
PHE
SER
ARG
GLN
ILE
ILE
THR
THR
ASN
GLY
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.79Å 80.39Å 125.21Å 90.00° 104.72° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	47.8 (49.71-2.70) 47.8 (49.71-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.261 0.202 , 0.278	Depositor DCC
R_{free} test set	1324 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 100.00 % 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 0.0000e+00. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, 2S3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	1/728 (0.1%)	1.07	1/982 (0.1%)
2	B	1.53	33/4558 (0.7%)	1.50	41/6178 (0.7%)
All	All	1.46	34/5286 (0.6%)	1.45	42/7160 (0.6%)

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	3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	TRP	CZ2-CH2	33.00	2.00	1.37
2	B	512	TRP	CA-C	16.44	1.72	1.52
2	B	512	TRP	CG-CD2	12.99	1.67	1.43
2	B	512	TRP	CD1-NE1	12.56	1.64	1.37
2	B	511	LEU	C-O	10.03	1.36	1.24
2	B	512	TRP	CA-CB	8.88	1.69	1.53
2	B	511	LEU	C-N	8.86	1.45	1.33
2	B	464	ALA	CA-CB	-8.32	1.39	1.53
2	B	512	TRP	C-O	8.14	1.33	1.24
2	B	513	MET	CA-C	-7.43	1.43	1.52
2	B	510	SER	N-CA	6.95	1.54	1.46
2	B	476	VAL	CA-CB	6.80	1.62	1.54
2	B	512	TRP	CD2-CE3	6.72	1.50	1.40
2	B	511	LEU	CA-C	6.71	1.60	1.52
2	B	259	VAL	CA-CB	6.12	1.60	1.54
2	B	509	ARG	N-CA	-6.08	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	TRP	CG-CD1	-6.03	1.21	1.36
2	B	512	TRP	CD2-CE2	5.87	1.51	1.41
2	B	462	SER	CA-C	-5.86	1.45	1.52
2	B	440	SER	CA-C	-5.85	1.45	1.52
2	B	512	TRP	N-CA	5.81	1.53	1.46
2	B	226	LYS	CA-C	-5.75	1.45	1.52
1	A	51	ILE	CA-CB	5.73	1.60	1.54
2	B	270	LEU	N-CA	-5.62	1.39	1.46
2	B	345	VAL	C-O	-5.57	1.18	1.24
2	B	416	THR	CA-CB	-5.53	1.44	1.53
2	B	438	SER	N-CA	-5.52	1.39	1.46
2	B	510	SER	C-N	5.36	1.40	1.33
2	B	460	MET	CA-C	-5.36	1.46	1.52
2	B	558	ILE	CA-CB	5.32	1.61	1.54
2	B	61	VAL	CA-CB	5.15	1.60	1.54
2	B	378	LEU	C-O	-5.14	1.17	1.24
2	B	431	CYS	CA-C	-5.11	1.47	1.53
2	B	138	SER	CA-C	5.03	1.59	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	512	TRP	CG-CD2-CE3	-18.35	115.55	133.90
2	B	511	LEU	CA-C-O	-13.47	105.81	120.36
2	B	512	TRP	N-CA-C	-12.36	89.69	109.59
2	B	510	SER	CA-C-O	-11.31	109.39	121.38
2	B	512	TRP	CE2-CD2-CE3	10.10	128.90	118.80
2	B	512	TRP	CB-CA-C	9.65	126.76	109.38
2	B	512	TRP	CA-CB-CG	-9.58	95.40	113.60
2	B	479	GLY	N-CA-C	9.21	125.71	113.37
2	B	243	GLY	N-CA-C	-9.12	99.92	112.13
2	B	336	THR	N-CA-C	8.99	120.69	111.07
2	B	512	TRP	NE1-CE2-CD2	-8.82	95.94	107.40
2	B	513	MET	N-CA-C	-8.46	93.71	108.69
1	A	9	LYS	N-CA-C	7.50	119.86	109.29
2	B	512	TRP	CH2-CZ2-CE2	-7.30	108.00	117.50
2	B	509	ARG	CA-C-O	-7.11	112.35	120.24
2	B	512	TRP	CE2-CD2-CG	6.95	115.54	107.20
2	B	511	LEU	N-CA-CB	-6.71	99.40	110.68
2	B	125	ILE	N-CA-C	-6.63	104.05	110.42
2	B	237	LEU	N-CA-C	6.58	120.03	110.42
2	B	486	LEU	N-CA-C	-6.48	99.25	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	VAL	N-CA-C	6.08	117.94	109.55
2	B	512	TRP	CA-C-O	-6.05	114.30	120.71
2	B	510	SER	CA-C-N	5.96	131.39	122.99
2	B	510	SER	C-N-CA	5.96	131.39	122.99
2	B	346	PHE	CA-C-N	-5.72	113.30	120.51
2	B	346	PHE	C-N-CA	-5.72	113.30	120.51
2	B	250	ARG	CA-C-N	-5.63	113.96	120.04
2	B	250	ARG	C-N-CA	-5.63	113.96	120.04
2	B	559	TYR	N-CA-C	5.58	117.48	108.32
2	B	289	SER	N-CA-C	-5.41	106.68	113.28
2	B	361	GLU	N-CA-C	-5.39	105.57	111.82
2	B	31	SER	N-CA-C	-5.37	105.99	112.54
2	B	356	ASN	N-CA-C	-5.28	107.22	113.97
2	B	510	SER	O-C-N	5.27	128.80	123.26
2	B	301	VAL	N-CA-CB	-5.21	102.63	111.23
2	B	234	ALA	CA-C-N	-5.18	114.28	119.56
2	B	234	ALA	C-N-CA	-5.18	114.28	119.56
2	B	475	HIS	N-CA-C	5.14	117.55	111.33
2	B	309	LEU	N-CA-C	5.12	117.53	111.33
2	B	490	ASP	N-CA-C	5.08	118.20	111.30
2	B	444	THR	N-CA-C	-5.03	102.45	109.69
2	B	260	ALA	O-C-N	5.02	127.31	122.09

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	LEU	Peptide
1	A	104	ALA	Peptide
1	A	28	THR	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	721	0	731	119	0
2	B	4461	0	4504	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	5	6	0
4	B	16	0	14	8	0
5	A	37	0	0	11	0
5	B	264	0	0	59	0
All	All	5535	0	5254	339	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 32.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD13	1:A:102:ILE:CD1	1.41	1.49
2:B:512:TRP:CH2	2:B:512:TRP:CZ2	1.99	1.48
1:A:29:ILE:CG2	1:A:30:ALA:H	1.18	1.46
1:A:101:LEU:HD22	1:A:102:ILE:N	1.48	1.28
2:B:569:MET:HE2	5:B:1088:HOH:O	1.39	1.21
2:B:576:MET:O	5:B:1006:HOH:O	1.56	1.19
1:A:102:ILE:N	1:A:102:ILE:HD13	1.54	1.17
1:A:102:ILE:CD1	1:A:102:ILE:H	1.56	1.15
4:B:1001:2S3:HAH	4:B:1001:2S3:CAI	1.79	1.12
1:A:106:ASN:O	1:A:108:LEU:N	1.83	1.12
4:B:1001:2S3:HAIA	4:B:1001:2S3:CAH	1.84	1.08
1:A:101:LEU:HD13	1:A:102:ILE:HD12	1.15	1.07
1:A:101:LEU:CD1	1:A:102:ILE:CD1	2.30	1.07
1:A:29:ILE:HG23	1:A:30:ALA:N	1.64	1.06
1:A:29:ILE:CG2	1:A:30:ALA:N	1.86	1.05
2:B:66:PRO:HB3	5:B:1047:HOH:O	1.57	1.03
1:A:29:ILE:HG22	1:A:30:ALA:N	1.52	1.03
2:B:10:PRO:HB2	5:B:1091:HOH:O	1.57	1.02
2:B:109:GLU:HB3	2:B:134:VAL:HB	1.43	1.01
1:A:26:SER:O	1:A:29:ILE:CG2	2.12	0.97
2:B:569:MET:HE1	2:B:575:ASN:HB2	1.46	0.96
1:A:101:LEU:N	1:A:103:LEU:HG	1.82	0.95
2:B:287:VAL:HA	5:B:1256:HOH:O	1.66	0.95
1:A:101:LEU:N	1:A:103:LEU:HD21	1.80	0.95
1:A:101:LEU:N	1:A:103:LEU:CG	2.30	0.94
1:A:101:LEU:CD2	1:A:102:ILE:N	2.30	0.94
1:A:101:LEU:N	1:A:103:LEU:CD2	2.30	0.94
1:A:101:LEU:HD13	1:A:102:ILE:HD13	1.49	0.94
4:B:1001:2S3:HAH	4:B:1001:2S3:HAIA	0.94	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:O	1:A:29:ILE:HG22	1.66	0.92
1:A:103:LEU:HD23	1:A:103:LEU:H	1.32	0.91
1:A:28:THR:HG21	1:A:107:TYR:O	1.71	0.91
1:A:101:LEU:CD2	1:A:101:LEU:C	2.46	0.89
1:A:102:ILE:HD13	1:A:102:ILE:H	0.74	0.88
1:A:160:GLU:HG3	2:B:28:ASN:ND2	1.88	0.88
2:B:432:LYS:HZ3	2:B:432:LYS:HB2	1.39	0.88
2:B:22:GLN:O	2:B:47:LYS:NZ	2.07	0.88
1:A:101:LEU:O	1:A:104:ALA:HB3	1.73	0.87
1:A:130:PRO:HD2	5:A:191:HOH:O	1.72	0.86
1:A:28:THR:OG1	1:A:108:LEU:HA	1.75	0.86
1:A:101:LEU:HD22	1:A:101:LEU:C	2.01	0.86
2:B:576:MET:O	5:B:1237:HOH:O	1.93	0.86
1:A:29:ILE:HG22	1:A:30:ALA:H	0.69	0.85
2:B:362:GLN:HB2	5:B:1218:HOH:O	1.79	0.83
1:A:101:LEU:HB3	1:A:102:ILE:HD13	1.59	0.83
2:B:309:LEU:HD23	2:B:309:LEU:O	1.80	0.82
2:B:432:LYS:HB2	2:B:432:LYS:NZ	1.93	0.82
1:A:56:ILE:C	1:A:58:TYR:H	1.89	0.81
1:A:101:LEU:CB	1:A:102:ILE:HD13	2.10	0.81
1:A:101:LEU:HD22	1:A:102:ILE:H	1.41	0.80
4:B:1001:2S3:CAI	4:B:1001:2S3:CAH	2.52	0.80
2:B:111:ARG:HH11	2:B:111:ARG:HG2	1.47	0.79
1:A:101:LEU:O	1:A:104:ALA:CB	2.30	0.79
2:B:144:SER:HB3	2:B:169:ASP:HB3	1.65	0.76
2:B:389:LEU:HG	5:B:1264:HOH:O	1.85	0.76
1:A:106:ASN:O	1:A:107:TYR:C	2.29	0.76
4:B:1001:2S3:CAH	4:B:1001:2S3:CAJ	2.62	0.76
1:A:101:LEU:HB3	1:A:102:ILE:CD1	2.15	0.75
2:B:352:VAL:O	2:B:382:ARG:NH2	2.18	0.75
2:B:63:ARG:HB3	5:B:1071:HOH:O	1.84	0.75
1:A:101:LEU:HD13	1:A:102:ILE:HD11	1.63	0.75
2:B:255:SER:O	2:B:259:VAL:HG23	1.85	0.75
1:A:104:ALA:O	1:A:106:ASN:C	2.30	0.74
2:B:384:MET:SD	5:B:1264:HOH:O	2.46	0.74
2:B:281:LEU:O	2:B:284:VAL:HG22	1.88	0.74
1:A:101:LEU:CG	1:A:102:ILE:HD13	2.19	0.73
2:B:233:ARG:HD2	5:B:1111:HOH:O	1.86	0.73
2:B:288:CYS:HB3	2:B:312:GLN:HB2	1.70	0.73
1:A:104:ALA:C	1:A:106:ASN:N	2.47	0.73
2:B:394:ARG:HD2	5:B:1152:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HG3	2:B:28:ASN:HD22	1.53	0.72
2:B:73:LEU:HB3	2:B:115:MET:CE	2.20	0.72
2:B:10:PRO:HD2	5:B:1089:HOH:O	1.88	0.71
1:A:102:ILE:C	1:A:104:ALA:H	1.97	0.71
2:B:284:VAL:O	2:B:287:VAL:HB	1.90	0.71
1:A:28:THR:O	1:A:29:ILE:HD13	1.91	0.70
2:B:459:GLU:OE1	2:B:484:ARG:NH1	2.24	0.70
2:B:545:ASP:HB3	5:B:1192:HOH:O	1.90	0.70
1:A:101:LEU:CD1	1:A:102:ILE:HD13	2.12	0.70
1:A:27:GLN:O	1:A:27:GLN:HG3	1.93	0.69
2:B:566:ARG:NH1	2:B:568:ASP:OD1	2.26	0.68
2:B:111:ARG:HH11	2:B:111:ARG:CG	2.07	0.68
2:B:409:PRO:HA	5:B:1029:HOH:O	1.92	0.68
1:A:10:SER:HA	5:A:167:HOH:O	1.94	0.67
2:B:72:GLU:HB2	5:B:1151:HOH:O	1.92	0.67
2:B:178:HIS:NE2	5:B:1014:HOH:O	1.67	0.67
1:A:102:ILE:HG23	1:A:117:THR:OG1	1.95	0.67
2:B:174:HIS:O	2:B:178:HIS:HD2	1.76	0.67
2:B:325:ILE:HG13	2:B:329:GLY:HA3	1.76	0.67
2:B:39:GLU:OE2	2:B:42:ARG:NH1	2.28	0.67
2:B:389:LEU:N	5:B:1264:HOH:O	2.25	0.67
1:A:101:LEU:O	1:A:102:ILE:C	2.36	0.66
1:A:106:ASN:C	1:A:108:LEU:N	2.54	0.66
2:B:73:LEU:HB3	2:B:115:MET:HE1	1.76	0.66
2:B:94:TYR:HB3	2:B:95:PRO:HD3	1.78	0.66
2:B:185:SER:O	5:B:1031:HOH:O	2.13	0.66
2:B:287:VAL:CG1	2:B:291:LEU:HD13	2.26	0.65
1:A:101:LEU:C	1:A:103:LEU:N	2.50	0.65
1:A:101:LEU:O	1:A:103:LEU:N	2.30	0.65
1:A:108:LEU:O	1:A:109:ASN:HB2	1.95	0.65
1:A:56:ILE:O	1:A:58:TYR:N	2.30	0.65
1:A:101:LEU:O	1:A:104:ALA:N	2.30	0.65
2:B:539:ASP:OD2	2:B:541:ARG:HD2	1.97	0.65
2:B:286:SER:HB3	5:B:1223:HOH:O	1.98	0.65
2:B:534:ASN:HD21	2:B:565:PRO:HA	1.62	0.64
1:A:104:ALA:O	1:A:106:ASN:N	2.30	0.64
1:A:102:ILE:O	1:A:104:ALA:N	2.30	0.64
2:B:378:LEU:HD11	2:B:380:PHE:CE1	2.31	0.64
2:B:232:GLN:HG3	5:B:1079:HOH:O	1.96	0.64
2:B:285:TYR:HA	2:B:288:CYS:SG	2.37	0.64
2:B:422:ILE:HG12	5:B:1080:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:OG1	1:A:147:GLU:HG3	1.98	0.63
2:B:393:ALA:HB2	2:B:427:ILE:HD13	1.81	0.63
2:B:505:LEU:HD13	2:B:558:ILE:HG21	1.81	0.63
4:B:1001:2S3:CAH	4:B:1001:2S3:HAJA	2.29	0.63
1:A:102:ILE:C	1:A:104:ALA:N	2.57	0.63
2:B:281:LEU:HD11	2:B:301:VAL:HG21	1.80	0.62
1:A:28:THR:O	1:A:29:ILE:CD1	2.47	0.62
1:A:56:ILE:C	1:A:58:TYR:N	2.57	0.62
1:A:129:THR:HB	5:A:191:HOH:O	1.99	0.62
2:B:484:ARG:HG2	5:B:1099:HOH:O	1.99	0.62
1:A:48:THR:HG22	1:A:51:ILE:HD13	1.80	0.62
2:B:70:SER:OG	2:B:109:GLU:HG3	2.00	0.61
2:B:27:ARG:HB3	2:B:45:ARG:NH2	2.15	0.61
2:B:403:ARG:HG2	2:B:438:SER:HB3	1.81	0.61
1:A:135:THR:HG22	1:A:136:THR:N	2.17	0.60
2:B:512:TRP:NE1	2:B:514:SER:HB3	2.15	0.60
2:B:447:VAL:O	2:B:450:TYR:HB2	2.02	0.60
2:B:359:LEU:HD21	2:B:379:TYR:CZ	2.37	0.60
2:B:176:LEU:HD21	2:B:206:LEU:HD12	1.83	0.59
1:A:106:ASN:C	1:A:108:LEU:H	2.10	0.59
2:B:378:LEU:HD12	2:B:378:LEU:C	2.27	0.59
1:A:160:GLU:C	5:A:169:HOH:O	2.46	0.58
1:A:102:ILE:HG23	1:A:117:THR:CB	2.33	0.58
1:A:120:THR:O	1:A:123:ASP:HB2	2.04	0.58
2:B:414:TYR:HB2	5:B:1201:HOH:O	2.02	0.58
2:B:281:LEU:HB2	2:B:282:PRO:HD3	1.84	0.58
1:A:26:SER:O	1:A:29:ILE:HG21	2.01	0.58
1:A:27:GLN:HB3	1:A:109:ASN:HD22	1.69	0.58
2:B:64:ARG:NH2	5:B:1133:HOH:O	2.27	0.57
2:B:378:LEU:HD11	2:B:380:PHE:HE1	1.66	0.57
2:B:512:TRP:HE1	2:B:514:SER:CB	2.17	0.57
2:B:520:PHE:HE1	2:B:576:MET:HE1	1.69	0.57
1:A:107:TYR:CD2	1:A:108:LEU:HD23	2.40	0.57
2:B:42:ARG:HB2	2:B:64:ARG:O	2.05	0.57
2:B:63:ARG:HG3	5:B:1085:HOH:O	2.05	0.57
2:B:66:PRO:HA	5:B:1047:HOH:O	2.05	0.57
1:A:48:THR:HG22	1:A:51:ILE:CD1	2.35	0.56
1:A:144:THR:HB	5:A:175:HOH:O	2.04	0.56
2:B:160:GLU:CG	5:B:1105:HOH:O	2.53	0.56
2:B:485:LYS:NZ	3:B:1000:IHP:O31	2.37	0.56
2:B:309:LEU:HD23	2:B:309:LEU:C	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:TYR:O	2:B:326:GLU:HG3	2.04	0.56
1:A:101:LEU:C	1:A:101:LEU:HD23	2.28	0.56
2:B:131:ASN:O	2:B:133:LYS:HG3	2.06	0.56
2:B:539:ASP:O	2:B:572:PHE:HB2	2.06	0.55
2:B:100:MET:HG2	2:B:104:TYR:CD1	2.41	0.55
2:B:171:VAL:O	2:B:172:SER:HB3	2.06	0.55
2:B:445:ASP:OD1	2:B:468:ASP:HB2	2.07	0.55
2:B:10:PRO:HD3	5:B:1247:HOH:O	2.07	0.54
2:B:66:PRO:CA	5:B:1047:HOH:O	2.54	0.54
2:B:94:TYR:CE1	2:B:124:LEU:HD12	2.42	0.54
2:B:530:MET:HE2	5:B:1052:HOH:O	2.08	0.54
1:A:29:ILE:O	1:A:30:ALA:O	2.26	0.54
2:B:262:SER:HB3	2:B:286:SER:HB3	1.87	0.54
2:B:94:TYR:CE2	2:B:98:GLU:HG3	2.43	0.54
2:B:512:TRP:HE1	2:B:514:SER:HB3	1.70	0.54
2:B:174:HIS:O	2:B:178:HIS:CD2	2.60	0.54
2:B:234:ALA:HB1	2:B:237:LEU:HD13	1.90	0.54
2:B:93:VAL:HG12	2:B:116:VAL:O	2.07	0.54
2:B:413:ASP:C	2:B:413:ASP:OD1	2.50	0.54
1:A:101:LEU:CD2	1:A:102:ILE:H	2.11	0.53
2:B:454:TYR:O	2:B:456:LYS:N	2.42	0.53
1:A:104:ALA:O	1:A:105:ALA:C	2.51	0.53
2:B:86:PRO:HG3	5:B:1251:HOH:O	2.07	0.53
2:B:144:SER:CB	2:B:169:ASP:HB3	2.38	0.53
1:A:153:ARG:HD2	5:A:194:HOH:O	2.08	0.53
2:B:517:SER:C	5:B:1115:HOH:O	2.51	0.53
2:B:239:GLU:HB3	5:B:1018:HOH:O	2.09	0.53
2:B:569:MET:C	2:B:570:PRO:O	2.50	0.52
2:B:287:VAL:HG12	2:B:291:LEU:HD13	1.91	0.52
2:B:487:GLU:C	2:B:488:ILE:HG13	2.34	0.52
2:B:19:SER:O	2:B:22:GLN:NE2	2.42	0.52
2:B:62:ILE:HD13	5:B:1027:HOH:O	2.09	0.52
1:A:103:LEU:CD2	1:A:103:LEU:H	2.04	0.51
2:B:112:LEU:HD22	2:B:115:MET:HE3	1.92	0.51
2:B:288:CYS:CB	2:B:312:GLN:HB2	2.39	0.51
2:B:288:CYS:HA	2:B:291:LEU:HD22	1.92	0.51
2:B:236:GLN:OE1	2:B:236:GLN:N	2.37	0.51
2:B:282:PRO:HA	2:B:285:TYR:CZ	2.46	0.51
2:B:441:GLY:O	2:B:443:LEU:HG	2.10	0.51
2:B:484:ARG:NH2	3:B:1000:IHP:O31	2.42	0.51
2:B:97:ILE:O	2:B:101:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:O	1:A:109:ASN:N	2.44	0.51
2:B:160:GLU:HG3	5:B:1105:HOH:O	2.09	0.51
3:B:1000:IHP:O33	3:B:1000:IHP:O44	2.29	0.51
2:B:405:CYS:HB2	4:B:1001:2S3:HAI	1.93	0.51
2:B:190:ASN:HA	2:B:217:LYS:HB2	1.93	0.50
2:B:545:ASP:C	2:B:547:ARG:H	2.18	0.50
2:B:57:SER:O	2:B:58:PRO:C	2.55	0.50
2:B:63:ARG:NE	5:B:1109:HOH:O	2.44	0.50
1:A:102:ILE:CG2	1:A:117:THR:OG1	2.60	0.50
1:A:126:LYS:HB3	5:A:164:HOH:O	2.11	0.50
2:B:347:PRO:HG2	2:B:350:PRO:HG3	1.93	0.50
1:A:48:THR:CG2	1:A:51:ILE:CD1	2.90	0.50
2:B:238:GLU:C	2:B:239:GLU:HG3	2.36	0.50
2:B:62:ILE:HG22	5:B:1216:HOH:O	2.12	0.49
2:B:66:PRO:CB	5:B:1047:HOH:O	2.32	0.49
2:B:388:ALA:HB3	5:B:1264:HOH:O	2.12	0.49
1:A:27:GLN:O	1:A:27:GLN:CG	2.60	0.49
1:A:125:ILE:O	1:A:126:LYS:C	2.53	0.49
2:B:569:MET:O	2:B:570:PRO:O	2.30	0.49
2:B:224:LEU:HD11	2:B:257:LEU:HD11	1.95	0.49
2:B:287:VAL:CG1	2:B:291:LEU:CD1	2.90	0.49
3:B:1000:IHP:O23	5:B:1044:HOH:O	2.19	0.49
1:A:20:GLU:HG2	1:A:20:GLU:O	2.12	0.49
1:A:121:VAL:C	1:A:123:ASP:N	2.69	0.49
2:B:164:ARG:O	2:B:166:SER:N	2.46	0.49
2:B:464:ALA:HB2	4:B:1001:2S3:HAD	1.95	0.49
2:B:569:MET:SD	2:B:573:VAL:HG12	2.53	0.49
1:A:121:VAL:C	1:A:123:ASP:H	2.20	0.48
1:A:160:GLU:HG3	2:B:28:ASN:HD21	1.75	0.48
2:B:304:TYR:O	2:B:307:VAL:HB	2.13	0.48
2:B:359:LEU:HD21	2:B:379:TYR:OH	2.13	0.48
2:B:10:PRO:C	5:B:1091:HOH:O	2.56	0.48
2:B:570:PRO:HG2	2:B:573:VAL:CG2	2.44	0.48
2:B:118:THR:HA	2:B:142:GLY:O	2.14	0.48
2:B:436:ARG:HD2	2:B:460:MET:HE3	1.96	0.48
2:B:290:ARG:NH2	5:B:1256:HOH:O	2.46	0.48
2:B:569:MET:CE	5:B:1088:HOH:O	2.22	0.48
2:B:114:ARG:HA	2:B:139:SER:O	2.14	0.47
2:B:383:GLN:HG2	5:B:1053:HOH:O	2.14	0.47
1:A:101:LEU:CD1	1:A:102:ILE:HD11	2.32	0.47
1:A:103:LEU:HD23	1:A:103:LEU:N	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:ASP:C	2:B:547:ARG:N	2.72	0.47
2:B:325:ILE:O	2:B:329:GLY:HA3	2.13	0.47
2:B:512:TRP:CZ2	2:B:555:ARG:HD3	2.49	0.47
1:A:137:PHE:HB3	1:A:138:ASN:H	1.49	0.47
2:B:312:GLN:NE2	5:B:1095:HOH:O	2.48	0.47
2:B:460:MET:CE	5:B:1016:HOH:O	2.62	0.47
1:A:101:LEU:HD22	1:A:102:ILE:HD13	1.97	0.47
1:A:107:TYR:CD2	1:A:108:LEU:CD2	2.98	0.47
2:B:257:LEU:HD23	2:B:257:LEU:HA	1.81	0.47
2:B:79:PHE:CE2	2:B:489:ARG:HD3	2.50	0.46
2:B:294:LEU:HD21	2:B:296:LEU:HD11	1.97	0.46
2:B:510:SER:HB2	2:B:557:PHE:CE1	2.51	0.46
2:B:310:LEU:HD13	2:B:333:LEU:HD13	1.97	0.46
2:B:429:GLU:HB2	5:B:1259:HOH:O	2.15	0.46
2:B:518:VAL:O	2:B:552:PRO:HA	2.16	0.46
1:A:101:LEU:CD1	1:A:102:ILE:HD12	2.10	0.46
2:B:19:SER:HB3	5:B:1030:HOH:O	2.15	0.46
2:B:74:LYS:NZ	3:B:1000:IHP:H1	2.31	0.46
2:B:143:PHE:CE1	2:B:168:VAL:HG22	2.50	0.46
1:A:160:GLU:CG	2:B:28:ASN:HD22	2.27	0.46
2:B:170:ASP:OD1	2:B:196:SER:HB3	2.15	0.46
2:B:391:THR:O	2:B:392:ILE:C	2.60	0.45
2:B:543:ALA:O	2:B:546:SER:OG	2.28	0.45
2:B:202:ALA:O	2:B:206:LEU:HB2	2.17	0.45
2:B:570:PRO:HG2	2:B:573:VAL:HG23	1.97	0.45
1:A:101:LEU:HD22	1:A:102:ILE:CA	2.40	0.45
2:B:33:VAL:O	2:B:34:CYS:HB3	2.16	0.45
2:B:437:LEU:HG	2:B:438:SER:N	2.32	0.45
1:A:138:ASN:ND2	1:A:138:ASN:O	2.50	0.45
1:A:119:GLN:O	1:A:123:ASP:OD2	2.34	0.45
2:B:262:SER:HB3	2:B:286:SER:CB	2.46	0.45
2:B:548:PRO:O	2:B:550:SER:N	2.49	0.45
1:A:107:TYR:HD2	1:A:108:LEU:CD2	2.30	0.44
1:A:101:LEU:CD2	1:A:102:ILE:HD13	2.47	0.44
2:B:366:SER:O	2:B:367:VAL:C	2.59	0.44
2:B:228:ALA:HB3	5:B:1005:HOH:O	2.17	0.44
1:A:44:LEU:HD13	1:A:47:VAL:HG21	1.99	0.44
1:A:137:PHE:O	1:A:138:ASN:HB2	2.16	0.44
1:A:49:SER:HA	5:A:173:HOH:O	2.18	0.44
1:A:149:GLU:CB	5:A:189:HOH:O	2.64	0.44
1:A:149:GLU:HB3	5:A:162:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:LEU:C	2:B:309:LEU:CD2	2.91	0.44
1:A:102:ILE:HA	1:A:105:ALA:HB3	2.00	0.43
1:A:155:ASN:OD1	2:B:64:ARG:NH2	2.36	0.43
2:B:63:ARG:HD2	5:B:1209:HOH:O	2.17	0.43
2:B:109:GLU:CB	2:B:134:VAL:HB	2.31	0.43
2:B:210:CYS:HA	2:B:211:PRO:HD2	1.85	0.43
2:B:395:ASN:C	2:B:397:PRO:HD3	2.43	0.43
1:A:101:LEU:C	1:A:103:LEU:H	2.23	0.43
2:B:197:GLU:HG3	2:B:221:ALA:HB1	2.00	0.43
2:B:363:GLY:O	2:B:366:SER:HB2	2.19	0.43
2:B:94:TYR:HE2	2:B:98:GLU:OE1	2.01	0.43
2:B:195:ALA:O	2:B:196:SER:C	2.61	0.43
2:B:382:ARG:HG3	2:B:382:ARG:HH11	1.83	0.43
1:A:28:THR:HG23	1:A:108:LEU:O	2.18	0.43
2:B:525:LEU:O	2:B:528:GLN:HB2	2.19	0.43
2:B:208:THR:HG23	5:B:1235:HOH:O	2.19	0.43
2:B:165:GLU:N	2:B:165:GLU:CD	2.77	0.43
2:B:239:GLU:CB	5:B:1018:HOH:O	2.67	0.43
2:B:424:PHE:CD2	2:B:439:LEU:HD23	2.54	0.42
1:A:149:GLU:HB2	5:A:189:HOH:O	2.19	0.42
1:A:48:THR:CG2	1:A:51:ILE:HD12	2.48	0.42
2:B:489:ARG:HD2	5:B:1048:HOH:O	2.19	0.42
2:B:30:VAL:HG23	2:B:41:GLU:HG3	2.02	0.42
2:B:324:TYR:O	2:B:325:ILE:C	2.59	0.42
2:B:382:ARG:HG3	2:B:382:ARG:NH1	2.34	0.42
2:B:104:TYR:HA	5:B:1090:HOH:O	2.19	0.42
2:B:435:ARG:HA	2:B:458:MET:HA	2.02	0.42
2:B:285:TYR:N	5:B:1239:HOH:O	2.52	0.42
2:B:305:ASP:O	2:B:306:LEU:C	2.60	0.42
1:A:143:PHE:HB3	1:A:148:GLU:HB2	2.02	0.42
2:B:344:ARG:HG2	2:B:378:LEU:HB3	2.01	0.42
2:B:548:PRO:O	2:B:549:GLU:C	2.62	0.42
1:A:20:GLU:OE1	1:A:24:LEU:HD11	2.18	0.42
2:B:56:VAL:HG22	2:B:57:SER:N	2.35	0.42
2:B:88:GLY:O	2:B:89:TRP:C	2.61	0.42
2:B:374:LEU:HD23	2:B:374:LEU:HA	1.93	0.42
2:B:444:THR:HB	2:B:468:ASP:OD2	2.20	0.42
2:B:472:GLY:O	2:B:473:MET:C	2.59	0.42
2:B:62:ILE:HG21	5:B:1027:HOH:O	2.20	0.41
1:A:101:LEU:N	1:A:103:LEU:CD1	2.82	0.41
2:B:15:GLU:CD	5:B:1189:HOH:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LEU:HD12	2:B:291:LEU:HD21	2.01	0.41
2:B:137:LEU:O	2:B:166:SER:OG	2.35	0.41
2:B:288:CYS:HB3	2:B:312:GLN:CB	2.45	0.41
2:B:378:LEU:C	2:B:378:LEU:CD1	2.92	0.41
2:B:405:CYS:HA	2:B:440:SER:OG	2.20	0.41
2:B:173:GLY:HA3	2:B:197:GLU:O	2.20	0.41
2:B:287:VAL:HG13	2:B:291:LEU:HD13	1.97	0.41
3:B:1000:IHP:O25	3:B:1000:IHP:O16	2.38	0.41
1:A:9:LYS:HB3	1:A:10:SER:H	1.65	0.41
2:B:371:CYS:O	2:B:373:LYS:N	2.53	0.41
2:B:396:ARG:C	2:B:398:ASN:H	2.28	0.41
2:B:496:LYS:HZ3	2:B:496:LYS:HG3	1.76	0.41
1:A:22:VAL:HG13	1:A:22:VAL:O	2.21	0.41
1:A:127:GLY:HA2	2:B:26:ASP:OD1	2.21	0.41
1:A:101:LEU:HB3	1:A:102:ILE:HD11	1.99	0.41
2:B:73:LEU:HB3	2:B:115:MET:HE2	2.01	0.41
2:B:85:VAL:HG22	2:B:512:TRP:CH2	2.56	0.41
2:B:178:HIS:NE2	5:B:1231:HOH:O	2.37	0.41
2:B:396:ARG:C	2:B:398:ASN:N	2.78	0.41
2:B:477:LEU:HD23	2:B:477:LEU:HA	1.77	0.41
1:A:44:LEU:HA	1:A:45:PRO:HD3	1.97	0.40
2:B:335:SER:HA	2:B:338:LYS:HZ3	1.85	0.40
2:B:268:ARG:HD3	2:B:268:ARG:HA	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	82/160 (51%)	58 (71%)	10 (12%)	14 (17%)	0	0
2	B	565/594 (95%)	508 (90%)	47 (8%)	10 (2%)	6	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	647/754 (86%)	566 (88%)	57 (9%)	24 (4%)	2 6

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ALA
1	A	29	ILE
1	A	57	GLU
1	A	105	ALA
1	A	107	TYR
2	B	165	GLU
2	B	570	PRO
1	A	102	ILE
1	A	103	LEU
1	A	109	ASN
1	A	138	ASN
2	B	549	GLU
1	A	106	ASN
1	A	135	THR
1	A	136	THR
2	B	225	GLU
2	B	455	ALA
2	B	164	ARG
2	B	172	SER
2	B	283	ALA
1	A	145	PRO
2	B	196	SER
1	A	45	PRO
2	B	131	ASN

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	81/137 (59%)	65 (80%)	16 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	500/525 (95%)	436 (87%)	64 (13%)	4	11
All	All	581/662 (88%)	501 (86%)	80 (14%)	3	9

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	47	VAL
1	A	51	ILE
1	A	52	LEU
1	A	101	LEU
1	A	102	ILE
1	A	103	LEU
1	A	111	LYS
1	A	114	LEU
1	A	120	THR
1	A	135	THR
1	A	137	PHE
1	A	139	ILE
1	A	145	PRO
1	A	149	GLU
1	A	153	ARG
2	B	12	GLU
2	B	21	ILE
2	B	33	VAL
2	B	35	LYS
2	B	62	ILE
2	B	68	VAL
2	B	87	ASP
2	B	98	GLU
2	B	102	SER
2	B	109	GLU
2	B	111	ARG
2	B	115	MET
2	B	123	GLU
2	B	124	LEU
2	B	139	SER
2	B	141	GLU
2	B	156	ARG
2	B	164	ARG
2	B	165	GLU
2	B	167	ASP

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Mol	Chain	Res	Type
2	B	177	SER
2	B	182	THR
2	B	184	THR
2	B	192	SER
2	B	198	VAL
2	B	199	SER
2	B	201	SER
2	B	206	LEU
2	B	213	LEU
2	B	227	LEU
2	B	237	LEU
2	B	238	GLU
2	B	248	GLU
2	B	262	SER
2	B	275	ASP
2	B	286	SER
2	B	291	LEU
2	B	301	VAL
2	B	309	LEU
2	B	312	GLN
2	B	325	ILE
2	B	364	LEU
2	B	369	MET
2	B	374	LEU
2	B	378	LEU
2	B	381	CYS
2	B	408	GLU
2	B	432	LYS
2	B	438	SER
2	B	440	SER
2	B	462	SER
2	B	471	LEU
2	B	483	LEU
2	B	490	ASP
2	B	495	ASP
2	B	525	LEU
2	B	530	MET
2	B	534	ASN
2	B	541	ARG
2	B	545	ASP
2	B	549	GLU
2	B	561	THR

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Mol	Chain	Res	Type
2	B	575	ASN
2	B	576	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	119	GLN
2	B	28	ASN
2	B	178	HIS
2	B	232	GLN
2	B	317	GLN
2	B	383	GLN
2	B	534	ASN
2	B	575	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.29	3 (8%)	60,60,60	3.06	28 (46%)
4	2S3	B	1001	-	17,17,17	2.43	5 (29%)	21,23,23	2.79	11 (52%)

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	-	-	6/30/54/54	0/1/1/1
4	2S3	B	1001	-	-	6/11/11/11	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	2S3	CAH-CAN	7.92	1.45	1.36
3	B	1000	IHP	P3-O13	4.83	1.68	1.59
4	B	1001	2S3	CAP-CAN	-3.09	1.38	1.44
3	B	1000	IHP	P4-O14	2.92	1.64	1.59
4	B	1001	2S3	CAG-CAP	2.80	1.44	1.39
4	B	1001	2S3	CAF-CAO	2.53	1.43	1.39
3	B	1000	IHP	P1-O11	2.45	1.63	1.59
4	B	1001	2S3	CAD-CAF	2.16	1.42	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	IHP	O13-C3-C2	9.31	128.56	108.76
3	B	1000	IHP	O12-C2-C3	6.83	123.28	108.76
3	B	1000	IHP	C3-C2-C1	6.70	125.14	110.43
3	B	1000	IHP	P6-O16-C6	-5.78	107.99	123.43
3	B	1000	IHP	C4-C3-C2	-5.71	97.89	110.43
4	B	1001	2S3	CAQ-CAN-CAH	-5.05	119.51	126.75
4	B	1001	2S3	CAG-CAP-CAO	4.98	124.00	118.84
3	B	1000	IHP	O11-C1-C6	4.92	119.23	108.76
4	B	1001	2S3	CAF-CAO-CAP	-4.90	117.45	122.19
4	B	1001	2S3	CAN-CAH-NL	-4.85	106.37	110.31
3	B	1000	IHP	C6-C5-C4	4.79	120.95	110.43
3	B	1000	IHP	O11-C1-C2	4.52	118.39	108.76
3	B	1000	IHP	O15-C5-C6	4.49	118.31	108.76
3	B	1000	IHP	O16-C6-C5	4.29	117.88	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	IHP	P4-O14-C4	-4.02	112.69	123.43
3	B	1000	IHP	P5-O15-C5	3.94	133.97	123.43
3	B	1000	IHP	O14-C4-C3	3.88	117.02	108.76
3	B	1000	IHP	C5-C4-C3	3.69	118.52	110.43
3	B	1000	IHP	C6-C1-C2	-3.69	102.34	110.43
3	B	1000	IHP	O31-P1-O11	-3.60	91.82	105.85
4	B	1001	2S3	CAE-CAD-CAF	3.56	124.62	120.24
3	B	1000	IHP	O42-P2-O12	-3.44	92.45	105.85
3	B	1000	IHP	O16-C6-C1	3.42	116.03	108.76
3	B	1000	IHP	O33-P3-O13	3.03	117.67	105.85
4	B	1001	2S3	CAG-CAP-CAN	-3.03	128.51	133.68
4	B	1001	2S3	CAP-CAN-CAQ	2.97	131.95	126.56
3	B	1000	IHP	C5-C6-C1	2.96	116.93	110.43
4	B	1001	2S3	CAP-CAN-CAH	2.87	108.45	106.25
3	B	1000	IHP	O43-P3-O13	-2.79	94.97	105.85
3	B	1000	IHP	O36-P6-O16	-2.67	95.45	105.85
4	B	1001	2S3	OAB-CAM-CAQ	-2.55	111.68	120.19
3	B	1000	IHP	O43-P3-O23	2.53	120.69	110.83
4	B	1001	2S3	CAP-CAO-NL	2.48	109.59	107.52
3	B	1000	IHP	O46-P6-O36	2.43	116.92	107.80
4	B	1001	2S3	OAC-CAM-CAQ	2.43	124.77	116.50
3	B	1000	IHP	O45-P5-O35	2.28	116.34	107.80
3	B	1000	IHP	O12-P2-O22	-2.12	101.79	109.33
3	B	1000	IHP	O14-C4-C5	2.06	113.15	108.76
3	B	1000	IHP	O15-C5-C4	2.03	113.07	108.76

There are no chirality outliers.

All (12) torsion outliers are listed below:

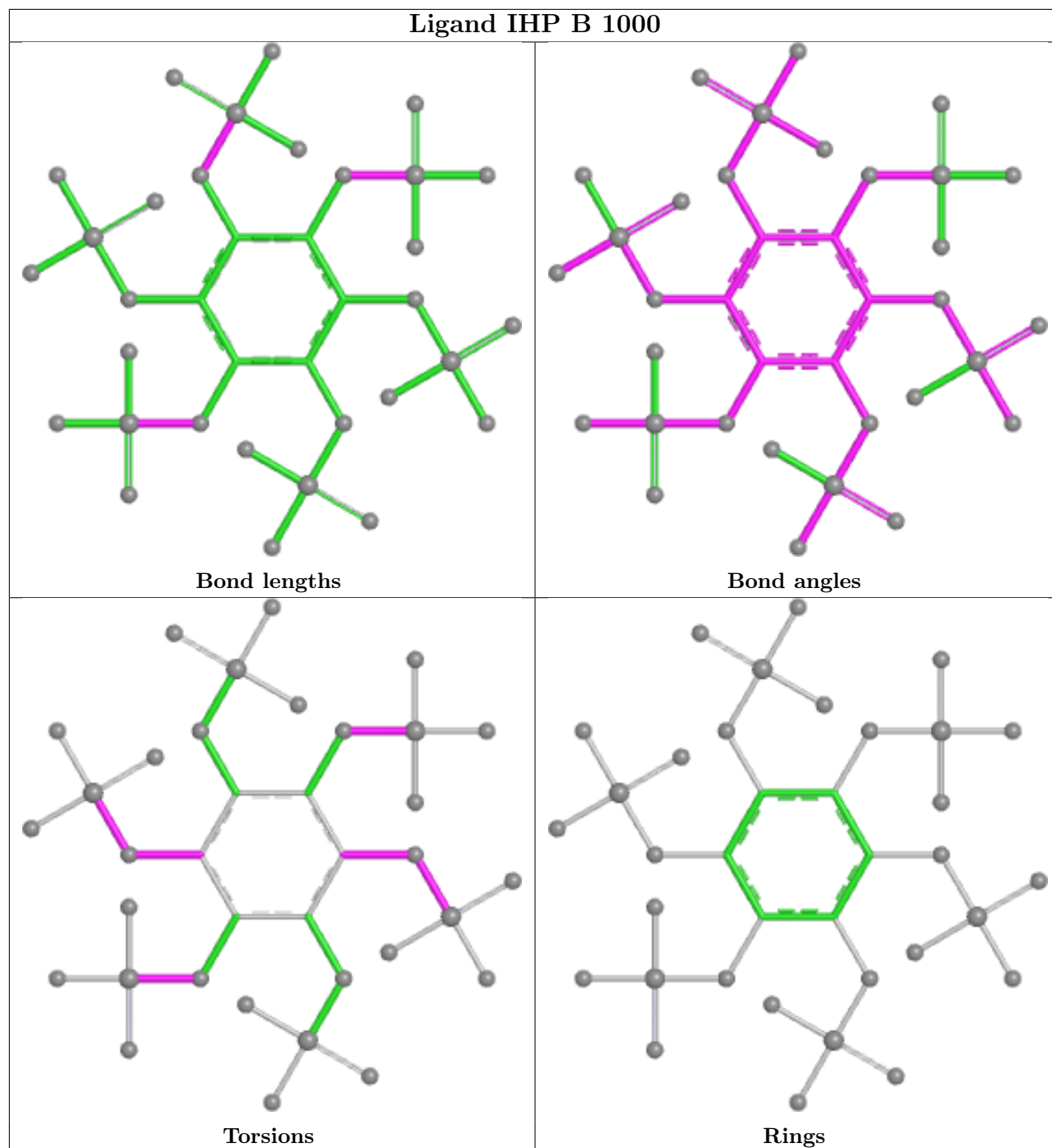
Mol	Chain	Res	Type	Atoms
3	B	1000	IHP	C3-C2-O12-P2
3	B	1000	IHP	C6-C5-O15-P5
4	B	1001	2S3	CAJ-CAK-CAQ-CAM
4	B	1001	2S3	CAJ-CAK-CAQ-CAN
4	B	1001	2S3	CAI-CAJ-CAK-CAQ
3	B	1000	IHP	C4-O14-P4-O24
4	B	1001	2S3	CAH-CAN-CAQ-CAM
4	B	1001	2S3	CAH-CAN-CAQ-CAK
3	B	1000	IHP	C2-O12-P2-O22
4	B	1001	2S3	CAP-CAN-CAQ-CAM
3	B	1000	IHP	C1-O11-P1-O31
3	B	1000	IHP	C5-O15-P5-O35

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	IHP	6	0
4	B	1001	2S3	8	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	90/160 (56%)	0.56	5 (5%) 30 26	29, 59, 69, 70	0
2	B	567/594 (95%)	-0.51	1 (0%) 91 90	25, 41, 56, 73	0
All	All	657/754 (87%)	-0.36	6 (0%) 81 80	25, 42, 63, 73	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	ILE	3.4
1	A	23	ALA	2.7
1	A	43	PRO	2.6
1	A	44	LEU	2.3
1	A	103	LEU	2.3
2	B	528	GLN	2.3

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](#)

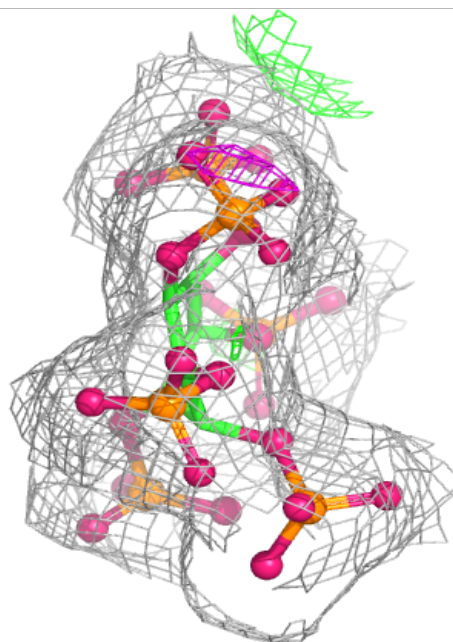
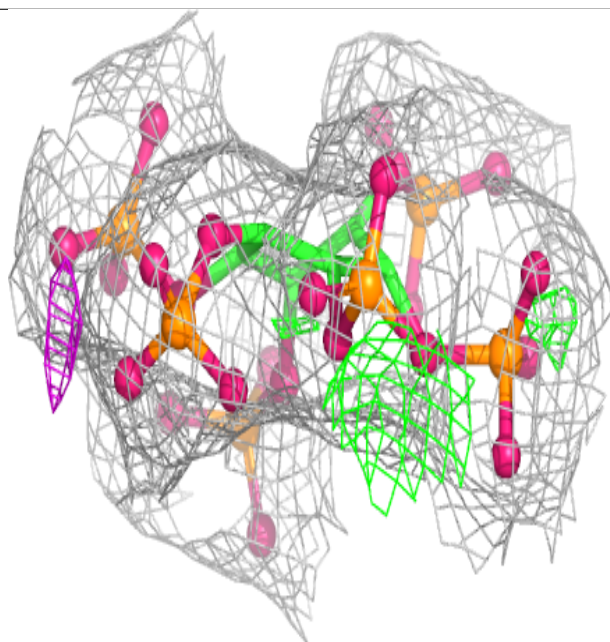
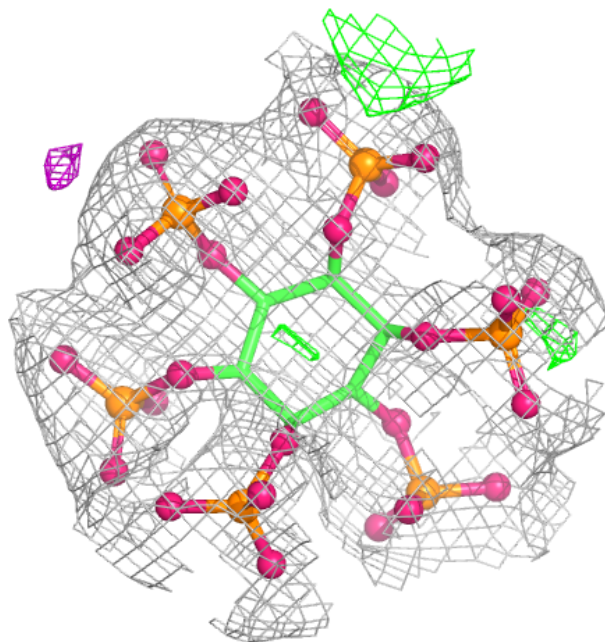
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	IHP	B	1000	36/36	0.89	0.09	67,78,99,101	0
4	2S3	B	1001	16/16	0.93	0.18	77,80,84,85	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.