



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:35 am GMT

PDB ID : 3C6N
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

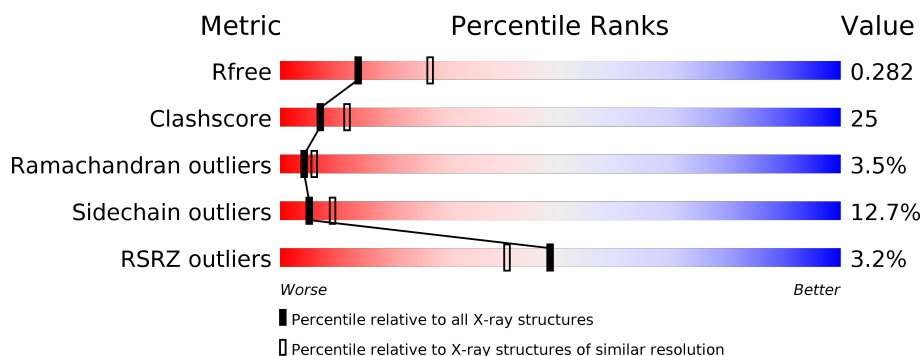
1 Overall quality at a glance

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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	2S8	B	1001	-	-	-	X

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.

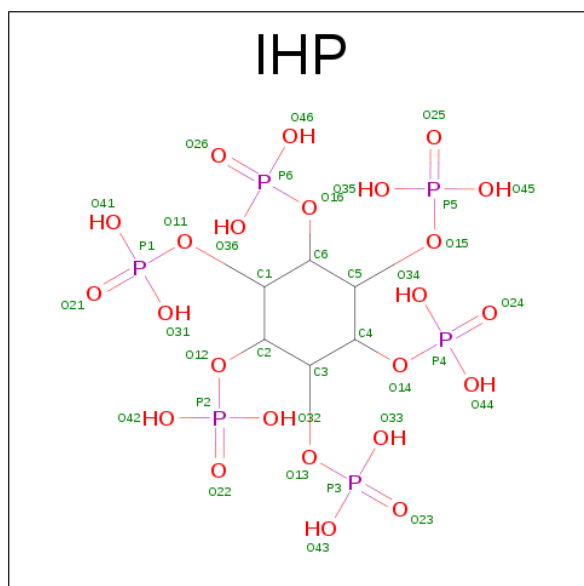
- Molecule 1 is a protein called SKP1-like protein 1A.

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.

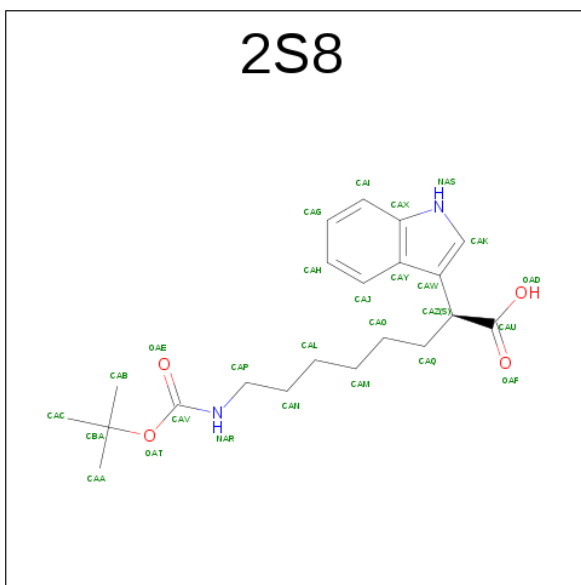
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	567	Total	C	N	O	S	0	0	0
			4461	2850	754	820	37			

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: 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)OCTA NOIC ACID (three-letter code: 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 16 16	0	0
5	B	161	Total O 161 161	0	0

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

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 (5.43%)	DCC
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 , 50.9	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	0.94	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, 2S8

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	1/478 (0.2%)	1.17	3/646 (0.5%)
2	B	1.64	50/4558 (1.1%)	1.45	47/6178 (0.8%)
All	All	1.61	51/5036 (1.0%)	1.42	50/6824 (0.7%)

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 (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	CYS	CB-SG	9.84	1.99	1.82
2	B	71	VAL	CB-CG1	-8.97	1.34	1.52
2	B	311	CYS	CB-SG	-8.00	1.68	1.82
2	B	557	PHE	CD1-CE1	7.51	1.54	1.39
2	B	64	ARG	CZ-NH1	7.15	1.42	1.33
2	B	441	GLY	CA-C	7.06	1.63	1.51
2	B	506	GLU	CG-CD	6.74	1.62	1.51
2	B	512	TRP	CD1-NE1	6.73	1.49	1.38
2	B	89	TRP	CB-CG	-6.70	1.38	1.50
2	B	380	PHE	CE1-CZ	6.64	1.50	1.37
2	B	65	PHE	N-CA	6.59	1.59	1.46
2	B	155	CYS	CB-SG	-6.53	1.71	1.82
2	B	331	GLU	CG-CD	6.46	1.61	1.51
2	B	326	GLU	N-CA	6.44	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	196	SER	CB-OG	6.26	1.50	1.42
2	B	480	CYS	CB-SG	6.25	1.92	1.82
2	B	239	GLU	CG-CD	6.25	1.61	1.51
2	B	380	PHE	CD2-CE2	6.11	1.51	1.39
2	B	438	SER	N-CA	-6.11	1.34	1.46
2	B	193	CYS	CB-SG	6.10	1.92	1.82
2	B	214	LYS	CD-CE	5.99	1.66	1.51
2	B	280	TYR	CE1-CZ	5.94	1.46	1.38
2	B	302	GLN	CG-CD	5.91	1.64	1.51
2	B	449	GLU	C-O	5.83	1.34	1.23
2	B	374	LEU	C-O	5.75	1.34	1.23
2	B	420	LEU	C-O	5.67	1.34	1.23
2	B	12	GLU	CG-CD	5.67	1.60	1.51
2	B	232	GLN	CG-CD	5.65	1.64	1.51
2	B	379	TYR	CE2-CZ	5.63	1.45	1.38
2	B	408	GLU	CG-CD	5.57	1.60	1.51
2	B	522	ALA	CA-CB	-5.53	1.40	1.52
2	B	46	ARG	CG-CD	5.51	1.65	1.51
2	B	331	GLU	CD-OE2	5.49	1.31	1.25
2	B	553	VAL	CA-CB	-5.47	1.43	1.54
2	B	63	ARG	CG-CD	5.44	1.65	1.51
1	A	149	GLU	CG-CD	5.41	1.60	1.51
2	B	85	VAL	CB-CG2	-5.38	1.41	1.52
2	B	106	TRP	CB-CG	5.36	1.59	1.50
2	B	536	GLU	CG-CD	5.34	1.59	1.51
2	B	94	TYR	CG-CD1	5.34	1.46	1.39
2	B	175	TRP	CE3-CZ3	5.33	1.47	1.38
2	B	574	TRP	CZ3-CH2	5.29	1.48	1.40
2	B	464	ALA	CA-CB	-5.27	1.41	1.52
2	B	65	PHE	CE1-CZ	5.23	1.47	1.37
2	B	432	LYS	CE-NZ	5.21	1.62	1.49
2	B	106	TRP	CG-CD1	5.19	1.44	1.36
2	B	375	GLU	CB-CG	-5.12	1.42	1.52
2	B	301	VAL	CB-CG2	-5.11	1.42	1.52
2	B	454	TYR	CD1-CE1	5.08	1.47	1.39
2	B	476	VAL	CA-CB	5.05	1.65	1.54
2	B	94	TYR	CE1-CZ	5.02	1.45	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	ARG	NE-CZ-NH2	-13.43	113.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	ARG	NE-CZ-NH1	9.46	125.03	120.30
2	B	401	ARG	NE-CZ-NH1	-8.27	116.16	120.30
2	B	421	ASP	CB-CG-OD1	8.19	125.67	118.30
2	B	243	GLY	N-CA-C	-8.13	92.77	113.10
2	B	270	LEU	CB-CG-CD2	-7.98	97.43	111.00
2	B	115	MET	CA-CB-CG	-7.08	101.26	113.30
2	B	378	LEU	CB-CG-CD1	6.83	122.60	111.00
2	B	404	LEU	CB-CG-CD2	-6.81	99.42	111.00
2	B	576	MET	CG-SD-CE	6.59	110.75	100.20
2	B	486	LEU	N-CA-C	-6.49	93.47	111.00
2	B	124	LEU	CB-CG-CD1	-6.45	100.03	111.00
2	B	526	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	A	110	ILE	CB-CA-C	6.23	124.06	111.60
2	B	114	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	B	220	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	B	325	ILE	C-N-CA	-6.14	106.34	121.70
2	B	434	LEU	CA-CB-CG	-6.04	101.40	115.30
2	B	576	MET	CA-CB-CG	5.95	123.41	113.30
2	B	458	MET	CA-CB-CG	-5.93	103.22	113.30
2	B	359	LEU	CA-CB-CG	-5.91	101.70	115.30
2	B	496	LYS	CD-CE-NZ	-5.88	98.18	111.70
2	B	408	GLU	C-N-CD	5.87	140.72	128.40
2	B	114	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	B	405	CYS	CA-CB-SG	-5.85	103.47	114.00
2	B	479	GLY	N-CA-C	5.83	127.67	113.10
2	B	73	LEU	CA-CB-CG	5.75	128.53	115.30
2	B	436	ARG	NE-CZ-NH2	5.75	123.17	120.30
2	B	440	SER	N-CA-CB	5.74	119.11	110.50
2	B	137	LEU	CB-CG-CD1	-5.67	101.36	111.00
2	B	325	ILE	CA-C-N	5.67	129.67	117.20
2	B	230	LEU	CB-CG-CD1	-5.61	101.47	111.00
2	B	311	CYS	CA-CB-SG	-5.60	103.92	114.00
2	B	170	ASP	CB-CG-OD2	5.55	123.30	118.30
2	B	309	LEU	CA-CB-CG	-5.55	102.54	115.30
2	B	458	MET	CB-CG-SD	-5.53	95.80	112.40
2	B	509	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	B	401	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	B	111	ARG	CA-CB-CG	5.39	125.26	113.40
2	B	325	ILE	O-C-N	-5.39	114.08	122.70
1	A	144	THR	C-N-CD	5.32	139.58	128.40
1	A	107	TYR	N-CA-C	-5.30	96.68	111.00
2	B	64	ARG	NE-CZ-NH1	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	ASP	CB-CG-OD1	5.29	123.06	118.30
2	B	316	LEU	CB-CG-CD1	-5.24	102.10	111.00
2	B	483	LEU	CB-CG-CD2	5.12	119.70	111.00
2	B	445	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	111	ARG	NE-CZ-NH1	-5.06	117.77	120.30
2	B	194	LEU	CA-CB-CG	-5.02	103.75	115.30
2	B	575	ASN	N-CA-C	5.02	124.55	111.00

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

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	28	0
2	B	4461	0	4504	225	0
3	B	36	0	6	4	0
4	B	27	0	29	4	0
5	A	16	0	0	5	0
5	B	161	0	0	24	0
All	All	5172	0	4992	252	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 25.

All (252) 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:HH11	2:B:111:ARG:CG	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:CG	1:A:148:GLU:O	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
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:354:GLU:O	2:B:355:PRO:C	2.19	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:NH1	2:B:111:ARG:CG	2.43	0.76
2:B:79:PHE:CE2	2:B:489:ARG:HG2	2.21	0.76
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:CG2	2:B:33:VAL:O	2.40	0.70
1:A:140:LYS:CE	1:A:140:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:TYR:C	2:B:325:ILE:O	2.27	0.69
2:B:575:ASN:C	2:B:575:ASN:HD22	1.96	0.68
2:B:352:VAL:HG13	2:B:354:GLU:HG2	1.71	0.68
2:B:22:GLN:O	2:B:47:LYS:NZ	2.25	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:104:TYR:HA	5:B:1073:HOH:O	1.97	0.64
2:B:97:ILE:HG22	2:B:124:LEU:HD13	1.79	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:11:GLU:N	2:B:11:GLU:OE1	2.34	0.60
2:B:544:PRO:HA	2:B:547:ARG:NH2	2.16	0.60
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:THR:O	2:B:417:LEU:HB2	2.04	0.58
2:B:83:ASN:HA	5:B:1051:HOH:O	2.04	0.57
2:B:33:VAL:HG23	2:B:33:VAL:O	2.03	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: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:63:ARG:C	2:B:64:ARG:O	2.41	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: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:104:TYR:C	5:B:1073:HOH:O	2.44	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:135:LEU:HD11	2:B:137:LEU:HD21	1.88	0.55
2:B:565:PRO:HB3	2:B:575:ASN:OD1	2.07	0.55
2:B:93:VAL:HG12	2:B:116:VAL:O	2.07	0.55
2:B:57:SER:O	2:B:58:PRO:C	2.46	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:174:HIS:C	2:B:174:HIS:CD2	2.82	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:575:ASN:ND2	2:B:575:ASN:C	2.62	0.53
2:B:268:ARG:HH12	2:B:290:ARG:HD3	1.72	0.53
2:B:10:PRO:C	2:B:11:GLU:OE1	2.47	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:512:TRP:C	2:B:512:TRP:CD1	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:ASP:O	2:B:434:LEU:C	2.48	0.52
2:B:312:GLN:CD	5:B:1079:HOH:O	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:41:GLU:O	2:B:42:ARG:C	2.48	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:254:TYR:C	2:B:254:TYR:CD2	2.85	0.50
2:B:309:LEU:HD23	2:B:309:LEU:C	2.26	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:174:HIS:CD2	5:B:1066:HOH:O	2.64	0.50
2:B:43:TRP:CZ3	2:B:66:PRO:HG2	2.47	0.50
2:B:510:SER:HB2	2:B:557:PHE:CE1	2.47	0.50
2:B:252:ASP:N	2:B:252:ASP:OD2	2.45	0.50
2:B:282:PRO:HA	2:B:285:TYR:CZ	2.47	0.50
2:B:505:LEU:HD23	2:B:505:LEU:N	2.27	0.49
2:B:42:ARG:HB2	2:B:65:PHE:H	1.75	0.49
2:B:324:TYR:O	2:B:325:ILE:C	2.50	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
1:A:143:PHE:HB3	1:A:148:GLU:HB2	1.94	0.49
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: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
1:A:119:GLN:HG2	2:B:20:PHE:CD2	2.48	0.48
2:B:412:PRO:O	2:B:413:ASP:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:CAB	4:B:1001:2S8:OAE	2.62	0.46
2:B:277:VAL:O	2:B:278:PRO:C	2.55	0.46
1:A:118:CYS:HB2	2:B:20:PHE:HE1	1.79	0.46
2:B:194:LEU:HD23	2:B:194:LEU:HA	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: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:309:LEU:CD2	2:B:309:LEU:C	2.85	0.45
1:A:107:TYR:CE2	5:A:174:HOH:O	2.52	0.45
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:353:MET:HG2	2:B:353:MET:H	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:270:LEU:HD22	2:B:273:PHE:CZ	2.52	0.44
2:B:495:ASP:OD1	2:B:495:ASP:N	2.49	0.44
2:B:33:VAL:HG22	2:B:33:VAL:O	2.17	0.44
2:B:179:PHE:CD2	2:B:183:TYR:CD2	3.05	0.43
2:B:56:VAL:HG22	2:B:57:SER:N	2.33	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:450:TYR:O	2:B:451:ILE:C	2.56	0.43
2:B:460:MET:CE	2:B:485:LYS:HZ2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:GLY:HA2	2:B:517:SER:O	2.19	0.43
1:A:147:GLU:C	1:A:149:GLU:H	2.22	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:528:GLN:O	2:B:529:LYS:C	2.53	0.43
2:B:68:VAL:HB	2:B:104:TYR:CZ	2.53	0.43
2:B:227:LEU:HA	2:B:227:LEU:HD23	1.57	0.43
2:B:88:GLY:O	2:B:89:TRP:C	2.54	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:N	2:B:380:PHE:CD1	2.87	0.42
2:B:457:LYS:O	2:B:458:MET:C	2.55	0.42
2:B:100:MET:HG2	2:B:104:TYR:HD1	1.82	0.42
2:B:471:LEU:HA	2:B:471:LEU:HD23	1.54	0.42
2:B:308:LYS:HB2	2:B:308:LYS:HE3	1.86	0.41
2:B:498:LEU:HD12	2:B:498:LEU:HA	1.66	0.41
1:A:160:GLU:CD	2:B:25:LYS:HD2	2.41	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:359:LEU:HD21	2:B:379:TYR:CZ	2.55	0.41
2:B:470:ASP:HB3	2:B:497:ALA:HB2	2.02	0.41
2:B:241:GLY:HA2	2:B:271:SER:O	2.21	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:199:SER:HG	2:B:202:ALA:HB3	1.85	0.41
2:B:438:SER:OG	4:B:1001:2S8:CAK	2.69	0.41
2:B:509:ARG:HG2	2:B:509:ARG:O	2.20	0.41
2:B:553:VAL:O	5:B:1147:HOH:O	2.21	0.41
2:B:364:LEU:HD23	2:B:364:LEU:HA	1.84	0.41
2:B:143:PHE:CE1	2:B:168:VAL:HG22	2.56	0.41
2:B:510:SER:HB2	2:B:557:PHE:HE1	1.85	0.41
3:B:1000:IHP:O44	3:B:1000:IHP:O33	2.38	0.41
2:B:179:PHE:CD2	2:B:183:TYR:CE2	3.08	0.41
2:B:224:LEU:O	2:B:227:LEU:HB2	2.22	0.40
2:B:485:LYS:NZ	3:B:1000:IHP:O31	2.50	0.40
2:B:13:VAL:O	2:B:17:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:SER:OG	2:B:239:GLU:HG2	2.21	0.40
2:B:388:ALA:C	2:B:392:ILE:HD12	2.42	0.40
2:B:464:ALA:HA	2:B:489:ARG:O	2.21	0.40
2:B:215:SER:OG	2:B:239:GLU:CG	2.70	0.40
2:B:413:ASP:C	2:B:413:ASP:OD1	2.59	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	55/160 (34%)	42 (76%)	6 (11%)	7 (13%)	0	0
2	B	565/594 (95%)	483 (86%)	67 (12%)	15 (3%)	6	10
All	All	620/754 (82%)	525 (85%)	73 (12%)	22 (4%)	4	6

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

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Mol	Chain	Res	Type
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%)	38 (73%)	14 (27%)	0	1
2	B	500/525 (95%)	444 (89%)	56 (11%)	7	12
All	All	552/662 (83%)	482 (87%)	70 (13%)	5	9

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	107	TYR
1	A	108	LEU
1	A	112	ASN
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	147	GLU
1	A	149	GLU
1	A	153	ARG

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Mol	Chain	Res	Type
2	B	11	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	42	ARG
2	B	63	ARG
2	B	101	SER
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	167	ASP
2	B	174	HIS
2	B	182	THR
2	B	184	THR
2	B	192	SER
2	B	201	SER
2	B	206	LEU
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	290	ARG
2	B	307	VAL
2	B	309	LEU
2	B	331	GLU
2	B	349	GLU
2	B	364	LEU
2	B	369	MET

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Mol	Chain	Res	Type
2	B	374	LEU
2	B	381	CYS
2	B	438	SER
2	B	440	SER
2	B	449	GLU
2	B	460	MET
2	B	483	LEU
2	B	489	ARG
2	B	512	TRP
2	B	525	LEU
2	B	530	MET
2	B	561	THR
2	B	575	ASN
2	B	576	MET

Some 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
2	B	317	GLN
2	B	383	GLN
2	B	395	ASN
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 carbohydrates 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	0.98	2 (5%)	54,60,60	0.69	0
4	2S8	B	1001	-	24,28,28	1.17	3 (12%)	29,38,38	1.55	6 (20%)

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	-	-	0/30/54/54	0/1/1/1
4	2S8	B	1001	-	-	0/16/23/23	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	IHP	P6-O16	-2.81	1.54	1.59
4	B	1001	2S8	CAK-NAS	-2.41	1.31	1.36
4	B	1001	2S8	CAI-CAX	-2.14	1.38	1.41
3	B	1000	IHP	P5-O15	-2.10	1.55	1.59
4	B	1001	2S8	OAT-CAV	3.34	1.41	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	2S8	CAU-CAZ-CAW	-2.44	107.65	111.20
4	B	1001	2S8	CAW-CAY-CAX	-2.43	104.31	106.83
4	B	1001	2S8	OAT-CAV-OAE	-2.08	121.50	125.56
4	B	1001	2S8	CAJ-CAY-CAX	2.93	122.06	118.17
4	B	1001	2S8	CAP-NAR-CAV	3.54	127.72	121.88
4	B	1001	2S8	OAT-CAV-NAR	3.92	116.05	109.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	IHP	4	0
4	B	1001	2S8	4	0

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	57/160 (35%)	1.09	16 (28%) 1 0	26, 53, 62, 63	0
2	B	567/594 (95%)	-0.46	4 (0%) 87 85	17, 36, 51, 64	0
All	All	624/754 (82%)	-0.32	20 (3%) 48 40	17, 37, 56, 64	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	LEU	6.9
2	B	353	MET	5.1
1	A	107	TYR	3.9
2	B	13	VAL	3.6
1	A	108	LEU	3.6
1	A	120	THR	3.6
1	A	117	THR	3.4
1	A	113	LEU	3.4
1	A	112	ASN	3.0
2	B	354	GLU	3.0
1	A	138	ASN	2.9
2	B	14	LEU	2.8
1	A	110	ILE	2.8
1	A	123	ASP	2.4
1	A	139	ILE	2.3
1	A	137	PHE	2.2
1	A	119	GLN	2.1
1	A	135	THR	2.1
1	A	136	THR	2.0
1	A	114	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	2S8	B	1001	27/27	0.86	0.28	5.53	70,76,124,125	0
3	IHP	B	1000	36/36	0.92	0.19	0.76	50,64,87,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.