Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 10:18 PM EDT

PDB ID	:	7T1Z
Title	:	Structure of the Fbw7-Skp1-MycNdegron complex
Authors	:	Wang, B.; Rusnac, D.V.; Clurman, B.E.; Zheng, N.
Deposited on	:	2021-12-02
Resolution	:	2.77 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 (i) 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 (1)) were used in the production of this report:

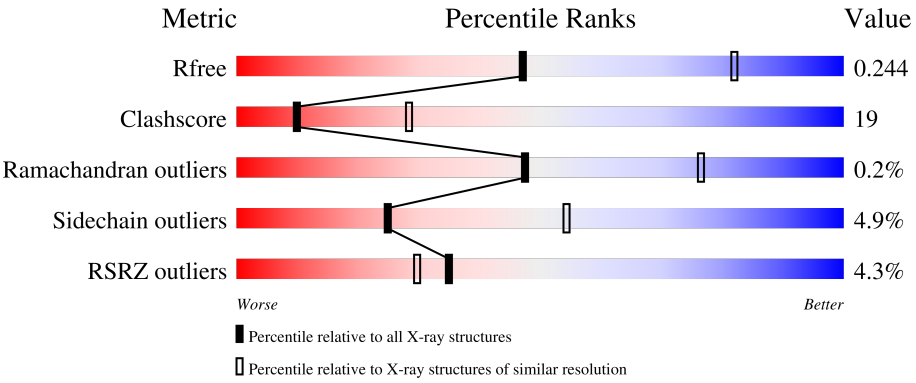
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	149	11% 58% 26% . 13%
2	B	457	2% 65% 29% . .
3	C	20	5% 15% 45% 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4701 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 S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1018	650	167	196	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P63208
A	84	GLY	PRO	linker	UNP P63208
A	85	GLY	PRO	linker	UNP P63208
A	86	SER	PRO	linker	UNP P63208
A	87	GLY	GLU	linker	UNP P63208
A	88	THR	ASP	linker	UNP P63208
A	?	-	ARG	deletion	UNP P63208
A	?	-	THR	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ILE	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	VAL	deletion	UNP P63208
A	?	-	TRP	deletion	UNP P63208
A	160	THR	CYS	conflict	UNP P63208
A	163	GLU	LYS	conflict	UNP P63208

- Molecule 2 is a protein called F-box/WD repeat-containing protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	438	Total	C	N	O	S	0	0	0
			3455	2168	621	645	21			

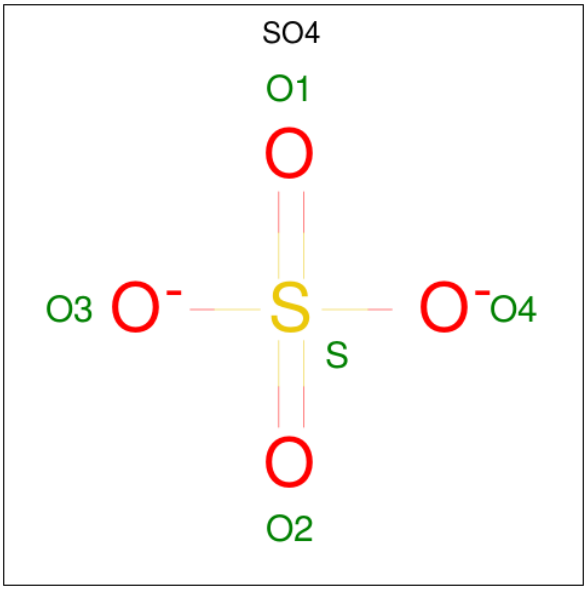
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	251	SER	-	expression tag	UNP Q969H0
B	252	HIS	-	expression tag	UNP Q969H0
B	253	HIS	-	expression tag	UNP Q969H0
B	254	HIS	-	expression tag	UNP Q969H0
B	255	HIS	-	expression tag	UNP Q969H0
B	256	HIS	-	expression tag	UNP Q969H0
B	257	HIS	-	expression tag	UNP Q969H0
B	258	GLY	-	expression tag	UNP Q969H0
B	259	GLY	-	expression tag	UNP Q969H0
B	260	SER	-	expression tag	UNP Q969H0
B	261	GLY	-	expression tag	UNP Q969H0
B	262	MET	-	expression tag	UNP Q969H0

- Molecule 3 is a protein called Myc proto-oncogene N terminal degron.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			104	66	14	22	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	O	S		0	0
			5	4	1			
4	B	1	Total	O	S		0	0
			5	4	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

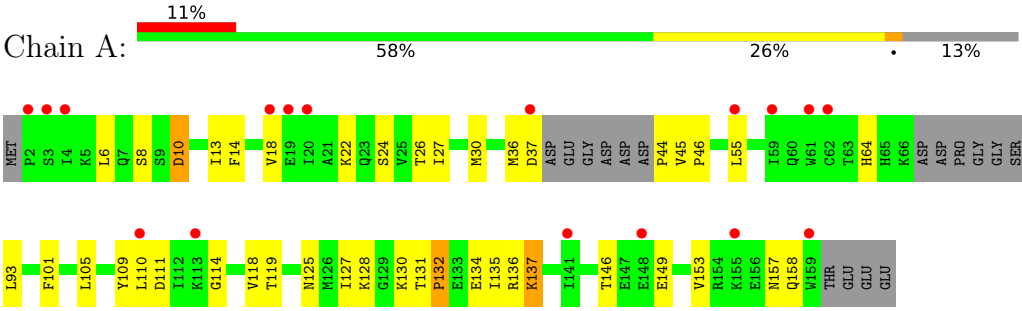
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	B	85	Total O 85 85	0	0
5	C	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

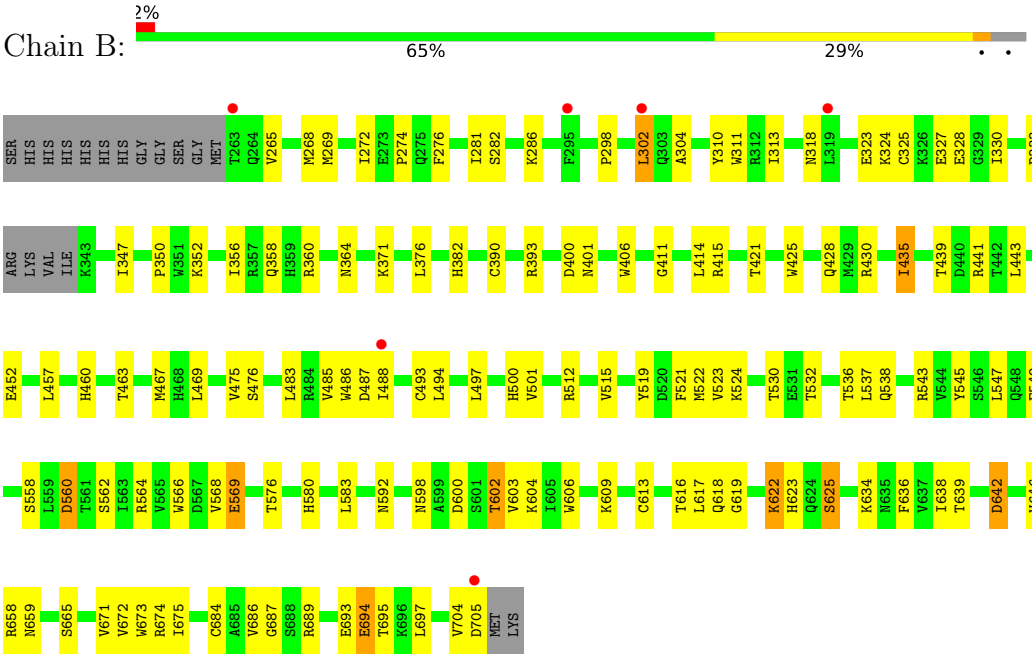
• Molecule 1: S-phase kinase-associated protein 1

Chain A:



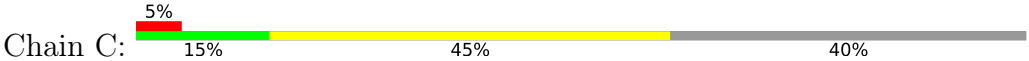
• Molecule 2: F-box/WD repeat-containing protein 7

Chain B:



• Molecule 3: Myc proto-oncogene N terminal degron

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	232.87Å 232.87Å 107.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.77 49.96 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.96-2.77) 93.9 (49.96-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.223 , 0.248 0.218 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4701	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPO, SEP, SO4

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	0.50	0/1032	0.69	0/1391
2	B	0.51	1/3525 (0.0%)	0.73	1/4777 (0.0%)
3	C	0.66	0/85	0.73	0/112
All	All	0.51	1/4642 (0.0%)	0.72	1/6280 (0.0%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	694	GLU	CG-CD	5.64	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	622	LYS	CA-CB-CG	-8.54	94.62	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	619	GLY	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	1018	0	1030	48	0
2	B	3455	0	3428	125	0
3	C	104	0	102	9	0
4	B	25	0	0	1	0
5	A	11	0	0	1	0
5	B	85	0	0	9	0
5	C	3	0	0	0	0
All	All	4701	0	4560	175	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 19.

All (175) 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:376:LEU:HD23	2:B:406:TRP:CE3	1.65	1.32
2:B:530:THR:HG22	2:B:532:THR:HG23	1.19	1.09
2:B:618:GLN:HA	2:B:622:LYS:HG3	1.30	1.08
1:A:14:PHE:CE1	1:A:55:LEU:HD23	1.91	1.06
2:B:530:THR:HG22	2:B:532:THR:CG2	1.89	1.01
2:B:695:THR:HG23	5:B:913:HOH:O	1.60	1.00
2:B:376:LEU:HD23	2:B:406:TRP:CD2	1.98	0.97
3:C:53:PHE:O	3:C:54:GLU:HG2	1.68	0.91
2:B:592:ASN:ND2	2:B:609:LYS:HE3	1.84	0.91
2:B:592:ASN:HD22	2:B:609:LYS:HE3	1.36	0.90
1:A:125:ASN:HD22	1:A:128:LYS:HD2	1.38	0.88
2:B:554:VAL:HG12	2:B:568:VAL:HG22	1.58	0.83
2:B:376:LEU:CD2	2:B:406:TRP:CE3	2.57	0.81
2:B:665:SER:OG	2:B:693:GLU:HG2	1.80	0.80
2:B:530:THR:CG2	2:B:532:THR:HG23	2.09	0.79
2:B:382:HIS:O	2:B:695:THR:HG21	1.82	0.78
1:A:36:MET:HE2	1:A:46:PRO:CD	2.14	0.78
2:B:530:THR:CG2	2:B:532:THR:CG2	2.63	0.76
2:B:336:ILE:HG22	2:B:336:ILE:O	1.88	0.74
2:B:687:GLY:HA3	2:B:695:THR:HG22	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:ASP:HB2	2:B:494:LEU:HD11	1.72	0.72
1:A:101:PHE:CE1	1:A:105:LEU:HD11	2.26	0.71
2:B:512:ARG:HD2	5:B:909:HOH:O	1.89	0.71
2:B:323:GLU:O	2:B:327:GLU:HG2	1.91	0.70
1:A:127:ILE:HG23	1:A:135:ILE:HD13	1.73	0.69
2:B:486:TRP:CZ3	2:B:493:CYS:HB2	2.26	0.69
1:A:27:ILE:HD11	1:A:110:LEU:CD2	2.23	0.69
2:B:515:VAL:HG12	2:B:547:LEU:HD21	1.74	0.69
2:B:695:THR:CG2	5:B:913:HOH:O	2.28	0.69
2:B:376:LEU:HD23	2:B:406:TRP:HE3	1.52	0.68
2:B:460:HIS:O	5:B:901:HOH:O	2.10	0.68
2:B:616:THR:OG1	5:B:902:HOH:O	2.11	0.68
2:B:592:ASN:ND2	2:B:609:LYS:CE	2.57	0.68
2:B:328:GLU:O	2:B:634:LYS:NZ	2.27	0.67
2:B:428:GLN:HG2	2:B:467:MET:HG3	1.75	0.67
2:B:625:SER:HB3	2:B:642:ASP:HB2	1.76	0.67
2:B:674:ARG:HG2	2:B:674:ARG:HH11	1.59	0.66
2:B:523:VAL:HB	2:B:537:LEU:HB2	1.76	0.65
1:A:14:PHE:CD1	1:A:55:LEU:HD23	2.33	0.64
2:B:552:ILE:O	2:B:568:VAL:HG23	1.98	0.63
2:B:673:TRP:O	2:B:674:ARG:HG3	1.98	0.63
1:A:36:MET:CE	1:A:46:PRO:CD	2.78	0.62
2:B:642:ASP:OD2	3:C:55:LEU:HD22	2.00	0.61
2:B:549:PHE:HE1	2:B:568:VAL:HG21	1.64	0.61
1:A:27:ILE:HD11	1:A:110:LEU:HD21	1.82	0.61
1:A:130:LYS:HB3	1:A:134:GLU:HG3	1.82	0.61
2:B:638:ILE:HG22	2:B:675:ILE:HD12	1.82	0.60
1:A:6:LEU:HD23	1:A:45:VAL:HB	1.82	0.60
1:A:14:PHE:CE1	1:A:55:LEU:CD2	2.79	0.59
1:A:109:TYR:CD2	1:A:110:LEU:HD12	2.36	0.59
2:B:376:LEU:HD11	2:B:411:GLY:HA2	1.85	0.58
2:B:425:TRP:CD2	3:C:59:PRO:HG3	2.39	0.57
1:A:37:ASP:HB2	1:A:44:PRO:HD3	1.86	0.57
1:A:137:LYS:HA	1:A:137:LYS:HE2	1.87	0.57
2:B:524:LYS:NZ	2:B:536:THR:OG1	2.38	0.57
2:B:530:THR:CG2	2:B:532:THR:HG21	2.35	0.57
2:B:324:LYS:HA	2:B:327:GLU:HG3	1.87	0.57
2:B:475:VAL:HG22	2:B:485:VAL:HG22	1.87	0.57
2:B:530:THR:HG22	2:B:530:THR:O	2.04	0.57
2:B:415:ARG:HD3	4:B:805:SO4:O4	2.04	0.57
1:A:14:PHE:CZ	1:A:55:LEU:HD23	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:LYS:HE3	2:B:356:ILE:HD11	1.88	0.56
2:B:622:LYS:NZ	2:B:623:HIS:HB2	2.21	0.56
1:A:158:GLN:HB2	5:A:201:HOH:O	2.04	0.56
1:A:14:PHE:CD1	1:A:55:LEU:CD2	2.89	0.56
2:B:298:PRO:HD3	2:B:324:LYS:HD2	1.88	0.56
1:A:157:ASN:HB3	2:B:302:LEU:HD13	1.88	0.55
1:A:27:ILE:HD11	1:A:110:LEU:HD23	1.90	0.54
2:B:519:TYR:CD1	2:B:543:ARG:HB3	2.42	0.54
2:B:639:THR:O	2:B:646:VAL:HA	2.07	0.54
1:A:36:MET:CE	1:A:46:PRO:CG	2.85	0.54
2:B:415:ARG:HD2	2:B:451:GLY:HA3	1.90	0.54
1:A:8:SER:OG	1:A:10:ASP:OD1	2.26	0.53
1:A:36:MET:CE	1:A:46:PRO:HG2	2.38	0.53
1:A:125:ASN:ND2	1:A:128:LYS:HD2	2.16	0.53
2:B:447:ASN:OD1	2:B:450:THR:HG23	2.08	0.53
2:B:265:VAL:HG23	2:B:313:ILE:HG22	1.91	0.52
2:B:583:LEU:HD23	3:C:56:LEU:HD12	1.90	0.52
1:A:18:VAL:O	1:A:22:LYS:HG3	2.10	0.52
2:B:360:ARG:HB3	2:B:704:VAL:HG11	1.91	0.52
2:B:439:THR:HA	2:B:463:THR:OG1	2.10	0.52
2:B:564:ARG:HD3	2:B:566:TRP:CZ2	2.45	0.52
2:B:636:PHE:HB3	2:B:648:LEU:HD11	1.91	0.51
2:B:430:ARG:HB2	2:B:469:LEU:HD21	1.93	0.51
1:A:130:LYS:HB3	1:A:134:GLU:CG	2.41	0.51
3:C:61:LEU:HD22	3:C:61:LEU:N	2.26	0.51
2:B:674:ARG:HG2	2:B:674:ARG:NH1	2.23	0.51
1:A:93:LEU:HD22	1:A:119:THR:HG22	1.92	0.51
2:B:376:LEU:HD11	2:B:411:GLY:CA	2.41	0.50
1:A:36:MET:HE2	1:A:46:PRO:CG	2.40	0.50
1:A:137:LYS:HA	1:A:137:LYS:CE	2.40	0.50
2:B:522:MET:SD	2:B:538:GLN:HG2	2.51	0.50
2:B:674:ARG:NE	5:B:911:HOH:O	2.42	0.50
2:B:704:VAL:O	2:B:705:ASP:OD1	2.30	0.50
2:B:333:PRO:HB2	2:B:350:PRO:HB2	1.94	0.50
1:A:36:MET:CE	1:A:46:PRO:HD3	2.41	0.50
2:B:545:TYR:CG	2:B:583:LEU:HD11	2.47	0.50
2:B:393:ARG:NH2	2:B:414:LEU:HD11	2.26	0.50
2:B:376:LEU:HG	2:B:411:GLY:O	2.12	0.49
1:A:114:GLY:O	1:A:118:VAL:HG23	2.12	0.49
1:A:157:ASN:OD1	2:B:352:LYS:NZ	2.45	0.49
2:B:325:CYS:HB3	2:B:330:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ARG:CZ	2:B:414:LEU:HD11	2.43	0.49
1:A:36:MET:HE2	1:A:46:PRO:HD2	1.92	0.48
2:B:443:LEU:HD21	2:B:476:SER:HB3	1.94	0.48
2:B:603:VAL:HG21	2:B:639:THR:HG21	1.95	0.48
2:B:580:HIS:CE1	2:B:604:LYS:HG3	2.49	0.48
2:B:318:ASN:OD1	2:B:350:PRO:HD2	2.13	0.48
2:B:443:LEU:HB2	2:B:457:LEU:HB2	1.96	0.48
2:B:622:LYS:HD3	2:B:623:HIS:N	2.28	0.48
1:A:157:ASN:HB3	2:B:302:LEU:CD1	2.43	0.47
2:B:604:LYS:HD3	2:B:606:TRP:CZ2	2.48	0.47
1:A:36:MET:HE2	1:A:46:PRO:HG2	1.97	0.47
3:C:53:PHE:C	3:C:55:LEU:H	2.17	0.47
2:B:523:VAL:CG1	2:B:537:LEU:HD12	2.44	0.47
2:B:272:ILE:O	2:B:274:PRO:HD3	2.14	0.47
1:A:27:ILE:CD1	1:A:110:LEU:HD23	2.45	0.47
2:B:622:LYS:CD	2:B:623:HIS:H	2.27	0.46
2:B:598:ASN:HB3	2:B:600:ASP:OD1	2.15	0.46
2:B:269:MET:HG3	2:B:286:LYS:NZ	2.30	0.46
2:B:304:ALA:HB1	2:B:311:TRP:HE3	1.81	0.46
2:B:425:TRP:CG	3:C:59:PRO:HG3	2.51	0.46
2:B:488:ILE:HD13	2:B:488:ILE:HA	1.59	0.46
2:B:486:TRP:CE3	2:B:493:CYS:HB2	2.51	0.46
1:A:149:GLU:O	1:A:153:VAL:HG23	2.16	0.45
2:B:603:VAL:HB	2:B:617:LEU:HD12	1.99	0.45
2:B:371:LYS:HE3	2:B:371:LYS:HB2	1.65	0.45
2:B:376:LEU:HB3	2:B:406:TRP:CZ3	2.51	0.45
2:B:684:CYS:O	2:B:697:LEU:HA	2.17	0.45
1:A:131:THR:OG1	1:A:134:GLU:OE2	2.26	0.44
2:B:530:THR:CG2	2:B:530:THR:O	2.65	0.44
1:A:109:TYR:CD2	1:A:110:LEU:CD1	3.00	0.44
2:B:376:LEU:CD2	2:B:406:TRP:HB3	2.47	0.44
2:B:282:SER:HA	2:B:310:TYR:CE1	2.53	0.44
1:A:30:MET:HB3	1:A:36:MET:HG3	1.98	0.44
1:A:36:MET:HE3	1:A:46:PRO:HD3	1.98	0.44
2:B:647:LYS:HG2	2:B:659:ASN:OD1	2.17	0.44
2:B:500:HIS:HB2	5:B:906:HOH:O	2.17	0.44
2:B:558:SER:HB3	2:B:560:ASP:OD1	2.17	0.44
2:B:360:ARG:O	2:B:364:ASN:HB2	2.18	0.44
2:B:554:VAL:HG22	2:B:566:TRP:CD1	2.53	0.44
2:B:530:THR:HG21	2:B:532:THR:HG21	2.00	0.43
2:B:622:LYS:CD	2:B:623:HIS:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:PHE:O	3:C:54:GLU:CG	2.53	0.43
2:B:483:LEU:HB2	2:B:497:LEU:HB2	2.01	0.43
1:A:132:PRO:O	1:A:136:ARG:HG3	2.19	0.43
2:B:281:ILE:HG12	2:B:311:TRP:CZ2	2.54	0.43
2:B:602:THR:N	2:B:622:LYS:HZ1	2.16	0.43
2:B:268:MET:HG3	2:B:347:ILE:HD12	2.02	0.42
2:B:549:PHE:CE1	2:B:568:VAL:HG21	2.50	0.42
2:B:487:ASP:HB2	2:B:494:LEU:CD1	2.46	0.42
2:B:554:VAL:CG1	2:B:568:VAL:HG22	2.41	0.42
2:B:687:GLY:CA	2:B:695:THR:HG22	2.46	0.42
1:A:137:LYS:HE2	1:A:137:LYS:CA	2.49	0.42
1:A:26:THR:HB	1:A:110:LEU:HA	2.02	0.41
2:B:400:ASP:O	2:B:401:ASN:HB2	2.19	0.41
2:B:580:HIS:CE1	2:B:602:THR:HG22	2.55	0.41
2:B:672:VAL:HG22	2:B:686:VAL:HG22	2.02	0.41
2:B:569:GLU:OE2	5:B:904:HOH:O	2.22	0.41
2:B:642:ASP:HA	2:B:671:VAL:HG23	2.01	0.41
1:A:6:LEU:O	1:A:13:ILE:HA	2.20	0.41
2:B:704:VAL:HG23	2:B:705:ASP:N	2.36	0.41
2:B:336:ILE:O	2:B:336:ILE:CG2	2.59	0.41
2:B:447:ASN:CG	2:B:450:THR:HG23	2.42	0.41
2:B:606:TRP:CZ3	2:B:613:CYS:HB2	2.56	0.41
1:A:93:LEU:HD22	1:A:119:THR:CG2	2.51	0.41
2:B:330:ILE:HD11	2:B:358:GLN:HG2	2.03	0.41
3:C:61:LEU:N	3:C:61:LEU:CD2	2.84	0.41
2:B:435:ILE:HD12	2:B:488:ILE:HD12	2.02	0.40
1:A:14:PHE:CD1	1:A:14:PHE:N	2.90	0.40
2:B:512:ARG:HD3	5:B:942:HOH:O	2.22	0.40
2:B:450:THR:OG1	2:B:452:GLU:HB3	2.21	0.40
2:B:501:VAL:O	2:B:501:VAL:CG1	2.70	0.40
2:B:617:LEU:HB3	2:B:649:TRP:CE3	2.56	0.40
1:A:36:MET:O	1:A:37:ASP:C	2.60	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	123/149 (83%)	110 (89%)	12 (10%)	1 (1%)	19 47
2	B	434/457 (95%)	403 (93%)	31 (7%)	0	100 100
3	C	9/20 (45%)	7 (78%)	2 (22%)	0	100 100
All	All	566/626 (90%)	520 (92%)	45 (8%)	1 (0%)	47 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ASP

5.3.2 Protein sidechains (i)

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	114/133 (86%)	108 (95%)	6 (5%)	22 51
2	B	387/404 (96%)	369 (95%)	18 (5%)	26 56
3	C	10/18 (56%)	9 (90%)	1 (10%)	7 20
All	All	511/555 (92%)	486 (95%)	25 (5%)	25 54

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	24	SER
1	A	64	HIS
1	A	132	PRO
1	A	137	LYS
1	A	146	THR
2	B	276	PHE
2	B	302	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	390	CYS
2	B	421	THR
2	B	435	ILE
2	B	441	ARG
2	B	521	PHE
2	B	554	VAL
2	B	560	ASP
2	B	562	SER
2	B	569	GLU
2	B	576	THR
2	B	602	THR
2	B	625	SER
2	B	642	ASP
2	B	658	ARG
2	B	689	ARG
2	B	694	GLU
3	C	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	125	ASN
2	B	592	ASN
2	B	612	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TPO	C	58	3	8,10,11	1.54	1 (12%)	10,14,16	1.71	2 (20%)
3	SEP	C	62	3	8,9,10	1.84	2 (25%)	8,12,14	1.26	1 (12%)

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	TPO	C	58	3	-	5/9/11/13	-
3	SEP	C	62	3	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	62	SEP	P-O1P	3.85	1.63	1.50
3	C	58	TPO	P-O1P	3.03	1.60	1.50
3	C	62	SEP	P-O3P	2.19	1.63	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	58	TPO	CG2-CB-CA	-3.42	106.41	113.16
3	C	62	SEP	OG-P-O1P	2.53	113.58	106.47
3	C	58	TPO	P-OG1-CB	-2.03	117.06	123.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	58	TPO	N-CA-CB-OG1
3	C	58	TPO	O-C-CA-CB
3	C	58	TPO	CB-OG1-P-O1P
3	C	58	TPO	CB-OG1-P-O2P
3	C	58	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	804	-	4,4,4	0.12	0	6,6,6	0.34	0
4	SO4	B	802	-	4,4,4	0.27	0	6,6,6	0.49	0
4	SO4	B	803	-	4,4,4	0.21	0	6,6,6	0.22	0
4	SO4	B	801	-	4,4,4	0.32	0	6,6,6	0.34	0
4	SO4	B	805	-	4,4,4	0.18	0	6,6,6	0.38	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	805	SO4	1	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, 95^{th} 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	129/149 (86%)	0.93	17 (13%) 3 2	65, 85, 107, 118	0
2	B	438/457 (95%)	0.12	7 (1%) 72 69	25, 39, 84, 110	0
3	C	10/20 (50%)	0.40	1 (10%) 7 5	36, 63, 71, 73	0
All	All	577/626 (92%)	0.31	25 (4%) 35 30	25, 45, 96, 118	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	4.1
1	A	2	PRO	3.9
1	A	18	VAL	3.1
1	A	4	ILE	3.1
1	A	148	GLU	3.1
2	B	337	LYS	3.1
1	A	110	LEU	2.9
1	A	61	TRP	2.6
1	A	59	ILE	2.5
2	B	319	LEU	2.5
1	A	159	TRP	2.4
2	B	263	THR	2.3
1	A	19	GLU	2.3
1	A	62	CYS	2.2
2	B	705	ASP	2.2
2	B	302	LEU	2.2
1	A	55	LEU	2.2
1	A	3	SER	2.1
2	B	295	PHE	2.1
1	A	155	LYS	2.1
1	A	20	ILE	2.1
1	A	113	LYS	2.1
2	B	488	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	141	ILE	2.0
3	C	53	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SEP	C	62	10/11	0.78	0.21	54,83,90,93	0
3	TPO	C	58	11/12	0.98	0.16	30,34,40,42	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	801	5/5	0.91	0.14	57,60,79,87	0
4	SO4	B	803	5/5	0.93	0.12	71,73,84,96	0
4	SO4	B	804	5/5	0.94	0.16	61,66,71,79	0
4	SO4	B	802	5/5	0.97	0.11	48,57,66,68	0
4	SO4	B	805	5/5	0.97	0.14	51,55,62,65	0

6.5 Other polymers (i)

There are no such residues in this entry.