



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:08 AM UTC

PDB ID : 7T1Y / pdb_00007t1y
Title : Structure of the Fbw7-Skp1-MycCdegron complex
Authors : Wang, B.; Rusnac, D.V.; Clurman, B.E.; Zheng, N.
Deposited on : 2021-12-02
Resolution : 2.55 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
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

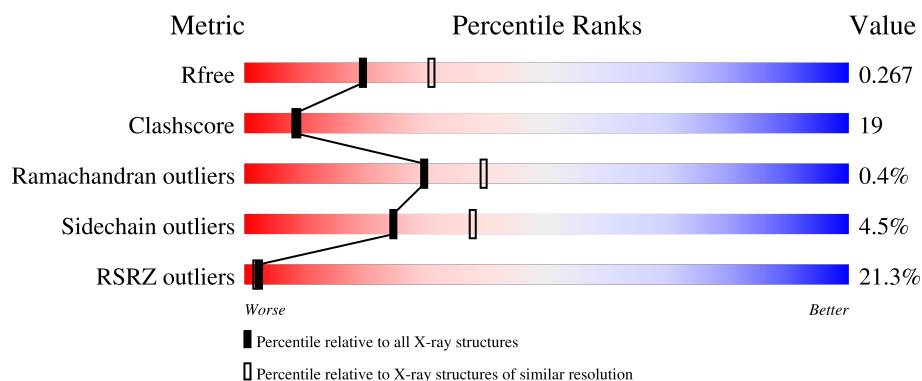
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	156	
2	B	457	
3	C	30	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4681 atoms, of which 5 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	133	Total	C	N	O	S	0	0	0
			1062	678	172	207	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	GLY	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	PRO	deletion	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
			3460	2170	623	645	22			

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

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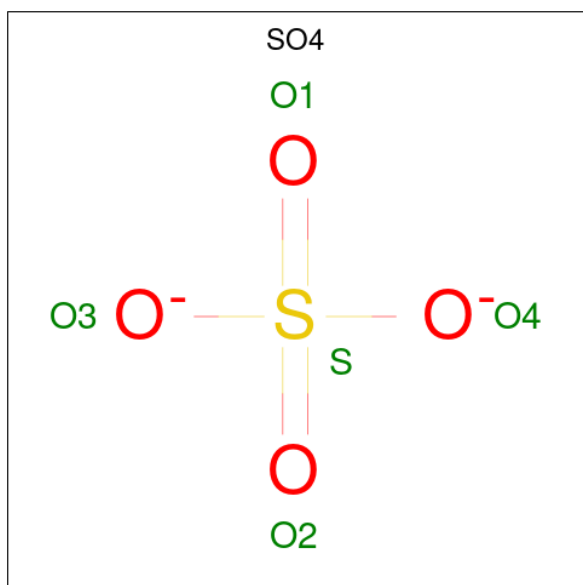
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Chain	Residue	Modelled	Actual	Comment	Reference
B	259	GLY	-	expression tag	UNP Q969H0
B	260	SER	-	expression tag	UNP Q969H0
B	261	GLY	-	expression tag	UNP Q969H0
B	262	MET	-	expression tag	UNP Q969H0

- Molecule 3 is a protein called Myc proto-oncogene protein C terminal degnon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	8	Total	C	H	N	O	P	0	0	0
			71	35	5	8	21	2			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		

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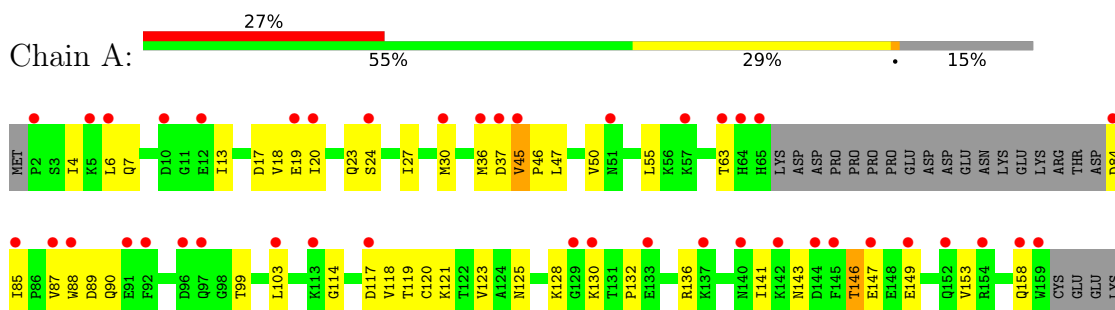
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	64	Total 64	O 64	0	0
5	C	2	Total 2	O 2	0	0

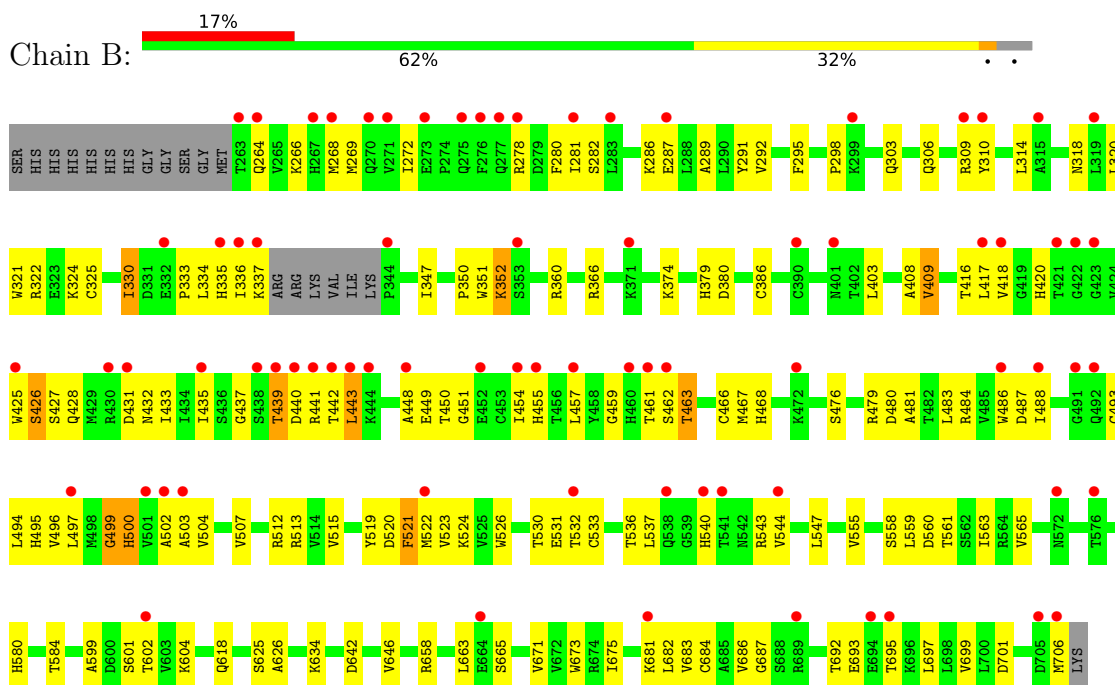
3 Residue-property plots

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

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



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



- Molecule 3: Myc proto-oncogene protein C terminal degnon



PRO	GLU	PRO	LEU	VAL	LEU	H241	H242	E243	T244	P245	P246	T247	T248	SER	SER	SER	ASP	SER	GLU	GLU	GLU	GLN	GLU	ASP	GLU	GLU	ILE	ASP	VAL	VAL

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	232.54Å 232.54Å 107.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.55 49.98 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.98-2.55) 94.4 (49.98-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.253 , 0.268 0.252 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4681	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: SO4, TPO

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	0.71	0/1079	1.11	3/1460 (0.2%)
2	B	0.52	0/3530	0.87	8/4782 (0.2%)
3	C	0.79	0/44	1.15	0/58
All	All	0.58	0/4653	0.93	11/6300 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	440	ASP	N-CA-C	-7.33	99.04	109.96
1	A	37	ASP	N-CA-C	-7.24	105.30	112.97
1	A	23	GLN	N-CA-C	-5.87	106.07	113.18
2	B	439	THR	N-CA-C	-5.79	105.10	111.82
1	A	130	LYS	N-CA-C	5.46	117.29	108.34
2	B	440	ASP	CB-CA-C	5.46	118.02	110.16
2	B	437	GLY	CA-C-O	-5.26	116.99	121.57
2	B	443	LEU	N-CA-C	-5.22	102.46	110.14
2	B	416	THR	CB-CA-C	5.15	118.71	110.16
2	B	439	THR	CB-CA-C	5.08	120.43	110.67
2	B	280	PHE	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

There are no planarity outliers.

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	1062	0	1065	56	0
2	B	3460	0	3436	129	1
3	C	66	5	45	1	0
4	B	15	0	0	0	0
5	A	7	0	0	0	0
5	B	64	0	0	1	0
5	C	2	0	0	0	0
All	All	4676	5	4546	175	1

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)
1:A:6:LEU:CD1	1:A:55:LEU:HD21	1.99	0.92
1:A:36:MET:HE2	1:A:46:PRO:CD	2.03	0.89
2:B:454:ILE:HG22	2:B:455:HIS:CE1	2.07	0.88
2:B:408:ALA:HB1	2:B:681:LYS:NZ	1.88	0.87
1:A:30:MET:CE	1:A:46:PRO:HD2	2.05	0.86
2:B:520:ASP:OD1	2:B:522:MET:HB2	1.74	0.85
1:A:85:ILE:HG22	1:A:90:GLN:HG3	1.59	0.82
2:B:558:SER:HB3	2:B:560:ASP:OD1	1.80	0.81
1:A:85:ILE:CG2	1:A:90:GLN:HG3	2.12	0.79
1:A:6:LEU:HD11	1:A:55:LEU:HD21	1.65	0.79
2:B:264:GLN:O	2:B:268:MET:HG2	1.83	0.78
2:B:681:LYS:HG2	2:B:701:ASP:HA	1.64	0.78
2:B:665:SER:OG	2:B:693:GLU:HG2	1.84	0.77
2:B:540:HIS:CD2	2:B:544:VAL:HG22	2.20	0.77
1:A:30:MET:SD	1:A:45:VAL:HG13	2.26	0.75
2:B:497:LEU:HD13	2:B:526:TRP:CG	2.22	0.74
2:B:408:ALA:O	2:B:681:LYS:NZ	2.21	0.74
2:B:524:LYS:NZ	2:B:536:THR:OG1	2.21	0.73
1:A:85:ILE:HG22	1:A:90:GLN:CG	2.17	0.73
2:B:642:ASP:HA	2:B:671:VAL:HG23	1.71	0.72
2:B:515:VAL:HG12	2:B:547:LEU:HD21	1.70	0.72
2:B:443:LEU:HB2	2:B:457:LEU:HB2	1.72	0.71
2:B:530:THR:HG22	2:B:532:THR:HB	1.73	0.71
2:B:408:ALA:CB	2:B:681:LYS:HZ1	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:PRO:HG3	2:B:351:TRP:CZ2	2.26	0.71
2:B:459:GLY:HA3	2:B:484:ARG:NH1	2.06	0.70
2:B:487:ASP:HB2	2:B:494:LEU:HD21	1.71	0.70
2:B:481:ALA:HB1	2:B:500:HIS:O	1.92	0.69
1:A:85:ILE:CG2	1:A:90:GLN:CG	2.69	0.69
2:B:495:HIS:HB3	2:B:531:GLU:HG2	1.73	0.69
2:B:435:ILE:HG22	2:B:467:MET:SD	2.33	0.69
2:B:502:ALA:HB3	2:B:520:ASP:N	2.08	0.68
2:B:530:THR:HG22	2:B:530:THR:O	1.93	0.68
1:A:30:MET:HE1	1:A:46:PRO:HD2	1.76	0.68
2:B:580:HIS:CE1	2:B:604:LYS:HD2	2.29	0.67
2:B:298:PRO:HD3	2:B:324:LYS:HE3	1.75	0.67
2:B:408:ALA:CB	2:B:681:LYS:NZ	2.57	0.67
1:A:125:ASN:HA	1:A:128:LYS:HG3	1.76	0.66
1:A:30:MET:HE2	1:A:45:VAL:HA	1.76	0.66
2:B:281:ILE:HG23	2:B:289:ALA:HB1	1.78	0.66
2:B:523:VAL:HB	2:B:537:LEU:HB2	1.78	0.65
2:B:486:TRP:CZ3	2:B:493:CYS:HB2	2.31	0.65
2:B:408:ALA:HB1	2:B:681:LYS:HZ2	1.61	0.65
1:A:85:ILE:HG13	1:A:121:LYS:HE3	1.79	0.64
2:B:526:TRP:CZ3	2:B:533:CYS:HB2	2.33	0.64
1:A:7:GLN:HB2	1:A:13:ILE:HG22	1.79	0.63
1:A:36:MET:HE2	1:A:46:PRO:HD3	1.78	0.63
1:A:6:LEU:HD13	1:A:55:LEU:HD21	1.78	0.63
2:B:360:ARG:HD2	2:B:706:MET:HE3	1.80	0.63
2:B:484:ARG:HG2	2:B:496:VAL:HG12	1.81	0.63
2:B:663:LEU:HD11	2:B:686:VAL:HG13	1.82	0.62
1:A:121:LYS:HG3	2:B:295:PHE:CD2	2.35	0.61
1:A:6:LEU:HD13	1:A:47:LEU:HD12	1.83	0.61
2:B:439:THR:HA	2:B:463:THR:OG1	2.01	0.60
2:B:268:MET:SD	2:B:347:ILE:HG13	2.40	0.60
2:B:408:ALA:C	2:B:681:LYS:NZ	2.59	0.60
2:B:462:SER:HB2	2:B:480:ASP:HB3	1.83	0.60
2:B:497:LEU:HD22	2:B:526:TRP:CE3	2.37	0.60
1:A:36:MET:HE2	1:A:46:PRO:HD2	1.84	0.60
1:A:4:ILE:HG23	1:A:18:VAL:HG22	1.83	0.59
2:B:269:MET:HG3	2:B:286:LYS:HE2	1.85	0.59
2:B:336:ILE:HG22	2:B:337:LYS:N	2.17	0.59
2:B:454:ILE:CG2	2:B:455:HIS:CE1	2.83	0.58
2:B:497:LEU:HD13	2:B:526:TRP:CD1	2.38	0.58
2:B:476:SER:O	2:B:483:LEU:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:PRO:HG3	2:B:351:TRP:CE2	2.38	0.58
1:A:24:SER:OG	1:A:27:ILE:HD12	2.04	0.57
1:A:30:MET:CE	1:A:45:VAL:HA	2.35	0.57
2:B:495:HIS:HB3	2:B:531:GLU:CG	2.34	0.57
1:A:153:VAL:HG12	2:B:306:GLN:HG2	1.86	0.57
2:B:320:LEU:O	2:B:324:LYS:HG2	2.05	0.57
2:B:432:ASN:HA	2:B:448:ALA:HB3	1.87	0.57
2:B:488:ILE:HD13	2:B:488:ILE:N	2.19	0.57
2:B:322:ARG:HE	2:B:351:TRP:NE1	2.03	0.56
1:A:99:THR:O	1:A:103:LEU:HG	2.05	0.56
2:B:530:THR:O	2:B:530:THR:CG2	2.52	0.56
1:A:30:MET:HE1	1:A:46:PRO:CD	2.36	0.56
1:A:85:ILE:HG22	1:A:90:GLN:CD	2.30	0.56
2:B:325:CYS:HB3	2:B:330:ILE:HB	1.88	0.56
2:B:540:HIS:HD2	2:B:544:VAL:HG22	1.67	0.56
1:A:30:MET:CE	1:A:46:PRO:CD	2.82	0.55
2:B:521:PHE:HD1	2:B:521:PHE:N	2.03	0.55
1:A:114:GLY:O	1:A:118:VAL:HG23	2.06	0.55
2:B:336:ILE:HG22	2:B:337:LYS:H	1.71	0.55
2:B:334:LEU:HD12	2:B:335:HIS:H	1.72	0.55
2:B:462:SER:HB3	2:B:480:ASP:N	2.21	0.55
2:B:521:PHE:N	2:B:521:PHE:CD1	2.74	0.55
2:B:540:HIS:HD2	2:B:544:VAL:CG2	2.20	0.55
2:B:563:ILE:HD11	2:B:584:THR:HG21	1.88	0.55
2:B:408:ALA:HB1	2:B:681:LYS:HZ1	1.61	0.55
2:B:502:ALA:H	2:B:520:ASP:HB3	1.73	0.55
2:B:321:TRP:CE2	2:B:352:LYS:HG3	2.43	0.54
1:A:17:ASP:HB3	1:A:19:GLU:OE1	2.08	0.53
2:B:427:SER:O	2:B:428:GLN:HG2	2.08	0.53
1:A:17:ASP:HB2	1:A:20:ILE:HD12	1.90	0.53
2:B:426:SER:HB2	2:B:467:MET:HG2	1.89	0.53
1:A:36:MET:CE	1:A:46:PRO:CD	2.83	0.52
2:B:432:ASN:O	2:B:433:ILE:HD13	2.10	0.52
2:B:443:LEU:HD21	2:B:476:SER:HB3	1.92	0.51
1:A:117:ASP:OD1	2:B:291:TYR:OH	2.19	0.51
1:A:121:LYS:HG3	2:B:295:PHE:HD2	1.74	0.51
2:B:454:ILE:HG22	2:B:455:HIS:ND1	2.24	0.50
2:B:318:ASN:OD1	2:B:350:PRO:HD2	2.11	0.50
2:B:479:ARG:HA	2:B:503:ALA:HB1	1.92	0.50
1:A:36:MET:CE	1:A:46:PRO:HD2	2.42	0.50
2:B:449:GLU:HA	2:B:449:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:CYS:HB2	2:B:507:VAL:HG12	1.92	0.49
2:B:530:THR:CG2	2:B:532:THR:HB	2.41	0.49
2:B:580:HIS:HB2	5:B:904:HOH:O	2.13	0.49
2:B:264:GLN:HG3	2:B:347:ILE:HG21	1.93	0.49
2:B:500:HIS:CE1	2:B:524:LYS:HD2	2.47	0.48
1:A:6:LEU:HD12	1:A:6:LEU:C	2.38	0.48
2:B:499:GLY:O	2:B:524:LYS:HE3	2.14	0.48
1:A:158:GLN:HA	1:A:158:GLN:OE1	2.13	0.47
2:B:403:LEU:HB2	2:B:417:LEU:HB2	1.96	0.47
2:B:425:TRP:CG	3:C:245:PRO:HG3	2.49	0.47
2:B:555:VAL:HG22	2:B:565:VAL:HG22	1.95	0.47
1:A:132:PRO:HD3	2:B:303:GLN:NE2	2.29	0.47
1:A:30:MET:HE3	1:A:46:PRO:HD2	1.93	0.47
2:B:450:THR:O	2:B:451:GLY:C	2.58	0.47
2:B:673:TRP:HZ3	2:B:695:THR:HG23	1.79	0.47
2:B:673:TRP:CH2	2:B:687:GLY:HA3	2.50	0.47
2:B:266:LYS:HE2	2:B:286:LYS:HD2	1.96	0.46
1:A:20:ILE:HD13	1:A:63:THR:HG22	1.98	0.46
1:A:120:CYS:HB3	2:B:292:VAL:HG22	1.98	0.46
1:A:158:GLN:HB3	2:B:360:ARG:HH21	1.80	0.46
1:A:120:CYS:CB	2:B:292:VAL:HG22	2.47	0.45
1:A:13:ILE:HD12	1:A:13:ILE:C	2.41	0.45
1:A:119:THR:O	1:A:123:VAL:HG23	2.16	0.45
1:A:143:ASN:OD1	1:A:143:ASN:C	2.60	0.45
2:B:435:ILE:HG22	2:B:467:MET:HE1	1.97	0.45
2:B:435:ILE:CG2	2:B:467:MET:SD	3.04	0.45
2:B:502:ALA:HB1	2:B:519:TYR:HB2	1.98	0.45
2:B:540:HIS:CD2	2:B:544:VAL:CG2	2.93	0.45
1:A:85:ILE:CD1	1:A:125:ASN:HD21	2.29	0.45
1:A:136:ARG:HA	1:A:141:ILE:HB	2.00	0.45
2:B:494:LEU:C	2:B:495:HIS:CG	2.95	0.45
2:B:432:ASN:OD1	2:B:449:GLU:HB2	2.17	0.44
2:B:599:ALA:HA	2:B:626:ALA:CB	2.48	0.44
1:A:85:ILE:HG21	1:A:90:GLN:CG	2.48	0.44
2:B:269:MET:HG3	2:B:286:LYS:CE	2.47	0.44
2:B:512:ARG:CZ	2:B:513:ARG:HD2	2.47	0.44
1:A:85:ILE:CG1	1:A:121:LYS:HE3	2.47	0.44
2:B:366:ARG:O	2:B:658:ARG:HD2	2.18	0.44
2:B:322:ARG:HE	2:B:351:TRP:HE1	1.63	0.43
1:A:50:VAL:HG11	1:A:55:LEU:HD13	1.99	0.43
2:B:646:VAL:HG11	2:B:682:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:SER:HA	2:B:310:TYR:CE1	2.53	0.43
2:B:513:ARG:HG3	2:B:513:ARG:HH11	1.83	0.43
2:B:675:ILE:HA	2:B:683:VAL:O	2.19	0.43
2:B:433:ILE:HG21	2:B:488:ILE:HG21	2.01	0.43
2:B:484:ARG:HD3	2:B:486:TRP:CH2	2.54	0.43
2:B:457:LEU:HD13	2:B:486:TRP:CG	2.54	0.42
2:B:663:LEU:HD13	2:B:693:GLU:HG3	2.00	0.42
2:B:314:LEU:HD23	2:B:314:LEU:HA	1.87	0.42
2:B:684:CYS:O	2:B:697:LEU:HA	2.20	0.42
2:B:428:GLN:OE1	2:B:468:HIS:HA	2.19	0.42
1:A:87:VAL:HG13	1:A:88:TRP:N	2.34	0.41
1:A:89:ASP:HB3	1:A:118:VAL:HG11	2.02	0.41
2:B:336:ILE:CG2	2:B:337:LYS:N	2.83	0.41
2:B:379:HIS:O	2:B:380:ASP:C	2.63	0.41
1:A:149:GLU:O	1:A:153:VAL:HG23	2.20	0.41
2:B:431:ASP:C	2:B:433:ILE:H	2.28	0.41
2:B:500:HIS:CD2	2:B:504:VAL:HG22	2.56	0.41
2:B:663:LEU:HD11	2:B:686:VAL:CG1	2.48	0.41
2:B:519:TYR:CD1	2:B:543:ARG:HB3	2.55	0.41
2:B:287:GLU:CD	2:B:287:GLU:H	2.28	0.41
2:B:435:ILE:HG22	2:B:467:MET:CE	2.49	0.41
2:B:374:LYS:HE3	2:B:409:VAL:O	2.20	0.41
1:A:24:SER:OG	1:A:27:ILE:HB	2.21	0.41
1:A:146:THR:HG23	2:B:309:ARG:HH21	1.84	0.41
2:B:386:CYS:SG	2:B:427:SER:HB2	2.61	0.41
2:B:559:LEU:HD12	2:B:559:LEU:O	2.20	0.40
2:B:681:LYS:HD2	2:B:699:VAL:HG12	2.03	0.40
1:A:149:GLU:OE1	2:B:309:ARG:NH2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:O	2:B:278:ARG:CD[10_775]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/156 (83%)	118 (92%)	11 (8%)	0	100	100
2	B	434/457 (95%)	402 (93%)	30 (7%)	2 (0%)	24	34
3	C	5/30 (17%)	5 (100%)	0	0	100	100
All	All	568/643 (88%)	525 (92%)	41 (7%)	2 (0%)	30	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	441	ARG
2	B	499	GLY

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	120/144 (83%)	116 (97%)	4 (3%)	33	50
2	B	388/404 (96%)	369 (95%)	19 (5%)	22	34
3	C	5/28 (18%)	5 (100%)	0	100	100
All	All	513/576 (89%)	490 (96%)	23 (4%)	24	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	84	ASP
1	A	146	THR
1	A	147	GLU
2	B	272	ILE
2	B	330	ILE
2	B	352	LYS
2	B	409	VAL
2	B	418	VAL
2	B	420	HIS
2	B	426	SER
2	B	442	THR
2	B	461	THR
2	B	463	THR
2	B	500	HIS
2	B	521	PHE
2	B	561	THR
2	B	601	SER
2	B	602	THR
2	B	618	GLN
2	B	625	SER
2	B	634	LYS
2	B	692	THR

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

Mol	Chain	Res	Type
2	B	306	GLN
2	B	358	GLN
2	B	388	GLN
2	B	420	HIS
2	B	455	HIS
2	B	540	HIS
2	B	618	GLN
2	B	635	ASN
2	B	679	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	248	3	8,10,11	0.73	0	10,14,16	1.16	1 (10%)
3	TPO	C	244	3	8,10,11	0.69	0	10,14,16	1.28	2 (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	TPO	C	248	3	-	4/9/11/13	-
3	TPO	C	244	3	-	2/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	248	TPO	O-C-CA	-3.02	117.00	124.77
3	C	244	TPO	O-C-CA	-2.65	117.96	124.77
3	C	244	TPO	P-OG1-CB	-2.20	117.36	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	244	TPO	N-CA-CB-OG1
3	C	244	TPO	O-C-CA-CB
3	C	248	TPO	N-CA-CB-OG1
3	C	248	TPO	C-CA-CB-CG2
3	C	248	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	C	248	TPO	N-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	803	-	4,4,4	0.38	0	6,6,6	0.10	0
4	SO4	B	802	-	4,4,4	0.44	0	6,6,6	0.09	0
4	SO4	B	801	-	4,4,4	0.35	0	6,6,6	0.21	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	133/156 (85%)	1.82	42 (31%) 1 0	63, 79, 97, 109	0
2	B	438/457 (95%)	0.93	77 (17%) 4 3	29, 51, 80, 101	0
3	C	6/30 (20%)	3.47	4 (66%) 0 0	70, 77, 89, 94	0
All	All	577/643 (89%)	1.16	123 (21%) 2 2	29, 57, 90, 109	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	241	HIS	6.6
2	B	278	ARG	6.0
2	B	273	GLU	5.8
1	A	2	PRO	5.7
1	A	37	ASP	5.5
1	A	30	MET	5.1
2	B	263	THR	4.9
1	A	36	MET	4.7
2	B	422	GLY	4.5
2	B	337	LYS	4.5
2	B	438	SER	4.4
1	A	87	VAL	4.4
2	B	319	LEU	4.3
3	C	247	THR	4.1
1	A	159	TRP	4.1
1	A	129	GLY	4.1
2	B	344	PRO	4.0
2	B	268	MET	4.0
2	B	281	ILE	4.0
2	B	576	THR	3.9
2	B	441	ARG	3.8
2	B	264	GLN	3.7
1	A	147	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	275	GLN	3.6
1	A	91	GLU	3.5
3	C	242	GLU	3.5
2	B	681	LYS	3.5
2	B	439	THR	3.5
2	B	336	ILE	3.5
2	B	267	HIS	3.5
2	B	457	LEU	3.3
2	B	501	VAL	3.3
2	B	705	ASP	3.3
2	B	706	MET	3.3
1	A	130	LYS	3.3
2	B	695	THR	3.3
1	A	137	LYS	3.3
1	A	57	LYS	3.2
2	B	277	GLN	3.2
2	B	440	ASP	3.2
2	B	430	ARG	3.2
1	A	133	GLU	3.2
3	C	243	GLU	3.2
1	A	85	ILE	3.2
1	A	152	GLN	3.2
2	B	538	GLN	3.1
1	A	6	LEU	3.1
2	B	462	SER	3.1
2	B	461	THR	3.1
2	B	315	ALA	3.1
1	A	84	ASP	3.1
2	B	371	LYS	3.0
2	B	492	GLN	3.0
2	B	503	ALA	3.0
1	A	88	TRP	3.0
1	A	63	THR	3.0
2	B	472	LYS	3.0
1	A	51	ASN	2.9
1	A	140	ASN	2.9
1	A	20	ILE	2.9
2	B	497	LEU	2.9
2	B	276	PHE	2.9
1	A	5	LYS	2.8
2	B	353	SER	2.8
2	B	310	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	455	HIS	2.8
2	B	486	TRP	2.7
2	B	309	ARG	2.7
1	A	64	HIS	2.7
2	B	418	VAL	2.6
1	A	65	HIS	2.6
2	B	460	HIS	2.6
1	A	142	LYS	2.6
1	A	24	SER	2.5
1	A	113	LYS	2.5
1	A	10	ASP	2.5
2	B	435	ILE	2.5
2	B	287	GLU	2.5
2	B	664	GLU	2.5
1	A	117	ASP	2.5
1	A	19	GLU	2.5
2	B	443	LEU	2.5
2	B	540	HIS	2.5
2	B	431	ASP	2.4
2	B	335	HIS	2.4
2	B	332	GLU	2.4
2	B	522	MET	2.4
2	B	544	VAL	2.4
1	A	149	GLU	2.4
2	B	541	THR	2.3
1	A	96	ASP	2.3
2	B	444	LYS	2.3
2	B	417	LEU	2.3
2	B	488	ILE	2.3
2	B	299	LYS	2.3
2	B	401	ASN	2.3
2	B	448	ALA	2.3
2	B	425	TRP	2.3
1	A	45	VAL	2.3
1	A	144	ASP	2.2
2	B	532	THR	2.2
2	B	270	GLN	2.2
2	B	602	THR	2.2
2	B	491	GLY	2.2
2	B	689	ARG	2.2
2	B	421	THR	2.2
1	A	103	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	390	CYS	2.2
2	B	454	ILE	2.2
1	A	145	PHE	2.2
2	B	423	GLY	2.1
2	B	442	THR	2.1
2	B	271	VAL	2.1
2	B	694	GLU	2.1
1	A	92	PHE	2.1
2	B	572	ASN	2.1
1	A	154	ARG	2.1
2	B	452	GLU	2.1
2	B	283	LEU	2.0
1	A	97	GLN	2.0
1	A	158	GLN	2.0
2	B	502	ALA	2.0
1	A	12	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TPO	C	248	11/12	0.59	0.26	80,97,117,120	0
3	TPO	C	244	11/12	0.92	0.13	50,61,69,70	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	803	5/5	0.77	0.25	68,83,99,110	0
4	SO4	B	801	5/5	0.87	0.20	68,69,87,90	0
4	SO4	B	802	5/5	0.89	0.18	61,64,71,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.