



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 5DSE / pdb_00005dse
Title : Crystal Structure of the TTC7B/Hyccin Complex
Authors : Wu, X.; Baskin, J.M.; Reinisch, K.M.; De Camilli, P.
Deposited on : 2015-09-17
Resolution : 2.90 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
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

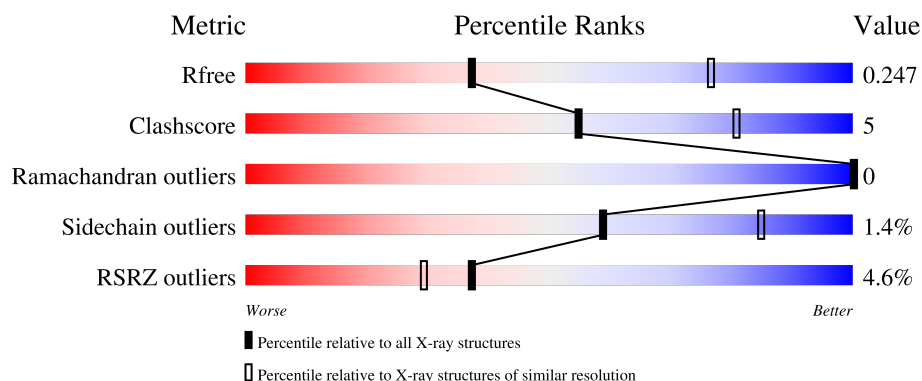
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	837	4% 57% 7% 36%
1	C	837	2% 75% 10% 15%
2	B	312	6% 62% 12% 26%
2	D	312	4% 69% 16% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13875 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 Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4242	2714	730	771	27			
1	C	712	Total	C	N	O	S	0	0	0
			5647	3591	982	1042	32			

- Molecule 2 is a protein called Hyccin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	231	Total	C	N	O	S	0	0	0
			1844	1205	293	334	12			
2	D	264	Total	C	N	O	S	0	0	0
			2091	1357	338	383	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9BYI3
B	-2	PRO	-	expression tag	UNP Q9BYI3
B	-1	LEU	-	expression tag	UNP Q9BYI3
B	0	GLY	-	expression tag	UNP Q9BYI3
B	1	SER	-	expression tag	UNP Q9BYI3
D	-3	GLY	-	expression tag	UNP Q9BYI3
D	-2	PRO	-	expression tag	UNP Q9BYI3
D	-1	LEU	-	expression tag	UNP Q9BYI3
D	0	GLY	-	expression tag	UNP Q9BYI3
D	1	SER	-	expression tag	UNP Q9BYI3

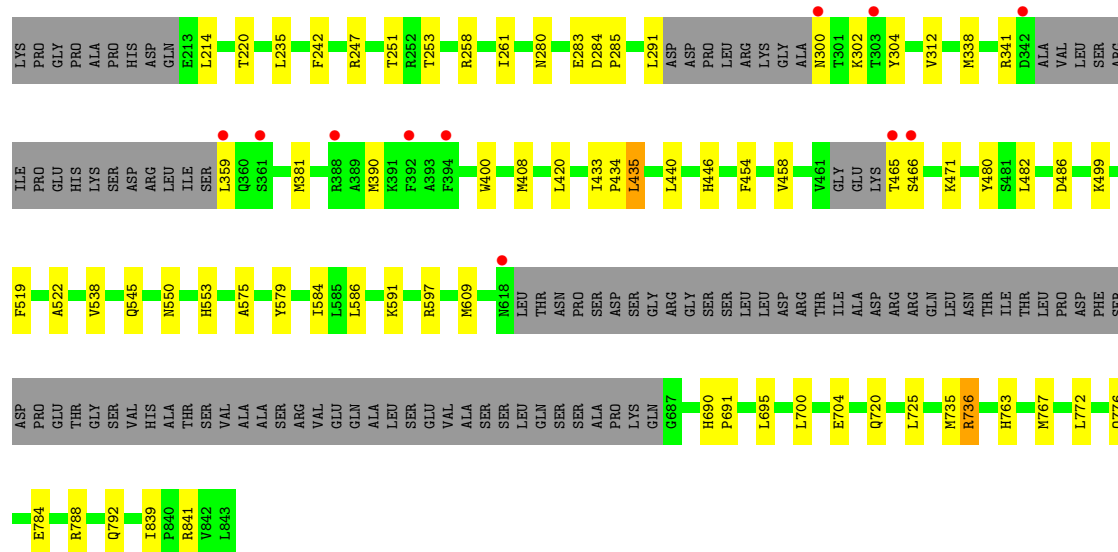
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		

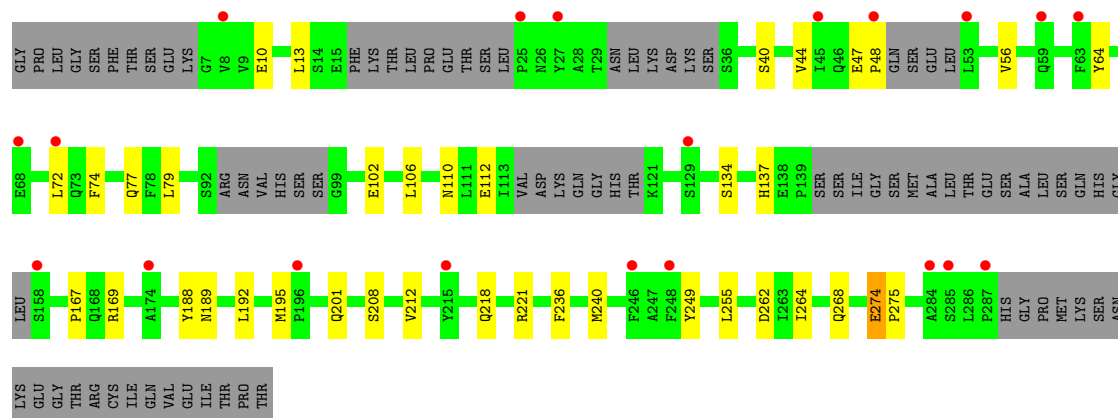
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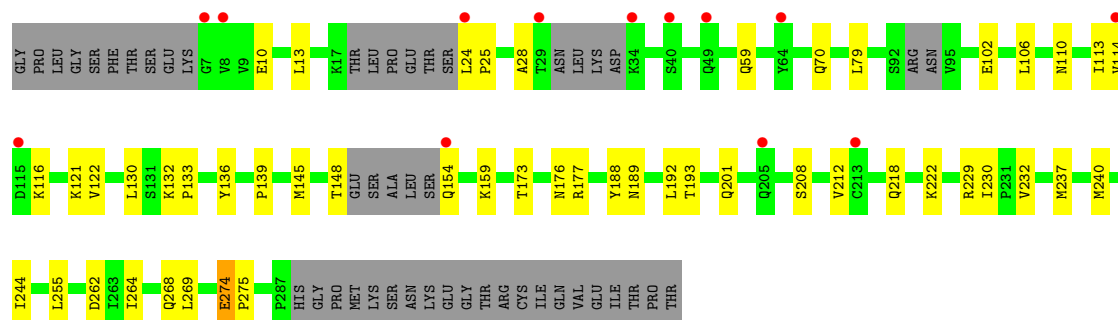
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total 32	O 32	0	0
3	D	2	Total 2	O 2	0	0



• Molecule 2: Hyccin



• Molecule 2: Hyccin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.78Å 168.07Å 239.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.90 29.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.96-2.90) 96.2 (29.96-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.32 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1630)	Depositor
R, R_{free}	0.212 , 0.242 0.217 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.5	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	0.93	EDS
Total number of atoms	13875	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.29	0/4319	0.69	0/5839
1	C	0.30	0/5747	0.72	4/7771 (0.1%)
2	B	0.29	0/1887	0.74	0/2560
2	D	0.31	0/2140	0.74	0/2903
All	All	0.30	0/14093	0.72	4/19073 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	VAL	CA-C-N	7.05	124.81	119.66
1	C	133	VAL	C-N-CA	7.05	124.81	119.66
1	C	284	ASP	CA-C-N	6.01	124.05	119.66
1	C	284	ASP	C-N-CA	6.01	124.05	119.66

There are no chirality outliers.

There are no planarity outliers.

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	4242	0	4292	39	0
1	C	5647	0	5715	48	0
2	B	1844	0	1847	22	0
2	D	2091	0	2096	32	0
3	A	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	0	0	0
3	D	2	0	0	0	0
All	All	13875	0	13950	134	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 5.

All (134) 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:D:274:GLU:HG2	2:D:275:PRO:HD3	1.58	0.85
2:B:274:GLU:HG2	2:B:275:PRO:HD3	1.61	0.83
1:C:482:LEU:HD23	1:C:841:ARG:HH11	1.55	0.72
1:A:187:LEU:HD21	1:A:253:THR:HB	1.73	0.70
1:A:180:GLY:HA3	1:A:241:ARG:HH22	1.55	0.70
1:C:280:ASN:HB2	1:C:283:GLU:HB2	1.75	0.69
1:A:334:ILE:HG22	1:A:338:MET:HE2	1.75	0.68
1:A:482:LEU:HD23	1:A:841:ARG:HH11	1.60	0.66
1:A:187:LEU:HG	1:A:251:THR:HG21	1.76	0.66
1:C:258:ARG:NH2	2:D:136:TYR:O	2.31	0.63
1:C:291:LEU:HD23	2:D:193:THR:HG21	1.81	0.63
2:B:106:LEU:O	2:B:110:ASN:ND2	2.33	0.61
2:D:10:GLU:HA	2:D:13:LEU:HD12	1.83	0.61
1:C:586:LEU:HD13	1:C:609:MET:HG2	1.83	0.58
1:A:187:LEU:HD23	1:A:254:THR:HG23	1.85	0.58
2:D:106:LEU:O	2:D:110:ASN:ND2	2.37	0.58
1:A:586:LEU:HD13	1:A:609:MET:HG2	1.86	0.56
1:C:482:LEU:HD23	1:C:841:ARG:NH1	2.20	0.56
1:A:700:LEU:HD22	1:A:735:MET:HG3	1.88	0.56
1:A:422:GLU:HG2	1:A:425:ARG:HH21	1.71	0.56
2:D:79:LEU:HD23	2:D:188:TYR:HB2	1.88	0.55
1:C:720:GLN:OE1	1:C:736:ARG:NH2	2.39	0.55
1:A:482:LEU:HD23	1:A:841:ARG:NH1	2.22	0.55
2:D:208:SER:OG	2:D:262:ASP:OD2	2.21	0.55
1:A:792:GLN:HG3	1:C:792:GLN:HG3	1.88	0.55
1:C:189:GLU:OE2	1:C:192:ARG:NH2	2.30	0.55
2:B:10:GLU:HA	2:B:13:LEU:HD12	1.88	0.54
2:B:189:ASN:HA	2:B:192:LEU:HG	1.89	0.54
1:C:181:ASP:OD2	1:C:304:TYR:OH	2.24	0.54
2:B:77:GLN:HA	2:B:195:MET:HE1	1.89	0.54
2:B:64:TYR:HA	2:B:72:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HD23	1:A:725:LEU:HD11	1.90	0.53
2:B:208:SER:OG	2:B:262:ASP:OD2	2.23	0.53
1:A:271:ARG:HD3	2:B:249:TYR:CG	2.44	0.53
1:C:435:LEU:HD21	1:C:471:LYS:HB3	1.90	0.53
1:C:242:PHE:HA	1:C:261:ILE:HD11	1.90	0.52
2:B:236:PHE:CE2	2:B:240:MET:HE3	2.45	0.52
1:A:575:ALA:O	1:A:579:TYR:N	2.41	0.52
2:D:189:ASN:HA	2:D:192:LEU:HG	1.92	0.52
2:D:133:PRO:HD3	2:D:139:PRO:HG3	1.92	0.51
1:C:54:GLU:OE2	1:C:105:LYS:NZ	2.44	0.51
1:C:553:HIS:HE1	1:C:584:ILE:HG22	1.77	0.50
2:D:218:GLN:O	2:D:222:LYS:N	2.44	0.50
1:A:267:GLU:O	1:A:271:ARG:HG2	2.11	0.50
2:B:201:GLN:HG2	2:B:255:LEU:HD12	1.93	0.50
1:C:79:ARG:O	1:C:83:THR:OG1	2.19	0.49
1:C:763:HIS:O	1:C:767:MET:HG3	2.12	0.49
2:D:110:ASN:HA	2:D:113:ILE:HG12	1.93	0.49
1:C:82:LEU:HD11	1:C:102:ILE:HG22	1.93	0.49
1:C:690:HIS:CG	1:C:691:PRO:HD3	2.47	0.49
1:A:370:THR:HG22	1:A:382:LEU:HD11	1.95	0.49
1:A:242:PHE:HB3	1:A:265:LEU:HD22	1.95	0.49
1:A:280:ASN:HD21	1:A:322:GLN:HG3	1.78	0.48
1:A:408:MET:HG3	1:A:440:LEU:HD11	1.96	0.48
1:A:420:LEU:HD22	1:A:433:ILE:HG23	1.93	0.48
1:C:420:LEU:HD22	1:C:433:ILE:HG23	1.94	0.48
2:D:13:LEU:HD23	2:D:59:GLN:OE1	2.13	0.48
2:D:145:MET:HA	2:D:148:THR:HG22	1.95	0.48
1:A:215:GLY:HA3	1:A:218:LEU:HD12	1.95	0.47
1:A:226:HIS:HA	1:A:229:TYR:HB2	1.95	0.47
1:A:386:LEU:O	1:A:390:MET:HG2	2.14	0.47
1:A:747:ASP:O	1:A:751:ARG:HG2	2.13	0.47
1:A:522:ALA:HB1	1:A:538:VAL:HG23	1.96	0.47
1:C:381:MET:HE3	2:D:154:GLN:HE21	1.78	0.47
1:C:522:ALA:HB1	1:C:538:VAL:HG23	1.95	0.47
1:C:465:THR:OG1	1:C:466:SER:N	2.47	0.47
1:C:258:ARG:NH1	1:C:338:MET:HE1	2.30	0.46
1:C:285:PRO:HG3	1:C:300:ASN:ND2	2.30	0.46
1:A:837:THR:HG22	1:A:841:ARG:HH21	1.80	0.46
1:C:251:THR:HG22	1:C:253:THR:H	1.81	0.46
1:A:478:LEU:HD22	1:A:841:ARG:HB3	1.97	0.46
1:C:446:HIS:NE2	1:C:486:ASP:OD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:GLU:O	1:C:788:ARG:HG2	2.16	0.45
2:D:116:LYS:HE3	2:D:122:VAL:H	1.80	0.45
1:A:417:VAL:HG12	1:A:421:LYS:HE3	1.97	0.45
2:D:28:ALA:HB1	2:D:70:GLN:HG3	1.98	0.45
1:C:700:LEU:HD22	1:C:735:MET:HG3	1.98	0.45
1:C:50:GLU:HB2	1:C:102:ILE:HD13	1.99	0.45
2:B:134:SER:OG	2:B:137:HIS:ND1	2.41	0.44
2:D:212:VAL:O	2:D:218:GLN:HB2	2.17	0.44
1:A:423:CYS:HB3	1:A:433:ILE:HD13	1.98	0.44
1:C:519:PHE:CZ	1:C:550:ASN:HB3	2.52	0.44
1:A:784:GLU:O	1:A:788:ARG:HG2	2.18	0.44
2:B:74:PHE:O	2:B:77:GLN:HG2	2.17	0.44
1:C:545:GLN:NE2	2:D:229:ARG:O	2.44	0.44
1:A:523:LEU:O	1:A:527:ILE:HG13	2.16	0.44
1:A:837:THR:O	3:A:901:HOH:O	2.21	0.44
2:B:167:PRO:HG2	2:B:169:ARG:HE	1.82	0.44
1:C:695:LEU:HD23	1:C:725:LEU:HD11	2.00	0.44
1:C:519:PHE:HZ	1:C:839:ILE:HG21	1.83	0.44
1:C:434:PRO:HG2	1:C:458:VAL:HG22	1.99	0.43
1:C:338:MET:HA	1:C:341:ARG:HD3	1.99	0.43
1:C:772:LEU:O	1:C:776:GLN:HG2	2.18	0.43
2:D:113:ILE:HG13	2:D:114:VAL:N	2.32	0.43
2:D:237:MET:O	2:D:240:MET:HB2	2.17	0.43
2:B:44:VAL:HG11	2:B:56:VAL:HG21	1.99	0.43
2:D:116:LYS:HE3	2:D:121:LYS:HA	2.01	0.43
2:B:79:LEU:HD23	2:B:188:TYR:HB2	2.01	0.43
2:D:176:ASN:OD1	2:D:177:ARG:N	2.51	0.43
2:B:208:SER:O	2:B:212:VAL:HG22	2.18	0.43
1:C:247:ARG:HB3	1:C:312:VAL:HG13	2.00	0.43
1:A:609:MET:HE3	1:A:698:ILE:HG23	2.01	0.43
1:C:597:ARG:HA	1:C:597:ARG:HD3	1.84	0.43
2:D:24:LEU:HB2	2:D:25:PRO:HD3	2.01	0.43
1:A:694:THR:O	1:A:698:ILE:HG13	2.19	0.42
2:B:47:GLU:HA	2:B:48:PRO:HD3	1.88	0.42
2:B:212:VAL:O	2:B:218:GLN:HB2	2.18	0.42
1:A:408:MET:HE2	1:A:420:LEU:HD11	2.00	0.42
2:B:64:TYR:OH	2:B:112:GLU:OE2	2.25	0.42
2:B:264:ILE:O	2:B:268:GLN:HG3	2.20	0.42
1:C:553:HIS:CE1	1:C:584:ILE:HG22	2.53	0.42
1:C:471:LYS:NZ	2:D:269:LEU:O	2.51	0.42
1:C:390:MET:HE1	1:C:400:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:MET:HG3	1:C:440:LEU:HD21	2.02	0.42
2:D:130:LEU:O	2:D:139:PRO:HB3	2.20	0.42
2:D:208:SER:O	2:D:212:VAL:HG22	2.20	0.42
2:D:132:LYS:HA	2:D:133:PRO:HD2	1.92	0.41
2:B:40:SER:O	2:B:44:VAL:HG23	2.20	0.41
1:C:134:PRO:HA	1:C:135:PRO:HD3	1.91	0.41
1:C:591:LYS:NZ	1:C:704:GLU:OE1	2.53	0.41
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.92	0.41
2:B:221:ARG:NH1	2:B:262:ASP:OD1	2.54	0.41
1:C:480:TYR:CD2	1:C:499:LYS:HB3	2.55	0.41
2:D:201:GLN:HG2	2:D:255:LEU:HD12	2.03	0.41
2:D:240:MET:O	2:D:244:ILE:HG12	2.21	0.41
1:A:586:LEU:O	1:A:590:VAL:HG23	2.21	0.41
1:C:150:LEU:HD21	1:C:220:THR:HG21	2.03	0.40
1:C:454:PHE:O	1:C:458:VAL:HG23	2.21	0.40
1:A:229:TYR:OH	1:A:237:ARG:NH1	2.53	0.40
1:A:432:THR:HG22	1:A:468:PHE:CE1	2.57	0.40
2:D:264:ILE:O	2:D:268:GLN:HG3	2.21	0.40
1:C:575:ALA:O	1:C:579:TYR:N	2.52	0.40
2:D:173:THR:O	2:D:177:ARG:HB3	2.22	0.40
2:D:230:ILE:O	2:D:232:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/837 (62%)	514 (98%)	9 (2%)	0	100	100
1	C	696/837 (83%)	687 (99%)	9 (1%)	0	100	100
2	B	217/312 (70%)	213 (98%)	4 (2%)	0	100	100
2	D	254/312 (81%)	247 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1690/2298 (74%)	1661 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	445/708 (63%)	440 (99%)	5 (1%)	65	88
1	C	601/708 (85%)	590 (98%)	11 (2%)	51	80
2	B	207/279 (74%)	205 (99%)	2 (1%)	68	89
2	D	236/279 (85%)	233 (99%)	3 (1%)	61	86
All	All	1489/1974 (75%)	1468 (99%)	21 (1%)	59	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LEU
1	A	191	GLU
1	A	229	TYR
1	A	524	GLN
1	A	581	GLU
2	B	102	GLU
2	B	274	GLU
1	C	17	CYS
1	C	37	LEU
1	C	83	THR
1	C	94	GLU
1	C	133	VAL
1	C	214	LEU
1	C	235	LEU
1	C	302	LYS
1	C	359	LEU
1	C	435	LEU

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Mol	Chain	Res	Type
1	C	736	ARG
2	D	102	GLU
2	D	159	LYS
2	D	274	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	GLN
1	A	730	HIS
1	A	792	GLN
1	C	32	GLN
1	C	280	ASN
1	C	508	HIS
1	C	516	GLN
1	C	792	GLN
1	C	811	GLN
2	D	154	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	537/837 (64%)	0.17	34 (6%) 26 20	43, 78, 176, 226	0
1	C	712/837 (85%)	-0.15	13 (1%) 67 59	43, 67, 136, 211	0
2	B	231/312 (74%)	0.56	20 (8%) 16 13	65, 113, 191, 233	0
2	D	264/312 (84%)	0.23	13 (4%) 35 27	51, 85, 156, 191	0
All	All	1744/2298 (75%)	0.10	80 (4%) 37 29	43, 77, 169, 233	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	114	VAL	6.0
2	D	8	VAL	5.1
1	A	140	VAL	4.7
2	D	34	LYS	4.3
1	A	235	LEU	4.0
1	A	151	CYS	3.9
1	C	359	LEU	3.8
2	D	24	LEU	3.6
2	B	53	LEU	3.5
1	A	249	VAL	3.5
1	C	394	PHE	3.4
1	A	214	LEU	3.4
1	C	300	ASN	3.3
1	A	254	THR	3.3
2	B	129	SER	3.2
2	D	7	GLY	3.2
1	C	37	LEU	3.1
1	A	273	MET	3.0
2	B	63	PHE	3.0
1	A	325	THR	3.0
1	A	173	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	171	ASP	2.9
1	A	150	LEU	2.9
2	B	285	SER	2.9
1	A	222	LEU	2.8
2	D	29	THR	2.8
2	D	154	GLN	2.8
2	B	45	ILE	2.8
1	A	395	GLU	2.8
2	B	48	PRO	2.8
1	A	193	VAL	2.7
1	A	323	GLU	2.7
1	C	361	SER	2.7
2	D	49	GLN	2.7
1	A	399	LEU	2.7
2	B	25	PRO	2.7
1	A	262	ALA	2.6
1	A	466	SER	2.6
1	A	141	ILE	2.6
2	B	8	VAL	2.6
1	A	228	LEU	2.6
2	B	72	LEU	2.5
1	A	319	PHE	2.5
2	B	287	PRO	2.5
2	B	158	SER	2.5
2	B	248	PHE	2.5
1	A	241	ARG	2.5
2	D	205	GLN	2.5
1	A	189	GLU	2.4
1	A	570	ASN	2.4
1	A	265	LEU	2.4
1	A	153	GLU	2.4
1	C	392	PHE	2.3
2	D	115	ASP	2.3
2	B	174	ALA	2.3
1	C	195	LEU	2.3
2	B	196	PRO	2.3
1	C	618	ASN	2.3
2	B	284	ALA	2.3
2	B	59	GLN	2.3
1	A	324	ASN	2.2
1	C	388	ARG	2.2
2	B	215	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	246	PHE	2.2
1	C	303	THR	2.2
1	A	392	PHE	2.2
1	A	467	GLU	2.2
1	C	465	THR	2.2
2	B	27	TYR	2.2
1	C	342	ASP	2.1
1	A	251	THR	2.1
1	A	426	LEU	2.1
2	D	213	CYS	2.1
2	B	68	GLU	2.1
1	A	255	GLN	2.1
1	A	266	ALA	2.1
2	D	40	SER	2.1
1	A	285	PRO	2.1
1	C	466	SER	2.0
2	D	64	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.