Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:15 pm BST

PDB ID	:	5DSE
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 following versions of software and data (see references ①) were used in the production of this report:

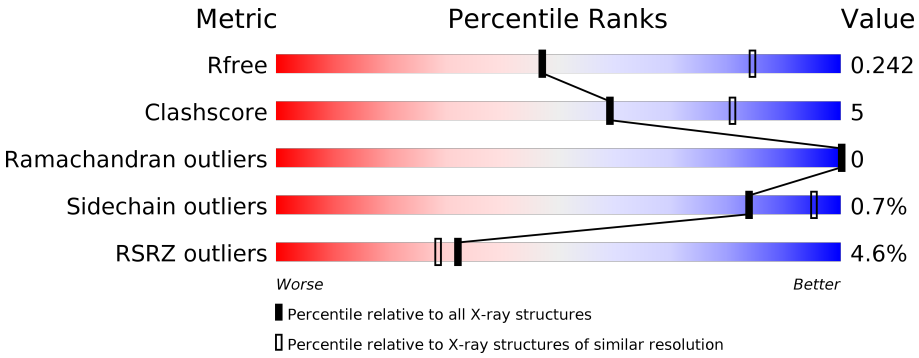
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 on 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	837	3% 57% 7% 36%
1	C	837	2% 75% 10% 15%
2	B	312	8% 63% 12% 26%
2	D	312	2% 69% 15% 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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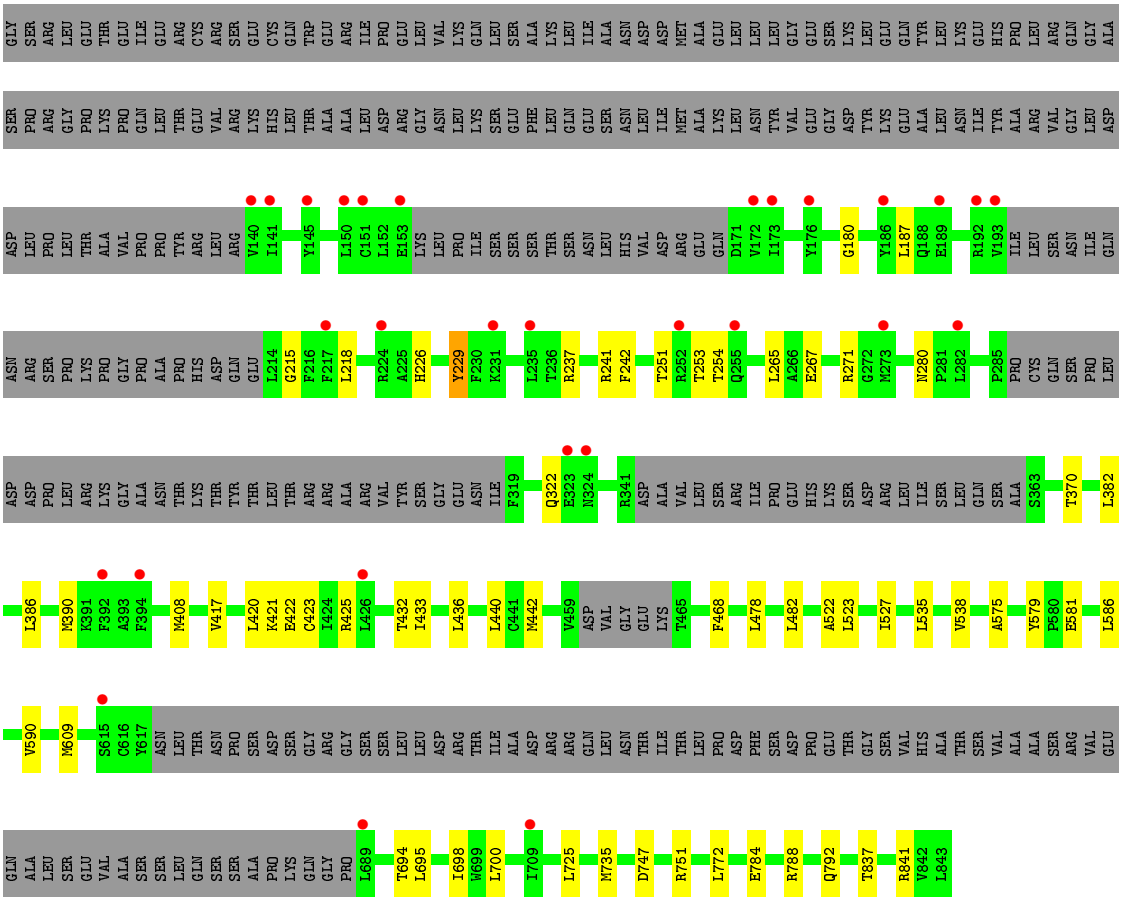
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	32	Total O 32 32	0	0
3	D	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

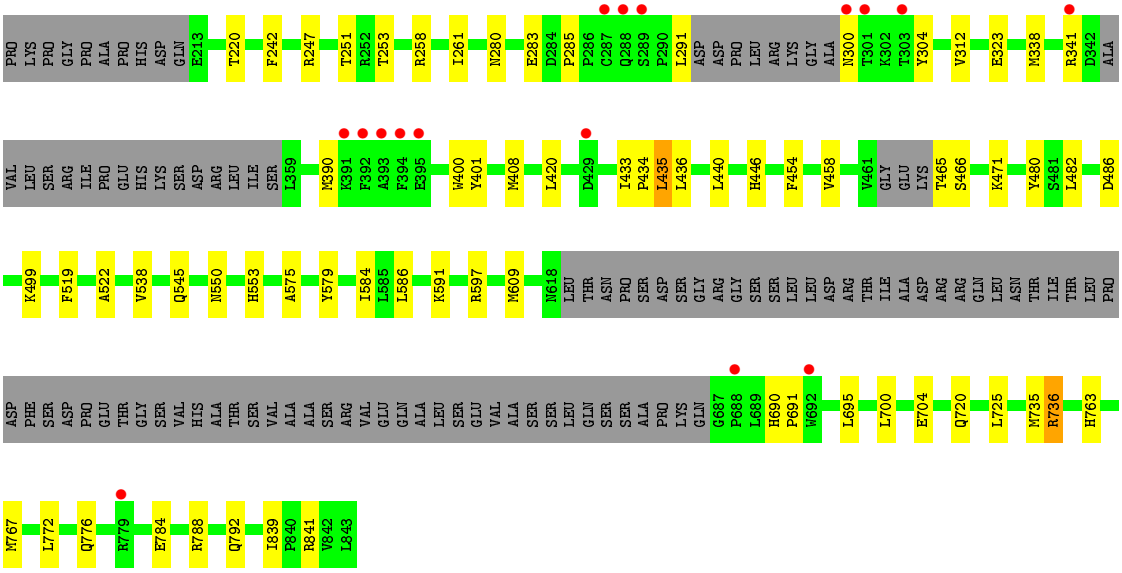
- Molecule 1: Tetratricopeptide repeat protein 7B

Chain A:



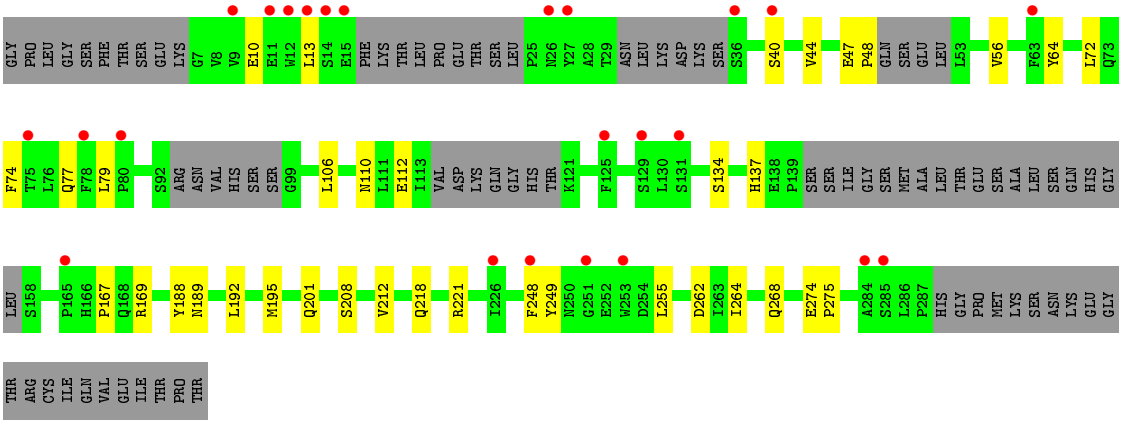
- Molecule 1: Tetratricopeptide repeat protein 7B

Chain C:



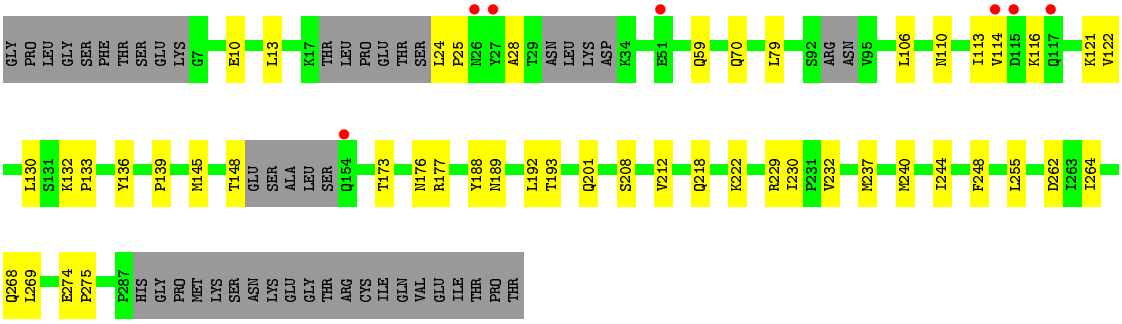
- Molecule 2: Hyccin

Chain B:



- Molecule 2: Hyccin

Chain D:



4 Data and refinement statistics (i)

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) 96.4 (29.96-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1630)	Depositor
R, R_{free}	0.212 , 0.242 0.215 , 0.242	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 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[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

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	0.23	0/4319	0.37	0/5839
1	C	0.23	0/5747	0.38	0/7771
2	B	0.23	0/1887	0.40	0/2560
2	D	0.24	0/2140	0.42	0/2903
All	All	0.23	0/14093	0.39	0/19073

There are no bond length outliers.

There are no bond angle outliers.

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	38	0
1	C	5647	0	5715	47	0
2	B	1844	0	1847	21	0
2	D	2091	0	2096	31	0
3	A	17	0	0	1	0
3	C	32	0	0	0	0
3	D	2	0	0	0	0
All	All	13875	0	13950	131	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 (131) 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: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
1:A:408:MET:HE1	1:A:436:LEU:HB3	1.90	0.54
2:B:64:TYR:HA	2:B:72:LEU:HD23	1.90	0.53
1:C:390:MET:HE1	1:C:400:TRP:CD2	2.44	0.53
1:A:695:LEU:HD23	1:A:725:LEU:HD11	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:442:MET:HE1	1:A:478:LEU:HD13	1.94	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: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: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
1:C:784:GLU:O	1:C:788:ARG:HG2	2.16	0.45
2:B:64:TYR:OH	2:B:112:GLU:OE2	2.25	0.45
2:D:116:LYS:HE3	2:D:122:VAL:H	1.80	0.45
2:B:77:GLN:HA	2:B:195:MET:HE1	1.98	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
2:B:208:SER:OG	2:B:262:ASP:OD2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:597:ARG:HD3	1:C:597:ARG:HA	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
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:408:MET:HE1	1:C:436:LEU:HB3	2.01	0.42
1:C:471:LYS:NZ	2:D:269:LEU:O	2.51	0.42
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
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
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	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
All	All	1690/2298 (74%)	1661 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	445/708 (63%)	442 (99%)	3 (1%)	84 95
1	C	601/708 (85%)	595 (99%)	6 (1%)	76 92
2	B	207/279 (74%)	206 (100%)	1 (0%)	88 96
2	D	236/279 (85%)	235 (100%)	1 (0%)	91 97
All	All	1489/1974 (75%)	1478 (99%)	11 (1%)	84 95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	TYR
1	A	581	GLU
1	A	772	LEU
2	B	248	PHE
1	C	17	CYS
1	C	37	LEU
1	C	323	GLU
1	C	401	TYR
1	C	435	LEU
1	C	736	ARG
2	D	248	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	775	HIS
1	C	811	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates 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, 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	537/837 (64%)	0.04	29 (5%) 25 22	43, 78, 176, 226	0
1	C	712/837 (85%)	-0.16	20 (2%) 53 49	43, 67, 136, 211	0
2	B	231/312 (74%)	0.47	24 (10%) 6 5	65, 113, 191, 233	0
2	D	264/312 (84%)	0.07	7 (2%) 54 50	51, 85, 156, 191	0
All	All	1744/2298 (75%)	0.02	80 (4%) 32 29	43, 77, 169, 233	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	CYS	8.2
2	D	114	VAL	5.9
1	C	300	ASN	5.6
1	A	189	GLU	5.1
1	A	150	LEU	4.7
1	C	688	PRO	4.4
1	C	392	PHE	4.4
1	A	173	ILE	4.4
1	A	176	TYR	4.4
1	A	193	VAL	4.3
2	B	129	SER	4.2
1	A	153	GLU	4.0
2	D	27	TYR	4.0
1	A	141	ILE	4.0
2	B	36	SER	3.9
2	B	12	TRP	3.9
1	A	392	PHE	3.9
2	B	27	TYR	3.9
1	A	255	GLN	3.8
1	C	287	CYS	3.7
1	C	394	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	115	ASP	3.6
1	A	252	ARG	3.5
1	C	38	ILE	3.5
1	A	689	LEU	3.5
1	C	288	GLN	3.5
1	A	235	LEU	3.4
2	B	26	ASN	3.3
1	C	301	THR	3.2
2	B	15	GLU	3.2
1	A	323	GLU	3.2
1	C	289	SER	3.1
2	B	11	GLU	3.1
2	B	165	PRO	3.0
2	D	26	ASN	3.0
2	B	131	SER	2.9
2	B	63	PHE	2.9
1	C	90	ASN	2.9
1	A	140	VAL	2.9
2	B	248	PHE	2.8
1	C	393	ALA	2.8
1	A	426	LEU	2.8
2	B	285	SER	2.8
1	C	9	ARG	2.8
1	A	224	ARG	2.8
1	C	168	ARG	2.8
2	D	51	GLU	2.7
2	B	40	SER	2.7
1	A	282	LEU	2.7
1	C	692	TRP	2.7
1	A	615	SER	2.6
1	A	145	TYR	2.6
1	A	172	VAL	2.5
1	C	395	GLU	2.5
1	C	341	ARG	2.4
1	A	231	LYS	2.4
1	C	303	THR	2.4
2	D	117	GLN	2.4
1	C	429	ASP	2.3
2	B	284	ALA	2.3
1	A	192	ARG	2.3
1	A	186	TYR	2.2
1	A	324	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	78	PHE	2.2
1	A	273	MET	2.2
2	B	9	VAL	2.2
2	B	13	LEU	2.1
2	B	226	ILE	2.1
1	C	391	LYS	2.1
2	B	75	THR	2.1
2	B	251	GLY	2.1
2	B	253	TRP	2.1
1	A	709	ILE	2.1
2	B	14	SER	2.1
2	D	154	GLN	2.1
1	A	217	PHE	2.1
2	B	80	PRO	2.0
1	A	394	PHE	2.0
2	B	125	PHE	2.0
1	C	779	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.