



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:20 AM GMT

PDB ID : 1C9I
Title : PEPTIDE-IN-GROOVE INTERACTIONS LINK TARGET PROTEINS TO
THE B-PROPELLER OF CLATHRIN
Authors : ter Haar, E.; Harrison, S. C.; Kirchhausen, T.
Deposited on : 1999-08-02
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

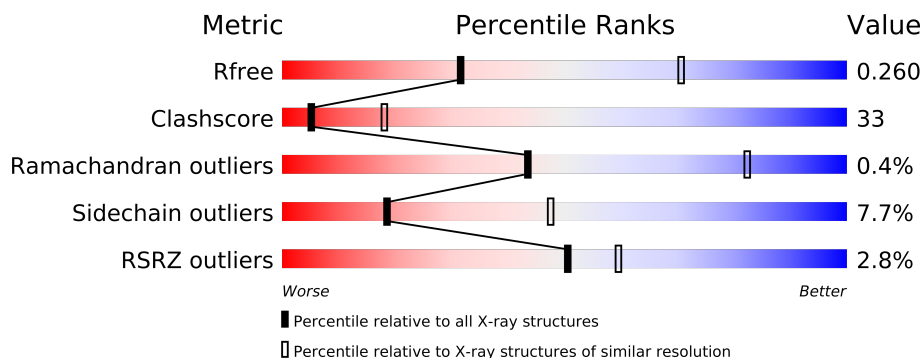
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
2	C	9	
2	D	9	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5671 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

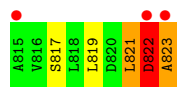
- Molecule 1 is a protein called CLATHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2779	1768	478	515	18			
1	B	355	Total	C	N	O	S	0	0	0
			2775	1766	477	514	18			

- Molecule 2 is a protein called B-ADAPTIN 3.

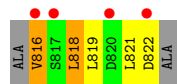
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			64	40	9	15			
2	D	7	Total	C	N	O	0	0	0
			53	34	7	12			

Chain C: 



● Molecule 2: B-ADAPTIN 3

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.04Å 131.28Å 79.01Å 90.00° 116.31° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.90 – 2.73	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.90) 95.7 (29.90-2.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.72Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.227 , 0.269 0.221 , 0.260	Depositor DCC
R_{free} test set	1251 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 16.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 32600 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5671	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.66	0/2837	0.88	2/3847 (0.1%)
1	B	0.66	2/2833 (0.1%)	0.85	2/3842 (0.1%)
2	C	1.43	1/63 (1.6%)	1.27	1/84 (1.2%)
2	D	0.94	0/52	1.63	1/70 (1.4%)
All	All	0.67	3/5785 (0.1%)	0.88	6/7843 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	823	ALA	C-OXT	9.75	1.41	1.23
1	B	294	TYR	N-CA	5.87	1.58	1.46
1	B	293	ILE	C-N	5.77	1.47	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLN	C-N-CA	-9.77	97.28	121.70
2	D	816	VAL	CB-CA-C	-8.14	95.92	111.40
1	B	280	GLY	N-CA-C	5.99	128.08	113.10
1	A	45	GLY	N-CA-C	-5.86	98.44	113.10
2	C	822	ASP	N-CA-CB	5.23	120.01	110.60
1	B	357	LEU	CB-CA-C	-5.19	100.34	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2779	0	2791	167	0
1	B	2775	0	2788	202	0
2	C	64	0	64	13	0
2	D	53	0	54	17	0
All	All	5671	0	5697	377	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (377) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:LEU:HD11	1:B:180:ALA:O	1.29	1.33
2:D:816:VAL:O	2:D:816:VAL:CG2	1.69	1.28
1:B:227:LYS:NZ	1:B:249:ASP:OD1	1.71	1.21
1:B:325:LEU:HD13	1:B:325:LEU:N	1.52	1.19
1:B:64:ARG:HD3	2:D:821:LEU:CD1	1.73	1.16
1:A:270:HIS:HA	1:A:355:ASN:ND2	1.62	1.15
1:B:64:ARG:HD3	2:D:821:LEU:HD12	1.21	1.14
1:B:50:VAL:HG23	1:B:66:ILE:HG12	1.29	1.12
1:B:325:LEU:H	1:B:325:LEU:HD13	0.94	1.10
1:B:325:LEU:CD1	1:B:325:LEU:N	2.10	1.10
1:A:270:HIS:CA	1:A:355:ASN:ND2	2.19	1.05
1:B:90:ILE:HG21	1:B:132:MET:HE2	1.37	1.02
1:A:73:MET:CE	1:A:79:VAL:O	2.08	1.02
1:B:296:ASN:HD22	1:B:297:ARG:N	1.59	0.99
1:A:73:MET:HE2	1:A:79:VAL:O	1.63	0.99
1:B:158:THR:HG22	1:B:159:ASP:O	1.64	0.98
1:A:270:HIS:C	1:A:355:ASN:ND2	2.18	0.96
2:C:822:ASP:O	2:C:823:ALA:CB	2.13	0.94
1:B:30:LEU:HD23	1:B:40:ILE:HG13	1.45	0.94
1:A:96:LYS:HA	2:C:821:LEU:HD13	1.52	0.91
1:A:90:ILE:HG12	1:A:132:MET:HE2	1.51	0.91
1:B:92:ASN:HD22	1:B:95:MET:H	1.16	0.90
1:B:64:ARG:CD	2:D:821:LEU:CD1	2.50	0.90
1:A:73:MET:HA	1:A:73:MET:HE3	1.52	0.90
1:A:270:HIS:CA	1:A:355:ASN:HD21	1.81	0.88
1:B:79:VAL:HG13	1:B:99:MET:HE1	1.56	0.87
2:C:822:ASP:O	2:C:823:ALA:HB2	1.75	0.86
1:B:16:GLN:NE2	1:B:22:PRO:HG3	1.91	0.86
1:B:16:GLN:HE22	1:B:22:PRO:HG3	1.40	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:323:GLN:OE1	1:B:325:LEU:HG	1.76	0.85
1:A:20:ILE:HG12	1:A:40:ILE:HD13	1.56	0.85
1:B:144:ARG:NH2	1:B:148:LEU:O	2.09	0.85
1:B:157:ARG:NH1	1:B:200:SER:HB2	1.91	0.85
1:A:7:ILE:HG21	1:A:284:LEU:HD21	1.60	0.84
1:B:176:ARG:HH12	1:B:222:GLY:HA2	1.42	0.83
1:B:92:ASN:ND2	1:B:95:MET:H	1.76	0.83
1:B:11:GLU:OE1	1:B:323:GLN:HG3	1.79	0.82
1:B:30:LEU:HD21	1:B:38:ILE:CG2	2.08	0.82
1:B:296:ASN:HD22	1:B:297:ARG:H	1.28	0.82
1:A:90:ILE:HG12	1:A:132:MET:CE	2.10	0.82
1:A:73:MET:CE	1:A:79:VAL:C	2.47	0.81
1:A:158:THR:HG21	1:A:162:GLN:HG2	1.62	0.81
1:A:155:ASN:HD21	1:A:157:ARG:HG3	1.45	0.81
1:A:154:ILE:HD13	1:A:170:ILE:HG12	1.61	0.80
1:A:253:PRO:HB2	1:A:255:GLU:OE1	1.82	0.80
1:B:96:LYS:NZ	2:D:822:ASP:OD2	2.15	0.80
1:B:265:GLN:HE21	1:B:308:PRO:N	1.80	0.79
1:A:51:VAL:HG22	1:A:63:ARG:HG2	1.64	0.79
1:B:148:LEU:CD1	1:B:180:ALA:O	2.23	0.78
1:B:284:LEU:HB3	1:B:293:ILE:HG13	1.65	0.78
1:B:166:LEU:HD22	1:B:216:PHE:HE1	1.49	0.77
1:B:323:GLN:HG2	1:B:325:LEU:HD12	1.66	0.77
1:B:72:ILE:HG13	1:B:81:ALA:HB3	1.67	0.77
1:B:284:LEU:HD12	1:B:293:ILE:HD11	1.66	0.77
1:A:281:TYR:CE2	1:A:297:ARG:HD2	2.20	0.76
1:A:255:GLU:H	1:A:255:GLU:CD	1.88	0.76
1:A:335:ILE:HB	1:A:336:PRO:HD3	1.68	0.76
1:A:166:LEU:HD22	1:A:216:PHE:HE1	1.52	0.75
1:A:270:HIS:C	1:A:355:ASN:HD22	1.89	0.74
1:A:6:PRO:HB2	1:A:334:ILE:HD12	1.68	0.74
1:A:73:MET:HE1	1:A:79:VAL:C	2.07	0.73
1:A:20:ILE:HG12	1:A:40:ILE:CD1	2.19	0.72
1:B:335:ILE:HB	1:B:336:PRO:HD3	1.70	0.72
1:A:309:HIS:HD2	1:A:312:THR:HG23	1.54	0.72
1:B:296:ASN:ND2	1:B:297:ARG:H	1.88	0.72
1:B:79:VAL:HG13	1:B:99:MET:CE	2.19	0.72
1:B:296:ASN:ND2	1:B:297:ARG:N	2.37	0.71
1:A:270:HIS:C	1:A:355:ASN:HD21	1.90	0.71
1:A:90:ILE:HG21	1:A:132:MET:CE	2.21	0.71
2:D:816:VAL:O	2:D:816:VAL:HG23	0.94	0.70
1:A:158:THR:HG22	1:A:159:ASP:O	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:GLN:HE22	1:B:22:PRO:CG	2.05	0.70
1:B:166:LEU:HD22	1:B:216:PHE:CE1	2.26	0.70
1:B:158:THR:HG23	1:B:162:GLN:HA	1.75	0.69
1:A:166:LEU:HD22	1:A:216:PHE:CE1	2.27	0.68
1:B:282:ILE:HG22	1:B:296:ASN:O	1.93	0.68
1:A:57:ASP:N	1:A:58:PRO:CD	2.56	0.68
1:B:312:THR:O	1:B:313:ALA:HB3	1.94	0.67
1:A:7:ILE:HD12	1:A:7:ILE:O	1.94	0.67
1:A:161:LYS:HE2	1:A:163:LYS:HZ2	1.59	0.67
1:B:57:ASP:N	1:B:58:PRO:CD	2.58	0.67
1:B:148:LEU:HD11	1:B:180:ALA:C	2.12	0.67
2:C:819:LEU:CD2	2:C:821:LEU:HD21	2.25	0.67
1:A:158:THR:HG21	1:A:162:GLN:CG	2.25	0.66
1:B:73:MET:HE1	1:B:78:LYS:HA	1.77	0.66
2:D:822:ASP:O	2:D:822:ASP:OD1	2.14	0.66
1:A:281:TYR:HE2	1:A:297:ARG:HD2	1.59	0.66
1:B:176:ARG:HH12	1:B:222:GLY:CA	2.09	0.65
1:B:51:VAL:HG22	1:B:63:ARG:HG2	1.79	0.65
1:A:57:ASP:N	1:A:58:PRO:HD3	2.11	0.65
1:B:98:LYS:HE2	1:B:101:ALA:HB2	1.77	0.65
1:A:323:GLN:OE1	1:A:325:LEU:HD23	1.96	0.65
1:B:272:VAL:CG1	1:B:284:LEU:HD22	2.27	0.65
1:A:246:LYS:HE2	1:A:288:GLU:O	1.97	0.65
1:A:227:LYS:HA	1:A:249:ASP:HA	1.79	0.65
1:B:148:LEU:HD12	1:B:180:ALA:CB	2.27	0.64
1:A:161:LYS:HE2	1:A:163:LYS:NZ	2.13	0.64
1:A:96:LYS:CA	2:C:821:LEU:HD13	2.27	0.63
1:A:7:ILE:HG21	1:A:284:LEU:CD2	2.28	0.63
1:B:323:GLN:OE1	1:B:325:LEU:CG	2.46	0.63
1:B:272:VAL:HG12	1:B:284:LEU:HD22	1.80	0.63
1:B:66:ILE:HD12	1:B:66:ILE:C	2.19	0.63
1:A:63:ARG:O	1:A:64:ARG:HD3	1.99	0.63
1:A:155:ASN:HD21	1:A:157:ARG:CG	2.10	0.62
1:B:4:ILE:HD12	1:B:333:ASN:HB2	1.80	0.62
1:A:174:GLN:NE2	1:A:223:GLN:HE22	1.97	0.62
1:B:64:ARG:CD	2:D:821:LEU:HD11	2.28	0.62
1:A:355:ASN:HB3	1:A:357:LEU:HD11	1.82	0.62
1:A:90:ILE:HG21	1:A:132:MET:HE1	1.80	0.62
1:B:128:TYR:N	1:B:128:TYR:CD1	2.67	0.62
1:A:267:SER:HB2	1:A:313:ALA:O	1.99	0.62
1:B:145:HIS:CD2	1:B:193:PRO:HG3	2.34	0.62
1:B:50:VAL:HG23	1:B:66:ILE:CG1	2.18	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:18:LEU:HD22	1:A:61:PRO:CG	2.30	0.62
1:A:207:GLU:OE1	1:B:256:ALA:HA	2.00	0.62
1:B:265:GLN:HB2	1:B:315:ILE:HD12	1.80	0.61
1:B:278:LYS:HG2	1:B:279:TYR:CE1	2.34	0.61
1:B:148:LEU:HD12	1:B:180:ALA:HB3	1.81	0.61
1:B:282:ILE:HG21	1:B:298:ILE:CG2	2.30	0.61
1:A:157:ARG:NH1	1:A:200:SER:HB2	2.16	0.61
1:A:232:GLU:HB2	1:A:243:PHE:HB3	1.83	0.61
1:A:18:LEU:HD13	1:A:53:ILE:HD13	1.83	0.61
1:B:325:LEU:HD12	1:B:325:LEU:N	2.10	0.60
2:C:822:ASP:O	2:C:823:ALA:HB3	1.97	0.60
1:A:16:GLN:NE2	1:A:22:PRO:HG3	2.16	0.60
1:B:59:SER:C	1:B:61:PRO:HD3	2.22	0.60
1:A:188:ARG:O	1:A:190:VAL:HG23	2.01	0.60
1:B:256:ALA:HB1	1:B:259:ASP:HB3	1.83	0.60
1:A:92:ASN:CG	1:A:95:MET:HG2	2.22	0.60
1:B:14:GLN:O	1:B:16:GLN:N	2.35	0.59
1:B:293:ILE:C	1:B:293:ILE:HD12	2.22	0.59
1:A:81:ALA:O	1:A:82:LEU:HD23	2.02	0.59
1:A:18:LEU:HD22	1:A:61:PRO:HG2	1.84	0.59
1:A:284:LEU:HB3	1:A:293:ILE:HB	1.85	0.59
1:B:209:ASN:HB3	1:B:240:ASN:ND2	2.18	0.58
1:B:338:ILE:HA	1:B:342:LEU:HD12	1.85	0.58
1:B:4:ILE:HD12	1:B:333:ASN:CB	2.33	0.58
1:A:50:VAL:HG22	1:A:66:ILE:CG2	2.34	0.58
1:A:309:HIS:CD2	1:A:312:THR:HG23	2.37	0.58
1:A:145:HIS:NE2	1:A:193:PRO:HG3	2.18	0.58
1:A:255:GLU:CD	1:A:255:GLU:N	2.57	0.58
1:B:255:GLU:O	1:B:257:GLN:HG3	2.03	0.58
1:B:50:VAL:CG2	1:B:66:ILE:HG12	2.20	0.57
1:B:264:MET:O	1:B:265:GLN:OE1	2.23	0.57
1:B:351:MET:O	1:B:357:LEU:HD12	2.05	0.57
1:A:312:THR:O	1:A:313:ALA:HB3	2.04	0.57
1:B:199:ALA:HB2	1:B:218:PHE:CB	2.34	0.56
1:A:237:PRO:O	1:A:240:ASN:HB2	2.04	0.56
1:B:148:LEU:CD1	1:B:180:ALA:CB	2.82	0.56
1:B:89:GLN:HE22	2:D:816:VAL:HG23	1.69	0.56
1:A:114:ILE:HD12	1:A:162:GLN:HE21	1.70	0.56
1:B:96:LYS:HA	2:D:821:LEU:HD23	1.88	0.56
1:A:155:ASN:ND2	1:A:157:ARG:HG3	2.17	0.56
1:A:51:VAL:CG2	1:A:63:ARG:NH1	2.69	0.56
1:B:83:LYS:NZ	1:B:108:VAL:O	2.27	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:VAL:O	1:A:356:ASN:ND2	2.38	0.56
1:A:296:ASN:CG	1:A:297:ARG:H	2.08	0.56
1:B:323:GLN:OE1	1:B:325:LEU:CD1	2.54	0.55
2:C:822:ASP:OD1	2:C:822:ASP:C	2.42	0.55
1:A:92:ASN:ND2	1:A:95:MET:H	2.03	0.55
1:A:173:GLN:HB2	1:A:178:VAL:HG21	1.87	0.55
1:B:323:GLN:CG	1:B:325:LEU:HD12	2.36	0.55
1:A:353:VAL:HG21	1:B:177:VAL:HG23	1.88	0.55
1:B:44:VAL:HB	1:B:49:GLN:NE2	2.21	0.55
1:B:338:ILE:HG22	1:B:348:ALA:HB2	1.87	0.55
1:B:50:VAL:HG12	1:B:52:ILE:HD12	1.88	0.55
1:B:90:ILE:HG13	1:B:132:MET:HE1	1.89	0.54
1:A:31:THR:HG21	1:A:72:ILE:HG22	1.88	0.54
1:B:52:ILE:HD12	1:B:52:ILE:N	2.21	0.54
2:C:819:LEU:HD21	2:C:821:LEU:CD2	2.37	0.54
1:B:333:ASN:HA	1:B:336:PRO:HD2	1.89	0.54
1:A:92:ASN:ND2	1:A:95:MET:HG2	2.22	0.54
1:B:221:ARG:HH21	1:B:252:PHE:CB	2.19	0.54
2:C:819:LEU:HD23	2:C:821:LEU:HD21	1.88	0.54
1:B:173:GLN:HB2	1:B:178:VAL:HG21	1.89	0.54
1:A:96:LYS:HA	2:C:821:LEU:CD1	2.32	0.54
1:B:164:TRP:HZ2	1:B:234:GLY:CA	2.21	0.54
1:B:158:THR:HG21	1:B:162:GLN:HG3	1.90	0.54
1:A:168:THR:OG1	1:A:181:MET:HG2	2.08	0.54
1:B:92:ASN:ND2	1:B:95:MET:N	2.52	0.53
1:A:278:LYS:O	1:A:302:THR:HG22	2.09	0.53
1:A:291:THR:HG21	1:A:347:LEU:HD22	1.90	0.53
1:A:158:THR:HG23	1:A:162:GLN:HA	1.91	0.53
1:A:355:ASN:HB3	1:A:357:LEU:CD1	2.38	0.53
1:B:251:PHE:CE2	1:B:253:PRO:HD3	2.43	0.53
1:B:25:ILE:HG22	1:B:25:ILE:O	2.08	0.53
1:A:335:ILE:HB	1:A:336:PRO:CD	2.38	0.53
1:B:39:CYS:SG	1:B:73:MET:HG2	2.49	0.53
1:B:291:THR:HG21	1:B:347:LEU:HD22	1.89	0.53
1:A:86:LYS:HB3	1:A:104:MET:O	2.09	0.53
1:B:57:ASP:H	1:B:58:PRO:HD3	1.74	0.53
1:A:283:HIS:HB3	1:A:285:TYR:CE1	2.43	0.53
1:B:148:LEU:CD1	1:B:180:ALA:HB1	2.38	0.52
1:A:158:THR:CG2	1:A:159:ASP:O	2.56	0.52
1:B:164:TRP:O	1:B:165:LEU:HD23	2.09	0.52
1:A:199:ALA:HB2	1:A:218:PHE:CB	2.38	0.52
1:B:282:ILE:CG2	1:B:298:ILE:CG2	2.87	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:LYS:NZ	1:B:257:GLN:NE2	2.57	0.52
1:A:128:TYR:CD2	1:A:140:LYS:HA	2.45	0.52
1:B:265:GLN:HE21	1:B:308:PRO:CD	2.22	0.52
1:B:89:GLN:NE2	2:D:816:VAL:HG23	2.25	0.52
1:B:157:ARG:HH12	1:B:200:SER:HB2	1.75	0.51
1:B:197:HIS:CD2	1:B:221:ARG:H	2.27	0.51
1:A:259:ASP:OD1	1:A:279:TYR:HD1	1.93	0.51
1:B:64:ARG:NE	2:D:821:LEU:HD11	2.25	0.51
1:B:293:ILE:HD12	1:B:293:ILE:O	2.11	0.51
1:B:282:ILE:CG2	1:B:298:ILE:HG23	2.40	0.51
1:B:158:THR:HG21	1:B:162:GLN:CG	2.40	0.51
1:B:312:THR:O	1:B:313:ALA:CB	2.57	0.51
1:B:188:ARG:HB2	1:B:190:VAL:HG12	1.92	0.51
1:A:18:LEU:HD21	1:A:58:PRO:O	2.11	0.51
1:A:50:VAL:HG22	1:A:66:ILE:HG21	1.93	0.51
1:B:54:ASP:O	1:B:58:PRO:HD3	2.11	0.50
1:B:339:THR:O	1:B:343:GLN:HA	2.12	0.50
1:B:282:ILE:HG21	1:B:298:ILE:HG21	1.93	0.50
1:B:57:ASP:N	1:B:58:PRO:HD3	2.26	0.50
1:A:166:LEU:HD11	1:A:181:MET:HE3	1.94	0.50
1:B:79:VAL:CG1	1:B:99:MET:HE1	2.34	0.50
2:C:819:LEU:CD2	2:C:821:LEU:CD2	2.89	0.50
1:B:112:LYS:HB2	1:B:112:LYS:NZ	2.26	0.50
1:B:211:GLU:H	1:B:240:ASN:HD21	1.60	0.49
1:B:306:THR:HG22	1:B:317:GLY:HA3	1.94	0.49
1:A:4:ILE:O	1:A:4:ILE:HD12	2.11	0.49
1:B:250:VAL:O	1:B:250:VAL:CG2	2.60	0.49
1:B:89:GLN:HG2	1:B:98:LYS:HE3	1.94	0.49
1:A:206:MET:HB2	1:A:209:ASN:OD1	2.12	0.49
2:C:819:LEU:HD21	2:C:821:LEU:HD21	1.94	0.49
1:B:267:SER:HB2	1:B:313:ALA:O	2.13	0.49
1:B:82:LEU:CD1	2:D:819:LEU:HB2	2.43	0.49
1:A:50:VAL:HG13	1:A:66:ILE:HD13	1.93	0.49
1:A:57:ASP:H	1:A:58:PRO:HD3	1.78	0.48
1:B:20:ILE:N	1:B:20:ILE:HD12	2.28	0.48
1:B:83:LYS:HB2	1:B:88:LEU:HD22	1.95	0.48
1:B:30:LEU:CD2	1:B:38:ILE:CG2	2.89	0.48
1:B:16:GLN:CD	1:B:22:PRO:HG3	2.33	0.48
1:B:49:GLN:OE1	1:B:63:ARG:HD3	2.13	0.48
1:A:11:GLU:HB2	1:A:323:GLN:HE21	1.78	0.48
1:B:282:ILE:HG22	1:B:298:ILE:HG23	1.96	0.48
1:B:128:TYR:N	1:B:128:TYR:HD1	2.09	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:145:HIS:NE2	1:B:193:PRO:HG3	2.29	0.47
1:B:221:ARG:HH21	1:B:252:PHE:HB3	1.79	0.47
1:A:50:VAL:HG22	1:A:66:ILE:HG23	1.96	0.47
1:A:206:MET:HE1	1:A:242:PRO:O	2.15	0.47
1:A:301:GLU:HA	1:A:301:GLU:OE1	2.14	0.47
1:B:333:ASN:C	1:B:336:PRO:HD2	2.34	0.47
1:A:92:ASN:HD22	1:A:95:MET:H	1.62	0.47
1:B:197:HIS:HD2	1:B:221:ARG:H	1.61	0.47
2:D:821:LEU:O	2:D:822:ASP:HB2	2.15	0.47
1:A:32:MET:CE	1:A:38:ILE:HD11	2.44	0.47
1:A:269:LYS:O	1:A:355:ASN:OD1	2.33	0.47
1:A:333:ASN:O	1:A:334:ILE:C	2.53	0.47
1:A:12:HIS:CD2	1:A:12:HIS:N	2.81	0.47
1:A:206:MET:O	1:A:209:ASN:HB2	2.15	0.46
1:B:164:TRP:CZ2	1:B:234:GLY:CA	2.98	0.46
1:B:86:LYS:HG3	1:B:107:ASP:OD1	2.15	0.46
1:B:72:ILE:HD11	1:B:111:TRP:CD2	2.50	0.46
1:A:174:GLN:O	1:A:175:ASN:HB2	2.16	0.46
1:B:262:VAL:HG12	1:B:276:ILE:O	2.16	0.46
1:B:250:VAL:CG2	1:B:252:PHE:HE1	2.29	0.46
1:B:69:ASP:C	1:B:69:ASP:OD2	2.53	0.46
1:A:18:LEU:CD1	1:A:53:ILE:HD13	2.44	0.46
1:A:30:LEU:HD22	1:A:304:PHE:CE1	2.51	0.46
1:B:286:ASP:OD2	1:B:289:THR:HG23	2.16	0.46
1:B:248:VAL:HG11	1:B:290:GLY:O	2.15	0.45
1:B:230:ILE:HD13	1:B:287:LEU:O	2.16	0.45
1:B:347:LEU:O	1:B:351:MET:HG3	2.17	0.45
1:B:84:ALA:CB	2:D:818:LEU:HD21	2.46	0.45
1:B:158:THR:CG2	1:B:162:GLN:HA	2.45	0.45
1:A:71:ALA:HA	1:A:82:LEU:HD23	1.98	0.45
1:A:309:HIS:HD2	1:A:312:THR:CG2	2.27	0.45
1:A:244:PRO:HB2	1:A:246:LYS:NZ	2.31	0.45
1:B:338:ILE:HG12	1:B:342:LEU:HD12	1.98	0.45
1:B:232:GLU:HB2	1:B:243:PHE:HB3	1.99	0.45
1:A:205:LYS:HE3	1:A:209:ASN:O	2.17	0.45
1:A:220:VAL:O	1:A:220:VAL:HG13	2.17	0.45
1:B:96:LYS:HG2	2:D:821:LEU:HD23	1.97	0.45
1:A:145:HIS:CE1	1:A:193:PRO:HG3	2.52	0.45
1:B:255:GLU:OE2	1:B:255:GLU:N	2.50	0.45
1:B:199:ALA:HB2	1:B:218:PHE:HB2	1.99	0.45
1:B:50:VAL:HG12	1:B:52:ILE:CD1	2.46	0.45
1:A:349:LEU:O	1:A:353:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:THR:CG2	1:A:162:GLN:HG2	2.41	0.45
1:A:92:ASN:C	1:A:92:ASN:HD22	2.19	0.45
2:D:818:LEU:HA	2:D:818:LEU:HD12	1.86	0.45
1:B:265:GLN:NE2	1:B:308:PRO:HD3	2.31	0.45
1:B:51:VAL:HG21	1:B:63:ARG:CZ	2.46	0.45
1:B:32:MET:CE	1:B:317:GLY:HA2	2.47	0.44
1:B:141:MET:O	1:B:142:PHE:HB3	2.16	0.44
1:A:73:MET:HA	1:A:73:MET:CE	2.35	0.44
1:A:73:MET:HE3	1:A:79:VAL:O	2.11	0.44
1:A:11:GLU:HB2	1:A:323:GLN:NE2	2.31	0.44
1:A:32:MET:CE	1:A:38:ILE:HG12	2.47	0.44
1:A:233:VAL:O	1:A:233:VAL:HG23	2.17	0.44
1:B:90:ILE:HG13	1:B:132:MET:CE	2.47	0.44
1:B:148:LEU:HD23	1:B:167:LEU:HG	1.99	0.44
1:A:73:MET:HE1	1:A:80:ILE:N	2.33	0.44
1:A:30:LEU:HD23	1:A:30:LEU:C	2.38	0.44
1:A:353:VAL:HG12	1:B:258:ASN:ND2	2.32	0.44
1:B:277:THR:HG23	1:B:281:TYR:HB2	1.98	0.44
1:B:309:HIS:HB2	1:B:316:ILE:HB	1.99	0.44
1:B:148:LEU:HD12	1:B:180:ALA:HB1	1.97	0.44
1:B:221:ARG:NH1	1:B:257:GLN:O	2.47	0.43
1:A:262:VAL:HG11	1:A:278:LYS:HA	1.99	0.43
1:B:14:GLN:O	1:B:17:ASN:N	2.51	0.43
1:B:255:GLU:CD	1:B:255:GLU:H	2.21	0.43
1:B:218:PHE:CE1	1:B:229:HIS:HD2	2.36	0.43
1:A:116:LEU:HD22	1:A:116:LEU:N	2.33	0.43
1:B:92:ASN:HD22	1:B:92:ASN:C	2.22	0.43
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.88	0.43
1:A:244:PRO:O	1:A:246:LYS:HD3	2.18	0.43
1:A:333:ASN:OD1	1:A:333:ASN:N	2.51	0.43
1:B:259:ASP:OD1	1:B:279:TYR:HD1	2.02	0.43
1:B:164:TRP:C	1:B:165:LEU:HD23	2.39	0.43
1:A:90:ILE:HG12	1:A:132:MET:HE1	1.96	0.43
1:A:13:LEU:HD21	1:A:58:PRO:HB3	2.00	0.43
1:A:24:ASN:ND2	1:A:42:GLU:HG2	2.34	0.43
1:B:318:VAL:HG22	1:B:324:VAL:HG22	2.00	0.43
1:B:90:ILE:HG22	1:B:99:MET:HE2	2.01	0.43
1:A:145:HIS:CE1	1:A:147:SER:HG	2.30	0.43
1:B:173:GLN:HB2	1:B:178:VAL:CG2	2.48	0.43
1:B:276:ILE:HA	1:B:281:TYR:O	2.19	0.43
1:A:165:LEU:HD12	1:A:184:TYR:HD2	1.84	0.43
1:B:337:TYR:CE1	1:B:341:VAL:HG11	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:ARG:HG2	1:B:50:VAL:HG22	2.00	0.42
1:A:20:ILE:CG2	1:A:21:ASN:N	2.82	0.42
1:B:157:ARG:HB3	1:B:157:ARG:HE	1.62	0.42
1:A:226:GLY:O	1:A:249:ASP:HB3	2.18	0.42
1:B:278:LYS:CG	1:B:279:TYR:CE1	3.01	0.42
1:A:73:MET:HE1	1:A:80:ILE:HB	2.01	0.42
1:A:57:ASP:CG	1:A:60:ASN:HD22	2.23	0.42
1:A:301:GLU:HG3	1:A:321:LYS:HB2	2.01	0.42
1:A:12:HIS:HE1	1:A:309:HIS:CE1	2.38	0.42
1:A:250:VAL:HG23	1:A:283:HIS:CE1	2.55	0.42
1:B:18:LEU:HB2	1:B:20:ILE:HD13	2.02	0.42
1:A:82:LEU:HD12	2:C:819:LEU:HB2	2.02	0.42
1:A:219:ALA:CB	1:A:275:LEU:HD11	2.49	0.42
1:B:66:ILE:C	1:B:66:ILE:CD1	2.87	0.42
1:B:77:SER:O	1:B:79:VAL:N	2.45	0.42
1:A:20:ILE:HD12	1:A:20:ILE:N	2.35	0.42
1:A:278:LYS:HG2	1:A:302:THR:HG22	2.01	0.42
1:A:109:THR:N	1:A:122:VAL:O	2.50	0.42
1:B:155:ASN:HD21	1:B:157:ARG:HG2	1.84	0.42
1:A:211:GLU:HB2	1:A:237:PRO:HB2	2.01	0.42
1:B:90:ILE:HG22	1:B:99:MET:CE	2.49	0.42
1:B:16:GLN:HE21	1:B:16:GLN:HA	1.84	0.42
1:B:256:ALA:HB1	1:B:259:ASP:CB	2.47	0.41
1:A:247:ALA:C	1:A:248:VAL:HG13	2.41	0.41
1:A:73:MET:CE	1:A:80:ILE:HB	2.50	0.41
1:B:30:LEU:HD21	1:B:38:ILE:HG22	1.94	0.41
1:B:25:ILE:HD13	1:B:322:GLY:HA2	2.02	0.41
1:B:277:THR:CG2	1:B:281:TYR:HB2	2.51	0.41
1:A:265:GLN:HG2	1:A:315:ILE:HD12	2.01	0.41
1:A:110:PHE:CZ	1:A:155:ASN:HA	2.55	0.41
1:B:343:GLN:C	1:B:345:PRO:HD3	2.41	0.41
1:A:235:THR:HA	1:A:236:PRO:HD3	1.90	0.41
1:B:231:ILE:HG22	1:B:245:LYS:HB2	2.03	0.41
1:B:92:ASN:C	1:B:92:ASN:ND2	2.74	0.41
1:B:13:LEU:HD21	1:B:58:PRO:CB	2.50	0.41
1:A:209:ASN:HD21	1:A:241:GLN:HB2	1.85	0.41
1:B:177:VAL:O	1:B:197:HIS:HE1	2.04	0.41
1:B:255:GLU:CD	1:B:255:GLU:N	2.74	0.41
1:A:156:TYR:OH	1:A:165:LEU:HB3	2.21	0.41
1:B:295:MET:HG3	1:B:295:MET:O	2.11	0.41
1:A:32:MET:HE3	1:A:38:ILE:HG12	2.02	0.41
1:A:350:ARG:O	1:A:354:ARG:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:PHE:HB2	1:A:261:PRO:CD	2.51	0.41
1:A:49:GLN:HA	1:A:66:ILE:HG12	2.03	0.41
1:B:172:ALA:O	1:B:173:GLN:HG2	2.21	0.41
1:A:226:GLY:O	1:A:249:ASP:CB	2.69	0.41
1:A:135:GLU:H	1:A:135:GLU:HG3	1.39	0.41
1:B:9:PHE:CD1	1:B:10:GLN:N	2.88	0.41
1:A:353:VAL:CG1	1:B:258:ASN:HD22	2.34	0.40
1:B:94:GLU:H	1:B:94:GLU:HG3	1.76	0.40
1:A:244:PRO:HG2	1:B:301:GLU:OE1	2.21	0.40
1:A:185:SER:OG	1:A:188:ARG:HG2	2.22	0.40
1:A:185:SER:CB	1:A:188:ARG:HG2	2.51	0.40
1:B:145:HIS:NE2	1:B:193:PRO:CG	2.85	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	353/359 (98%)	321 (91%)	31 (9%)	1 (0%)	50	85
1	B	353/359 (98%)	316 (90%)	36 (10%)	1 (0%)	50	85
2	C	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	1
2	D	5/9 (56%)	5 (100%)	0	0	100	100
All	All	718/736 (98%)	647 (90%)	68 (10%)	3 (0%)	43	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	LEU
1	A	320	ARG
2	C	822	ASP

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	306/307 (100%)	288 (94%)	18 (6%)	28	64
1	B	305/307 (99%)	278 (91%)	27 (9%)	14	40
2	C	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	D	7/7 (100%)	6 (86%)	1 (14%)	5	13
All	All	625/628 (100%)	577 (92%)	48 (8%)	18	47

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	50	VAL
1	A	55	MET
1	A	92	ASN
1	A	111	TRP
1	A	112	LYS
1	A	135	GLU
1	A	137	GLN
1	A	176	ARG
1	A	223	GLN
1	A	249	ASP
1	A	250	VAL
1	A	268	GLU
1	A	295	MET
1	A	302	THR
1	A	333	ASN
1	A	339	THR
1	A	357	LEU
1	B	4	ILE
1	B	11	GLU
1	B	16	GLN
1	B	47	GLN
1	B	92	ASN
1	B	105	THR
1	B	111	TRP
1	B	112	LYS

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	128	TYR
1	B	135	GLU
1	B	148	LEU
1	B	157	ARG
1	B	228	LEU
1	B	246	LYS
1	B	250	VAL
1	B	262	VAL
1	B	265	GLN
1	B	268	GLU
1	B	284	LEU
1	B	293	ILE
1	B	295	MET
1	B	296	ASN
1	B	310	GLU
1	B	325	LEU
1	B	333	ASN
1	B	357	LEU
2	C	817	SER
2	C	821	LEU
2	D	818	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	16	GLN
1	A	17	ASN
1	A	24	ASN
1	A	92	ASN
1	A	155	ASN
1	A	162	GLN
1	A	203	GLN
1	A	209	ASN
1	A	223	GLN
1	A	309	HIS
1	A	355	ASN
1	A	356	ASN
1	B	16	GLN
1	B	17	ASN
1	B	56	ASN

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	125	ASN
1	B	152	GLN
1	B	155	ASN
1	B	175	ASN
1	B	197	HIS
1	B	203	GLN
1	B	229	HIS
1	B	240	ASN
1	B	257	GLN
1	B	258	ASN
1	B	265	GLN
1	B	296	ASN
1	B	309	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	355/359 (98%)	-0.38	6 (1%) 67 76	3, 16, 38, 62	0
1	B	355/359 (98%)	-0.27	7 (1%) 62 71	5, 19, 38, 56	0
2	C	9/9 (100%)	1.97	3 (33%) 1 1	31, 46, 65, 72	0
2	D	7/9 (77%)	2.15	4 (57%) 0 0	47, 55, 67, 80	0
All	All	726/736 (98%)	-0.27	20 (2%) 50 59	3, 18, 41, 80	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	823	ALA	6.2
2	D	816	VAL	4.3
1	B	358	ALA	4.2
2	D	822	ASP	3.8
2	C	815	ALA	3.7
1	B	46	GLU	3.3
1	A	3	GLN	3.1
1	A	46	GLU	3.1
1	A	47	GLN	2.8
2	C	822	ASP	2.8
1	B	44	VAL	2.3
1	B	223	GLN	2.3
1	A	44	VAL	2.2
1	B	47	GLN	2.2
1	A	355	ASN	2.2
1	A	4	ILE	2.2
1	B	210	ALA	2.1
2	D	820	ASP	2.1
2	D	817	SER	2.1
1	B	4	ILE	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.