



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:44 PM GMT

PDB ID : 1C9L
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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

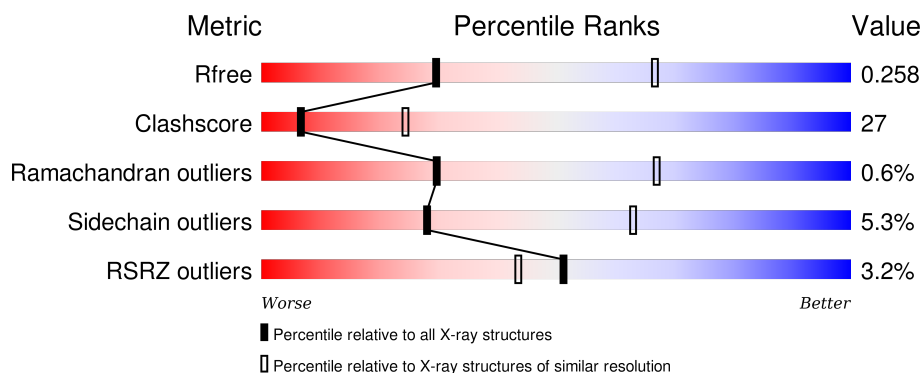
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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	357	<div> <div>3%</div> <div>60%</div> <div>37%</div> <div>.</div> </div>
1	B	357	<div> <div>3%</div> <div>53%</div> <div>44%</div> <div>.</div> </div>
2	C	8	<div> <div>25%</div> <div>38%</div> <div>38%</div> <div>25%</div> </div>
2	D	8	<div> <div>13%</div> <div>25%</div> <div>63%</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5716 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 CLATHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2789	1773	480	518	18			
1	B	357	Total	C	N	O	S	0	0	0
			2789	1773	480	518	18			

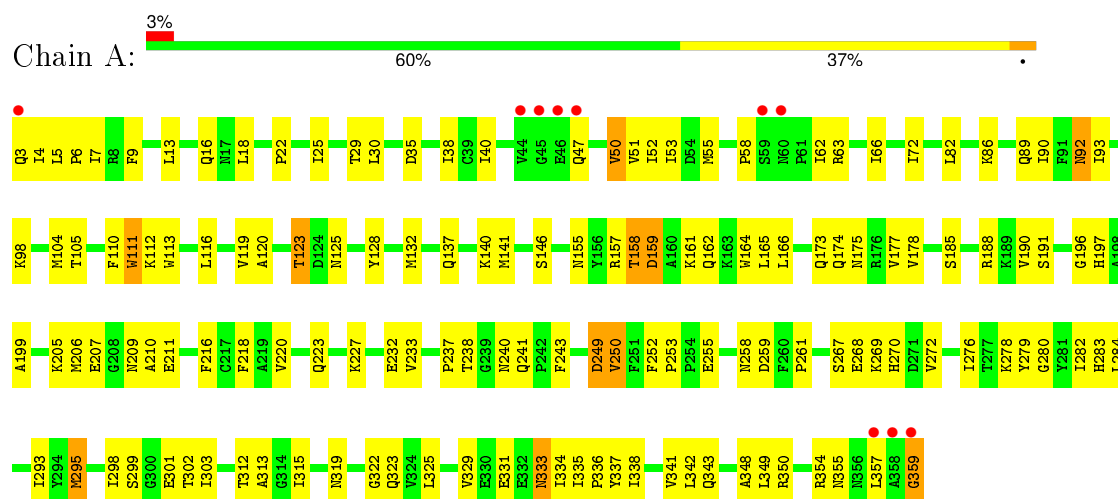
- Molecule 2 is a protein called B-ADAPTIN 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			69	43	9	17			
2	D	8	Total	C	N	O	0	0	0
			69	43	9	17			

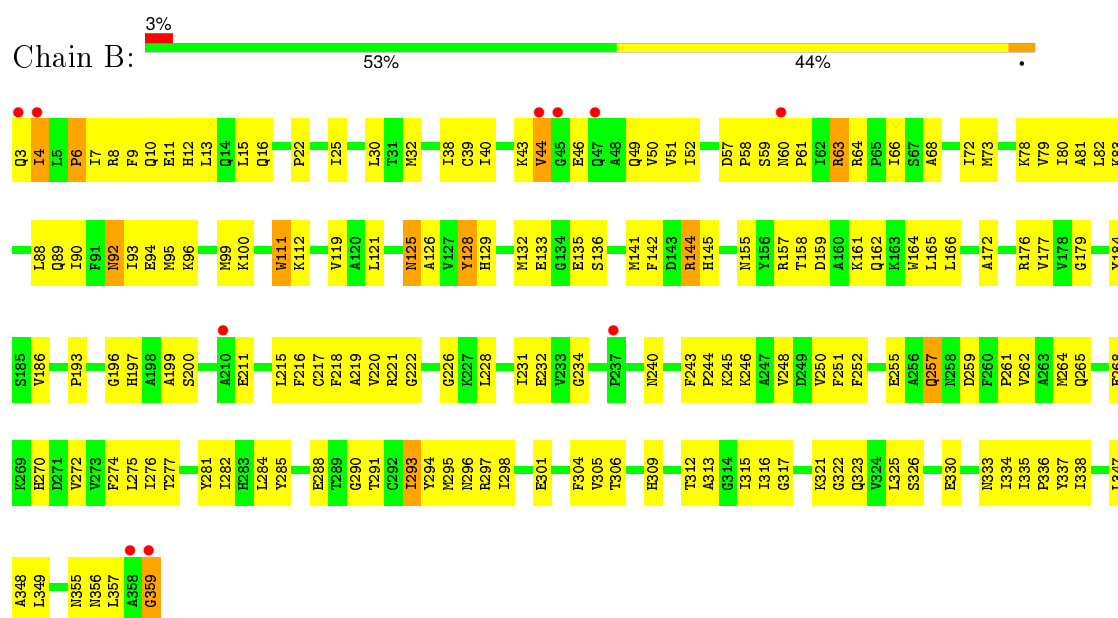
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: CLATHRIN



• Molecule 1: CLATHRIN



• Molecule 2: B-ADAPTIN 3





● Molecule 2: B-ADAPTIN 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.62Å 130.79Å 78.47Å 90.00° 115.47° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-2.90) 92.5 (29.94-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 2.90Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.221 , 0.263 0.217 , 0.258	Depositor DCC
R_{free} test set	1282 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25725 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.12	2/2847 (0.1%)	0.78	1/3859 (0.0%)
1	B	1.12	2/2847 (0.1%)	0.79	5/3859 (0.1%)
2	C	1.88	3/69 (4.3%)	1.57	1/91 (1.1%)
2	D	1.53	1/69 (1.4%)	1.50	1/91 (1.1%)
All	All	1.14	8/5832 (0.1%)	0.81	8/7900 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	GLY	C-OXT	53.00	2.24	1.23
1	B	359	GLY	C-OXT	53.00	2.24	1.23
2	C	377	GLU	C-OXT	9.93	1.42	1.23
2	D	377	GLU	C-OXT	9.75	1.41	1.23
2	C	377	GLU	N-CA	-6.50	1.33	1.46
2	C	376	PHE	C-N	-6.20	1.19	1.34
1	A	175	ASN	C-O	5.34	1.33	1.23
1	B	6	PRO	CA-C	-5.05	1.42	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	PRO	CA-C-N	-8.35	98.83	117.20
1	A	3	GLN	C-N-CA	-8.33	100.88	121.70
1	B	3	GLN	C-N-CA	-6.61	105.17	121.70
1	B	63	ARG	C-N-CA	6.47	137.86	121.70
2	C	377	GLU	N-CA-C	6.41	128.32	111.00
2	D	370	ASP	CA-C-N	-5.48	105.14	117.20
1	B	6	PRO	O-C-N	5.35	131.26	122.70
1	B	4	ILE	CA-C-N	-5.18	105.81	117.20

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	2789	0	2799	136	0
1	B	2789	0	2799	171	0
2	C	69	0	58	4	0
2	D	69	0	59	10	0
All	All	5716	0	5715	310	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 27.

All (310) 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:323:GLN:HE21	1:A:325:LEU:HD21	1.09	1.11
1:B:50:VAL:HG23	1:B:66:ILE:HG12	1.35	1.09
1:B:301:GLU:HG3	1:B:321:LYS:HG3	1.39	0.99
1:B:92:ASN:ND2	1:B:95:MET:H	1.61	0.97
1:B:51:VAL:HG22	1:B:63:ARG:HG2	1.46	0.95
1:A:4:ILE:HD12	1:A:333:ASN:HB3	1.47	0.94
1:A:209:ASN:HD21	1:A:241:GLN:H	1.16	0.92
1:B:335:ILE:HB	1:B:359:GLY:HA3	1.51	0.92
1:A:98:LYS:HE2	2:C:372:ASN:OD1	1.70	0.91
1:A:323:GLN:NE2	1:A:325:LEU:HD21	1.86	0.90
1:B:92:ASN:HD22	1:B:95:MET:H	1.19	0.88
1:B:89:GLN:NE2	2:D:371:THR:O	2.06	0.88
1:A:335:ILE:HB	1:A:359:GLY:HA3	1.54	0.87
1:A:335:ILE:HB	1:A:336:PRO:HD3	1.56	0.85
1:A:51:VAL:HG22	1:A:63:ARG:HG2	1.59	0.85
1:B:50:VAL:CG2	1:B:66:ILE:HG12	2.08	0.83
1:A:90:ILE:HG12	1:A:132:MET:CE	2.09	0.83
1:A:123:THR:HG22	1:A:125:ASN:H	1.43	0.83
1:A:209:ASN:ND2	1:A:241:GLN:H	1.77	0.81
1:A:90:ILE:HG12	1:A:132:MET:HE2	1.63	0.81
1:A:255:GLU:H	1:A:255:GLU:CD	1.84	0.80
1:B:79:VAL:HG13	1:B:99:MET:HE1	1.65	0.79
1:B:166:LEU:HD22	1:B:216:PHE:HE1	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:HD21	1:A:241:GLN:N	1.81	0.78
1:B:50:VAL:HG23	1:B:66:ILE:CG1	2.14	0.78
1:B:323:GLN:CD	1:B:325:LEU:HD21	2.03	0.77
1:A:252:PHE:HZ	1:A:261:PRO:HD3	1.47	0.77
1:A:253:PRO:HB2	1:A:255:GLU:OE1	1.84	0.77
1:A:5:LEU:HD23	1:A:7:ILE:HD11	1.67	0.76
1:B:30:LEU:HD23	1:B:40:ILE:HG13	1.65	0.76
1:A:359:GLY:C	1:A:359:GLY:OXT	2.24	0.76
1:A:166:LEU:HD22	1:A:216:PHE:HE1	1.51	0.76
1:B:338:ILE:HG22	1:B:348:ALA:HB2	1.68	0.76
1:B:293:ILE:HD12	1:B:334:ILE:HD11	1.69	0.75
1:B:9:PHE:CZ	1:B:325:LEU:HD22	2.22	0.74
1:B:158:THR:HG22	1:B:159:ASP:O	1.88	0.74
1:A:50:VAL:HG13	1:A:66:ILE:HD13	1.71	0.72
1:A:252:PHE:HZ	1:A:261:PRO:CD	2.04	0.71
1:B:306:THR:HG22	1:B:317:GLY:HA3	1.73	0.69
1:B:43:LYS:HZ2	1:B:46:GLU:HA	1.58	0.68
1:A:359:GLY:O	1:A:359:GLY:OXT	2.10	0.68
1:A:355:ASN:HB2	1:A:357:LEU:CD1	2.23	0.68
1:B:274:PHE:CE2	1:B:284:LEU:HD21	2.28	0.68
1:B:323:GLN:NE2	1:B:325:LEU:HD21	2.08	0.68
1:A:6:PRO:HG3	1:A:337:TYR:CG	2.29	0.67
1:A:16:GLN:NE2	1:A:22:PRO:HG3	2.09	0.67
1:B:93:ILE:HA	2:D:376:PHE:CE2	2.30	0.67
1:B:158:THR:HG21	1:B:162:GLN:HG2	1.76	0.67
1:B:79:VAL:HG13	1:B:99:MET:CE	2.25	0.66
1:A:13:LEU:HD11	1:A:58:PRO:HB3	1.77	0.66
1:B:6:PRO:HG3	1:B:337:TYR:CD2	2.31	0.66
1:B:30:LEU:CD2	1:B:40:ILE:HG13	2.26	0.66
2:D:371:THR:CG2	2:D:372:ASN:N	2.60	0.65
1:A:252:PHE:CZ	1:A:261:PRO:HD3	2.30	0.64
1:B:265:GLN:OE1	1:B:265:GLN:HA	1.96	0.64
1:B:90:ILE:HG21	1:B:132:MET:HE2	1.79	0.64
1:B:66:ILE:HD12	1:B:66:ILE:C	2.18	0.64
1:A:335:ILE:CB	1:A:359:GLY:HA3	2.27	0.64
1:B:211:GLU:H	1:B:240:ASN:HD21	1.46	0.63
1:A:90:ILE:HG21	1:A:132:MET:CE	2.28	0.63
1:B:83:LYS:HD3	1:B:111:TRP:CE2	2.33	0.63
1:B:284:LEU:CD1	1:B:293:ILE:HD11	2.29	0.63
1:A:50:VAL:HG22	1:A:66:ILE:HG23	1.81	0.63
1:B:246:LYS:HE2	1:B:288:GLU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:CD	1:B:255:GLU:H	2.02	0.63
1:B:277:THR:CG2	1:B:281:TYR:HB2	2.29	0.63
1:B:166:LEU:HD22	1:B:216:PHE:CE1	2.33	0.62
1:A:158:THR:HG21	1:A:162:GLN:CG	2.28	0.62
1:A:336:PRO:HD3	1:A:359:GLY:HA3	1.80	0.62
1:A:355:ASN:HB2	1:A:357:LEU:HD12	1.80	0.61
1:A:6:PRO:HG3	1:A:337:TYR:CD2	2.35	0.61
1:B:93:ILE:HA	2:D:376:PHE:HE2	1.66	0.61
1:A:158:THR:HG21	1:A:162:GLN:HG3	1.81	0.61
1:B:11:GLU:OE1	1:B:323:GLN:NE2	2.34	0.60
1:B:16:GLN:NE2	1:B:22:PRO:HG3	2.16	0.60
1:B:90:ILE:HG21	1:B:132:MET:CE	2.32	0.60
1:A:323:GLN:HE21	1:A:325:LEU:CD2	1.98	0.59
1:B:158:THR:HG23	1:B:162:GLN:HA	1.83	0.59
1:A:105:THR:O	1:A:105:THR:HG22	2.00	0.59
1:A:205:LYS:NZ	1:A:210:ALA:C	2.56	0.59
1:B:355:ASN:HB2	1:B:357:LEU:HD11	1.85	0.59
1:B:44:VAL:HB	1:B:49:GLN:HE21	1.67	0.58
1:B:335:ILE:HB	1:B:336:PRO:HD3	1.85	0.58
1:B:125:ASN:C	1:B:125:ASN:HD22	2.06	0.58
1:B:164:TRP:C	1:B:165:LEU:HD23	2.24	0.58
1:B:57:ASP:N	1:B:58:PRO:HD3	2.18	0.58
1:B:284:LEU:HD12	1:B:293:ILE:HD11	1.86	0.58
1:A:50:VAL:HG22	1:A:66:ILE:CG2	2.33	0.58
1:B:277:THR:HG23	1:B:281:TYR:HB2	1.85	0.58
1:B:51:VAL:HG22	1:B:63:ARG:CG	2.29	0.57
1:A:90:ILE:HG12	1:A:132:MET:HE1	1.82	0.57
1:B:232:GLU:HB2	1:B:243:PHE:HB3	1.86	0.57
1:B:44:VAL:HB	1:B:49:GLN:NE2	2.20	0.57
1:A:166:LEU:HD22	1:A:216:PHE:CE1	2.36	0.57
1:B:199:ALA:HB2	1:B:218:PHE:CB	2.35	0.57
1:B:261:PRO:HB3	1:B:275:LEU:HD11	1.87	0.57
1:A:188:ARG:O	1:A:190:VAL:HG23	2.04	0.56
1:A:270:HIS:CE1	1:A:329:VAL:HB	2.41	0.56
1:B:316:ILE:HG13	1:B:325:LEU:O	2.05	0.56
1:A:232:GLU:HB2	1:A:243:PHE:HB3	1.87	0.55
1:B:92:ASN:HB3	1:B:95:MET:HE3	1.88	0.55
1:A:259:ASP:OD1	1:A:279:TYR:HD1	1.90	0.55
1:A:141:MET:HA	1:A:141:MET:HE3	1.89	0.55
1:B:309:HIS:HD2	1:B:312:THR:OG1	1.89	0.55
1:B:72:ILE:HG13	1:B:81:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLN:NE2	1:B:22:PRO:CG	2.69	0.54
1:B:128:TYR:N	1:B:128:TYR:CD1	2.75	0.54
1:A:312:THR:O	1:A:313:ALA:HB3	2.07	0.54
1:B:32:MET:HG3	1:B:38:ILE:HG12	1.89	0.54
2:D:371:THR:HG22	2:D:372:ASN:N	2.23	0.54
1:B:43:LYS:NZ	1:B:46:GLU:HA	2.24	0.53
1:A:158:THR:HG23	1:A:162:GLN:HA	1.91	0.53
1:B:4:ILE:HD12	1:B:333:ASN:HB2	1.91	0.53
1:A:185:SER:OG	1:A:188:ARG:HG2	2.08	0.53
1:B:155:ASN:HD21	1:B:157:ARG:CG	2.22	0.53
1:A:86:LYS:HB3	1:A:104:MET:O	2.09	0.53
1:B:59:SER:C	1:B:61:PRO:HD3	2.30	0.53
1:A:155:ASN:HD21	1:A:157:ARG:HG3	1.74	0.53
1:A:335:ILE:HB	1:A:336:PRO:CD	2.33	0.52
1:B:12:HIS:O	1:B:13:LEU:HD23	2.09	0.52
1:A:196:GLY:HA2	1:A:220:VAL:HB	1.91	0.52
1:B:184:TYR:CE2	1:B:186:VAL:HA	2.45	0.52
1:A:7:ILE:HD12	1:A:7:ILE:C	2.30	0.52
1:A:302:THR:O	1:A:319:ASN:HB2	2.09	0.52
1:A:355:ASN:HB2	1:A:357:LEU:HD11	1.90	0.52
1:A:5:LEU:HD23	1:A:7:ILE:CD1	2.37	0.52
1:B:6:PRO:HG2	1:B:294:TYR:HB2	1.92	0.52
2:D:374:ILE:HG23	2:D:374:ILE:O	2.10	0.52
1:B:312:THR:O	1:B:313:ALA:HB3	2.10	0.51
1:A:301:GLU:HB2	1:A:319:ASN:ND2	2.24	0.51
1:A:280:GLY:HA3	1:A:299:SER:O	2.09	0.51
1:A:278:LYS:O	1:A:302:THR:HG22	2.11	0.51
1:A:293:ILE:O	1:A:342:LEU:HD11	2.09	0.51
2:D:371:THR:HG23	2:D:372:ASN:H	1.75	0.51
1:A:72:ILE:O	1:A:72:ILE:HG13	2.11	0.51
1:A:206:MET:O	1:A:209:ASN:HB2	2.11	0.51
2:D:371:THR:CG2	2:D:372:ASN:H	2.24	0.51
1:A:205:LYS:HZ2	1:A:210:ALA:C	2.13	0.51
1:A:199:ALA:HB2	1:A:218:PHE:CB	2.41	0.51
1:A:209:ASN:ND2	1:A:241:GLN:N	2.51	0.51
1:B:199:ALA:HB1	1:B:217:CYS:O	2.11	0.50
1:A:173:GLN:HB2	1:A:178:VAL:HG21	1.94	0.50
1:A:158:THR:HG21	1:A:162:GLN:HG2	1.93	0.50
1:B:49:GLN:OE1	1:B:63:ARG:HD3	2.12	0.50
1:B:11:GLU:CG	1:B:323:GLN:HE21	2.25	0.50
1:A:227:LYS:HA	1:A:249:ASP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HA	2:C:376:PHE:CE2	2.47	0.49
1:B:155:ASN:HD21	1:B:157:ARG:HG3	1.76	0.49
1:A:116:LEU:HD22	1:A:116:LEU:N	2.27	0.49
1:A:47:GLN:OE1	1:A:47:GLN:HA	2.13	0.49
1:A:207:GLU:OE2	1:B:257:GLN:HG3	2.13	0.49
1:B:25:ILE:HD13	1:B:322:GLY:CA	2.42	0.49
1:B:66:ILE:HD13	1:B:68:ALA:H	1.78	0.49
1:A:92:ASN:C	1:A:92:ASN:HD22	2.16	0.49
1:B:226:GLY:HA3	1:B:250:VAL:HG22	1.94	0.49
1:B:284:LEU:HD13	1:B:293:ILE:HD11	1.95	0.49
1:B:52:ILE:N	1:B:52:ILE:HD12	2.28	0.48
1:B:272:VAL:CG1	1:B:284:LEU:HD22	2.43	0.48
1:A:173:GLN:HB2	1:A:178:VAL:CG2	2.42	0.48
1:B:197:HIS:HD2	1:B:221:ARG:H	1.59	0.48
1:B:336:PRO:HG3	1:B:359:GLY:OXT	2.13	0.48
1:B:32:MET:HE1	1:B:316:ILE:HG12	1.95	0.48
1:B:349:LEU:C	1:B:349:LEU:HD13	2.34	0.48
1:B:250:VAL:HG23	1:B:250:VAL:O	2.13	0.48
1:B:9:PHE:CD1	1:B:10:GLN:N	2.81	0.48
1:B:184:TYR:HE2	1:B:186:VAL:HA	1.79	0.48
1:A:25:ILE:HD13	1:A:322:GLY:HA3	1.95	0.48
1:B:220:VAL:O	1:B:226:GLY:HA2	2.14	0.48
1:A:211:GLU:H	1:A:240:ASN:HD21	1.60	0.48
1:B:274:PHE:CD2	1:B:284:LEU:HD21	2.48	0.48
1:A:270:HIS:ND1	1:A:329:VAL:HB	2.29	0.48
1:A:161:LYS:HG2	1:A:161:LYS:O	2.14	0.48
1:B:179:GLY:HA3	1:B:196:GLY:O	2.13	0.48
1:A:349:LEU:HD22	1:B:172:ALA:HB2	1.96	0.48
1:A:338:ILE:HG22	1:A:348:ALA:HB2	1.96	0.47
1:B:50:VAL:HG12	1:B:52:ILE:HD12	1.96	0.47
1:B:338:ILE:CG2	1:B:348:ALA:HB2	2.41	0.47
1:B:83:LYS:HB2	1:B:88:LEU:CD2	2.44	0.47
1:B:129:HIS:CD2	1:B:141:MET:HG3	2.49	0.47
1:A:276:ILE:HG12	1:A:282:ILE:HD13	1.96	0.47
1:B:197:HIS:CD2	1:B:221:ARG:H	2.31	0.47
1:B:43:LYS:NZ	1:B:46:GLU:OE2	2.46	0.47
1:B:119:VAL:HG12	1:B:121:LEU:HD23	1.96	0.47
1:A:82:LEU:CD1	2:C:374:ILE:HB	2.44	0.47
1:A:25:ILE:HD13	1:A:322:GLY:CA	2.45	0.47
1:B:264:MET:HA	1:B:274:PHE:O	2.15	0.47
1:B:7:ILE:O	1:B:330:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ALA:N	1:B:144:ARG:HG3	2.30	0.47
1:A:111:TRP:HB2	1:A:120:ALA:O	2.14	0.47
1:A:62:ILE:O	1:A:62:ILE:HG13	2.15	0.46
1:B:291:THR:HG21	1:B:347:LEU:HD22	1.97	0.46
1:B:176:ARG:HH12	1:B:222:GLY:HA2	1.81	0.46
1:A:323:GLN:HG2	1:A:325:LEU:HD21	1.98	0.46
1:A:335:ILE:CG2	1:A:359:GLY:HA3	2.45	0.46
1:B:265:GLN:HG2	1:B:315:ILE:HD12	1.97	0.46
1:B:164:TRP:O	1:B:165:LEU:HD23	2.15	0.46
1:A:337:TYR:CZ	1:A:341:VAL:HG11	2.51	0.46
1:B:282:ILE:CG2	1:B:298:ILE:HG23	2.46	0.46
1:B:284:LEU:HB3	1:B:293:ILE:HG12	1.97	0.46
1:B:30:LEU:HD21	1:B:38:ILE:CG2	2.45	0.46
1:B:155:ASN:ND2	1:B:157:ARG:HG3	2.31	0.46
1:A:52:ILE:HD13	1:A:93:ILE:HD13	1.98	0.46
1:A:30:LEU:C	1:A:30:LEU:HD23	2.36	0.46
1:B:355:ASN:HB2	1:B:357:LEU:CD1	2.45	0.46
1:B:251:PHE:HB3	1:B:295:MET:HE1	1.98	0.46
1:A:51:VAL:HG21	1:A:63:ARG:CZ	2.45	0.45
1:B:92:ASN:CB	1:B:95:MET:HE3	2.45	0.45
1:A:255:GLU:N	1:A:255:GLU:CD	2.62	0.45
1:B:177:VAL:O	1:B:197:HIS:HE1	1.99	0.45
1:B:248:VAL:HG11	1:B:290:GLY:O	2.16	0.45
1:A:205:LYS:NZ	1:A:210:ALA:O	2.50	0.45
1:B:158:THR:CG2	1:B:159:ASP:O	2.59	0.45
1:B:12:HIS:NE2	1:B:326:SER:HB3	2.31	0.45
1:B:219:ALA:HB2	1:B:228:LEU:HD12	1.99	0.45
1:B:39:CYS:SG	1:B:73:MET:HG2	2.56	0.45
1:B:276:ILE:HG12	1:B:282:ILE:CD1	2.47	0.45
1:B:250:VAL:O	1:B:250:VAL:CG2	2.65	0.45
1:A:295:MET:HG3	1:A:295:MET:O	2.17	0.45
1:A:35:ASP:O	1:A:55:MET:HG3	2.17	0.45
1:A:9:PHE:CZ	1:A:325:LEU:HD22	2.52	0.45
1:B:252:PHE:CE2	1:B:259:ASP:O	2.69	0.45
1:B:304:PHE:CD1	1:B:305:VAL:HG12	2.52	0.44
1:B:276:ILE:HG12	1:B:282:ILE:HD13	1.98	0.44
1:B:30:LEU:HD23	1:B:40:ILE:CG1	2.41	0.44
1:B:262:VAL:HG12	1:B:276:ILE:O	2.18	0.44
1:B:6:PRO:HG3	1:B:337:TYR:CG	2.53	0.44
1:B:39:CYS:SG	1:B:73:MET:CG	3.05	0.44
1:B:96:LYS:HE2	2:D:377:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:MET:HE3	1:B:95:MET:HB2	1.87	0.44
1:B:11:GLU:HG3	1:B:323:GLN:HG3	1.99	0.43
1:A:267:SER:HB2	1:A:313:ALA:O	2.18	0.43
1:A:272:VAL:CG1	1:A:284:LEU:HD13	2.48	0.43
1:B:231:ILE:HG22	1:B:245:LYS:HB2	2.00	0.43
1:B:83:LYS:HB2	1:B:88:LEU:HD23	1.99	0.43
1:B:164:TRP:HZ2	1:B:234:GLY:CA	2.31	0.43
1:B:161:LYS:O	1:B:162:GLN:C	2.56	0.43
1:B:277:THR:HG21	1:B:281:TYR:HB2	2.00	0.43
1:B:145:HIS:CD2	1:B:193:PRO:HG3	2.52	0.43
1:A:113:TRP:CE3	1:A:119:VAL:HG22	2.52	0.43
1:A:93:ILE:HA	2:C:376:PHE:HE2	1.83	0.43
1:A:158:THR:CG2	1:A:159:ASP:O	2.66	0.43
1:A:155:ASN:ND2	1:A:157:ARG:HG3	2.33	0.43
1:A:250:VAL:HG23	1:A:283:HIS:CE1	2.54	0.43
1:A:128:TYR:CD2	1:A:140:LYS:HA	2.54	0.43
1:B:92:ASN:ND2	1:B:95:MET:N	2.46	0.42
1:A:205:LYS:HE3	1:A:209:ASN:O	2.19	0.42
1:B:142:PHE:CE2	1:B:165:LEU:HD12	2.54	0.42
1:B:96:LYS:CE	2:D:377:GLU:HG2	2.48	0.42
1:B:64:ARG:HA	1:B:64:ARG:HD3	1.83	0.42
1:A:89:GLN:C	1:A:90:ILE:HD12	2.39	0.42
1:A:51:VAL:CG2	1:A:63:ARG:CZ	2.98	0.42
1:B:282:ILE:HG22	1:B:296:ASN:O	2.19	0.42
1:B:79:VAL:CG1	1:B:99:MET:CE	2.94	0.42
1:A:269:LYS:HG2	1:A:270:HIS:CD2	2.54	0.42
1:B:60:ASN:N	1:B:61:PRO:HD3	2.35	0.42
1:A:333:ASN:O	1:A:334:ILE:C	2.58	0.42
1:B:355:ASN:O	1:B:356:ASN:HB2	2.19	0.42
1:B:199:ALA:HB2	1:B:218:PHE:HB3	2.02	0.42
1:A:233:VAL:HG23	1:A:233:VAL:O	2.20	0.42
1:A:350:ARG:NE	1:A:354:ARG:HD3	2.35	0.42
1:B:276:ILE:HA	1:B:281:TYR:O	2.20	0.42
1:A:173:GLN:O	1:A:174:GLN:C	2.56	0.42
1:A:272:VAL:HG11	1:A:284:LEU:HD13	2.01	0.42
1:A:51:VAL:CG2	1:A:63:ARG:NH1	2.82	0.41
1:B:323:GLN:CD	1:B:325:LEU:CD2	2.82	0.41
1:B:72:ILE:HD11	1:B:111:TRP:CD2	2.54	0.41
1:A:159:ASP:OD2	1:A:164:TRP:N	2.53	0.41
1:A:190:VAL:HG12	1:A:191:SER:N	2.36	0.41
1:B:157:ARG:CZ	1:B:200:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HB	1:A:298:ILE:HD13	2.02	0.41
1:A:4:ILE:HD12	1:A:333:ASN:CB	2.35	0.41
1:B:244:PRO:HG2	1:B:246:LYS:NZ	2.36	0.41
1:A:335:ILE:CB	1:A:336:PRO:HD3	2.39	0.41
1:B:285:TYR:HA	1:B:291:THR:O	2.19	0.41
1:A:38:ILE:HG22	1:A:40:ILE:HD11	2.01	0.41
1:B:50:VAL:CG2	1:B:66:ILE:HG21	2.50	0.41
1:B:316:ILE:O	1:B:316:ILE:HG23	2.20	0.41
1:A:276:ILE:CD1	1:A:315:ILE:HD13	2.50	0.41
1:A:237:PRO:O	1:A:238:THR:C	2.58	0.41
1:B:78:LYS:HB2	1:B:94:GLU:OE2	2.20	0.41
1:B:90:ILE:HG22	1:B:99:MET:CE	2.51	0.41
1:A:40:ILE:N	1:A:40:ILE:HD12	2.36	0.41
1:A:18:LEU:CD1	1:A:53:ILE:HD13	2.51	0.41
1:B:11:GLU:HB2	1:B:323:GLN:HE21	1.86	0.41
1:B:6:PRO:O	1:B:330:GLU:HB3	2.21	0.41
1:B:83:LYS:HD3	1:B:111:TRP:CZ2	2.56	0.41
1:B:270:HIS:C	1:B:355:ASN:ND2	2.74	0.41
1:B:58:PRO:O	1:B:61:PRO:HD3	2.21	0.41
1:B:221:ARG:NH1	1:B:257:GLN:O	2.52	0.41
1:B:92:ASN:ND2	1:B:95:MET:HG3	2.36	0.40
1:A:50:VAL:HG13	1:A:66:ILE:CD1	2.45	0.40
1:A:116:LEU:HD22	1:A:116:LEU:H	1.87	0.40
1:B:25:ILE:HD13	1:B:322:GLY:HA2	2.03	0.40
1:B:80:ILE:HD13	1:B:82:LEU:HD21	2.02	0.40
1:B:296:ASN:CG	1:B:297:ARG:N	2.75	0.40
1:B:125:ASN:ND2	1:B:125:ASN:C	2.73	0.40
1:A:110:PHE:CZ	1:A:155:ASN:HA	2.57	0.40
1:A:206:MET:HB2	1:A:209:ASN:OD1	2.21	0.40
1:A:90:ILE:HG21	1:A:132:MET:HE1	2.03	0.40
1:A:7:ILE:HD12	1:A:7:ILE:O	2.21	0.40
1:A:158:THR:HG22	1:A:159:ASP:O	2.21	0.40
1:B:142:PHE:CD2	1:B:165:LEU:HD12	2.57	0.40
1:A:303:ILE:HG12	1:A:319:ASN:HB3	2.02	0.40
1:B:196:GLY:HA2	1:B:220:VAL:HB	2.03	0.40
1:B:144:ARG:HB3	1:B:144:ARG:HE	1.60	0.40
1:B:284:LEU:CB	1:B:293:ILE:HG12	2.52	0.40
1:A:164:TRP:C	1:A:165:LEU:HD23	2.41	0.40
1:B:215:LEU:HD23	1:B:232:GLU:HA	2.04	0.40
1:A:272:VAL:HG11	1:A:284:LEU:CD1	2.52	0.40
1:A:177:VAL:O	1:A:197:HIS:HE1	2.05	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	355/357 (99%)	327 (92%)	28 (8%)	0	100	100
1	B	355/357 (99%)	328 (92%)	23 (6%)	4 (1%)	17	51
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	722/730 (99%)	666 (92%)	52 (7%)	4 (1%)	30	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	VAL
1	B	136	SER
1	B	15	LEU
1	B	135	GLU

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	306/306 (100%)	287 (94%)	19 (6%)	23	55
1	B	306/306 (100%)	294 (96%)	12 (4%)	39	75
2	C	8/8 (100%)	6 (75%)	2 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	8/8 (100%)	8 (100%)	0	100	100
All	All	628/628 (100%)	595 (95%)	33 (5%)	28	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	50	VAL
1	A	92	ASN
1	A	111	TRP
1	A	112	LYS
1	A	123	THR
1	A	137	GLN
1	A	146	SER
1	A	158	THR
1	A	159	ASP
1	A	223	GLN
1	A	249	ASP
1	A	250	VAL
1	A	258	ASN
1	A	268	GLU
1	A	295	MET
1	A	331	GLU
1	A	333	ASN
1	A	343	GLN
1	B	8	ARG
1	B	92	ASN
1	B	100	LYS
1	B	111	TRP
1	B	112	LYS
1	B	125	ASN
1	B	128	TYR
1	B	133	GLU
1	B	144	ARG
1	B	257	GLN
1	B	268	GLU
1	B	293	ILE
2	C	370	ASP
2	C	377	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	60	ASN
1	A	155	ASN
1	A	197	HIS
1	A	209	ASN
1	A	223	GLN
1	A	240	ASN
1	A	283	HIS
1	A	296	ASN
1	A	323	GLN
1	B	14	GLN
1	B	16	GLN
1	B	17	ASN
1	B	92	ASN
1	B	102	HIS
1	B	125	ASN
1	B	155	ASN
1	B	175	ASN
1	B	197	HIS
1	B	240	ASN
1	B	257	GLN
1	B	309	HIS
1	B	323	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 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	357/357 (100%)	-0.33	10 (2%) 56 50	6, 24, 52, 82	0
1	B	357/357 (100%)	-0.28	10 (2%) 56 50	7, 25, 51, 73	0
2	C	8/8 (100%)	0.89	2 (25%) 1 0	25, 44, 63, 79	0
2	D	8/8 (100%)	1.35	1 (12%) 5 3	39, 58, 70, 88	0
All	All	730/730 (100%)	-0.28	23 (3%) 51 43	6, 25, 55, 88	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	GLY	6.9
2	D	370	ASP	5.1
1	A	359	GLY	4.9
1	B	3	GLN	3.9
1	A	358	ALA	3.6
2	C	377	GLU	3.2
1	B	358	ALA	3.1
2	C	370	ASP	3.1
1	B	60	ASN	3.1
1	A	44	VAL	3.1
1	A	3	GLN	3.1
1	B	47	GLN	3.0
1	A	59	SER	2.9
1	B	44	VAL	2.7
1	A	47	GLN	2.6
1	A	60	ASN	2.6
1	B	4	ILE	2.5
1	B	45	GLY	2.4
1	B	237	PRO	2.4
1	A	357	LEU	2.3
1	A	46	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLY	2.1
1	B	210	ALA	2.1

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 carbohydrates 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.