Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 01:37 AM EDT

PDB ID	:	2ZUC
Title	:	Crystal structure of left-handed RadA filament
Authors	:	Chang, Y.W.; Ko, T.P.; Wang, T.F.; Wang, A.H.J.
Deposited on	:	2008-10-15
Resolution	:	3.30 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:

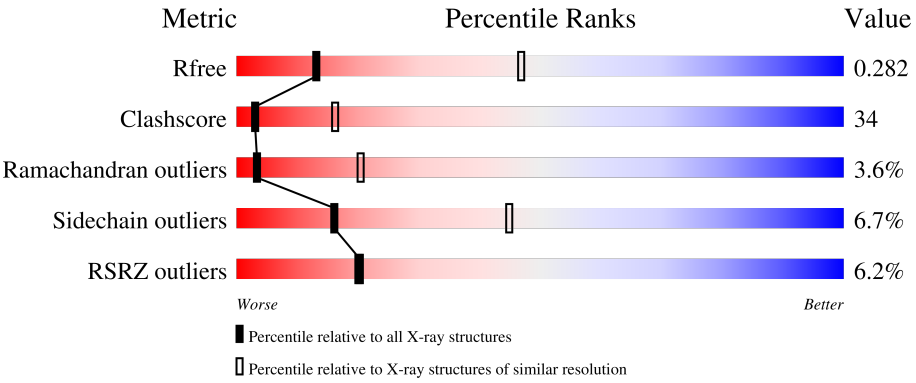
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	324	3%, 44%, 43%, 8%
1	B	324	8%, 45%, 44%, 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4673 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 DNA repair and recombination protein radA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2315	1459	411	439	6			
1	B	301	Total	C	N	O	S	0	0	0
			2346	1476	418	445	7			

- Molecule 2 is water.

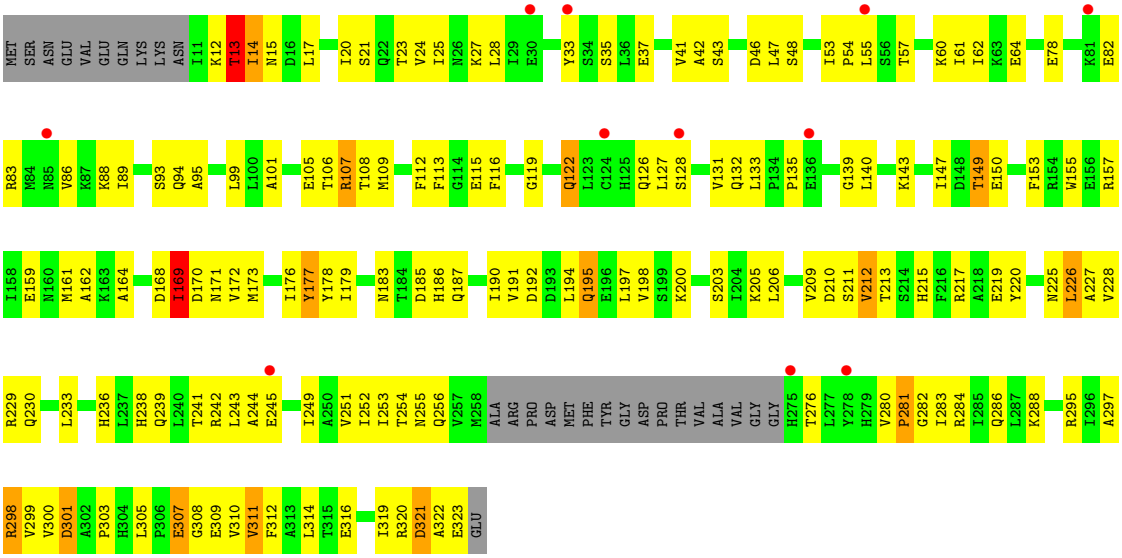
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	4	Total	O	0	0
			4	4		

3 Residue-property plots (i)

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

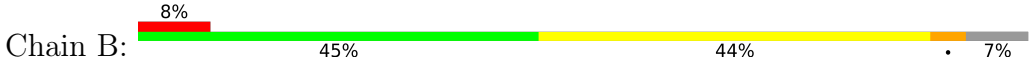
• Molecule 1: DNA repair and recombination protein radA

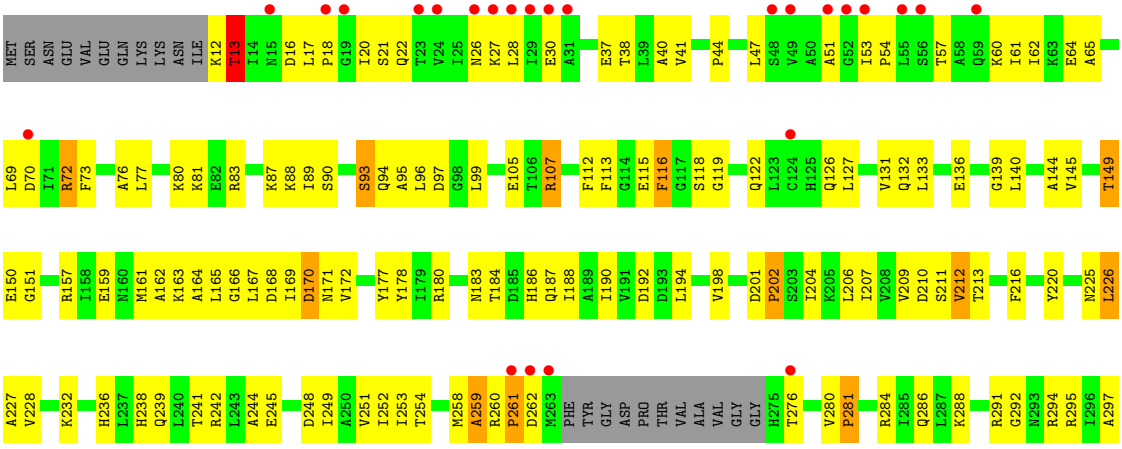
Chain A:

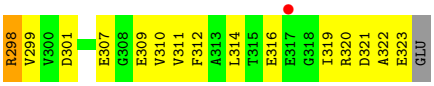


• Molecule 1: DNA repair and recombination protein radA

Chain B:






R298
V299
V300
D301
E307
G308
E309
V310
V311
F312
A313
L314
T315
E316
E317
G318
I319
R320
D321
A322
E323
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.14Å 114.79Å 136.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 24.86 – 3.31	Depositor EDS
% Data completeness (in resolution range)	82.7 (30.00-3.30) 83.2 (24.86-3.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.283 0.223 , 0.282	Depositor DCC
R_{free} test set	512 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	84.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4673	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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	0.70	1/2347 (0.0%)	0.79	1/3172 (0.0%)
1	B	0.72	1/2379 (0.0%)	0.81	0/3215
All	All	0.71	2/4726 (0.0%)	0.80	1/6387 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	GLU	CG-CD	6.44	1.61	1.51
1	B	307	GLU	CG-CD	5.21	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	THR	N-CA-C	5.17	124.96	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2315	0	2378	188	0
1	B	2346	0	2405	148	0
2	A	8	0	0	0	0
2	B	4	0	0	0	0
All	All	4673	0	4783	322	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 34.

All (322) 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:132:GLN:HE22	1:A:172:VAL:HA	1.22	1.01
1:A:212:VAL:HG23	1:A:213:THR:H	1.29	0.98
1:A:217:ARG:NH2	1:A:255:ASN:HD21	1.62	0.97
1:B:119:GLY:HA2	1:B:122:GLN:HE21	1.34	0.92
1:B:122:GLN:HG2	1:B:314:LEU:HD13	1.52	0.92
1:A:217:ARG:HH22	1:A:255:ASN:HD21	1.17	0.89
1:B:40:ALA:HB2	1:B:69:LEU:HD21	1.57	0.87
1:B:169:ILE:HG13	1:B:170:ASP:H	1.39	0.87
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.41	0.84
1:A:169:ILE:HD13	1:A:169:ILE:N	1.92	0.84
1:A:122:GLN:HG3	1:A:314:LEU:HD22	1.60	0.84
1:A:205:LYS:HD3	1:A:249:ILE:HG22	1.59	0.84
1:A:89:ILE:HD13	1:A:131:VAL:CG2	2.12	0.79
1:A:205:LYS:HA	1:A:249:ILE:HG22	1.64	0.78
1:A:89:ILE:HD13	1:A:131:VAL:HG22	1.66	0.77
1:A:122:GLN:H	1:A:122:GLN:NE2	1.81	0.77
1:B:119:GLY:HA2	1:B:122:GLN:NE2	1.98	0.77
1:B:207:ILE:HG12	1:B:249:ILE:HD12	1.66	0.76
1:A:319:ILE:O	1:A:320:ARG:HD3	1.86	0.76
1:A:35:SER:HB3	1:A:298:ARG:HH22	1.52	0.75
1:B:298:ARG:HG3	1:B:298:ARG:HH11	1.50	0.75
1:A:37:GLU:O	1:A:41:VAL:HG22	1.86	0.74
1:A:99:LEU:HD11	1:A:299:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:HG22	1:B:57:THR:HB	1.68	0.74
1:A:183:ASN:HB2	1:A:219:GLU:OE2	1.86	0.74
1:A:149:THR:HG22	1:A:150:GLU:HG3	1.70	0.73
1:B:169:ILE:HG13	1:B:170:ASP:N	2.03	0.73
1:B:99:LEU:HD11	1:B:299:VAL:HG23	1.70	0.73
1:A:12:LYS:HE3	1:A:300:VAL:O	1.89	0.72
1:A:99:LEU:HD22	1:A:310:VAL:HG12	1.70	0.71
1:A:131:VAL:HG21	1:A:206:LEU:HB2	1.73	0.71
1:A:133:LEU:O	1:A:139:GLY:HA3	1.89	0.71
1:B:127:LEU:HD12	1:B:252:ILE:HD13	1.73	0.71
1:A:212:VAL:HG23	1:A:213:THR:N	2.05	0.71
1:B:236:HIS:O	1:B:239:GLN:HB3	1.92	0.70
1:A:95:ALA:HB1	1:A:310:VAL:CG2	2.23	0.69
1:A:217:ARG:NH2	1:A:255:ASN:ND2	2.39	0.69
1:B:54:PRO:HB2	1:B:57:THR:OG1	1.92	0.69
1:A:177:TYR:CE2	1:A:197:LEU:HD11	2.28	0.69
1:B:149:THR:HG21	1:B:211:SER:O	1.93	0.69
1:A:126:GLN:HE22	1:A:161:MET:HG2	1.58	0.68
1:B:206:LEU:HD11	1:B:252:ILE:HD12	1.74	0.68
1:B:280:VAL:HB	1:B:281:PRO:HD3	1.74	0.68
1:B:188:ILE:HD13	1:B:236:HIS:CD2	2.28	0.67
1:A:95:ALA:HB1	1:A:310:VAL:HG21	1.77	0.67
1:B:310:VAL:HG22	1:B:311:VAL:N	2.09	0.67
1:A:57:THR:O	1:A:61:ILE:HG13	1.95	0.66
1:A:168:ASP:HB3	1:A:171:ASN:HB2	1.76	0.66
1:B:192:ASP:OD2	1:B:239:GLN:NE2	2.29	0.66
1:A:169:ILE:N	1:A:169:ILE:CD1	2.59	0.66
1:A:187:GLN:HE21	1:A:236:HIS:HE1	1.45	0.65
1:A:149:THR:HB	1:A:210:ASP:O	1.96	0.65
1:B:12:LYS:O	1:B:13:THR:O	2.14	0.65
1:A:225:ASN:O	1:A:227:ALA:N	2.30	0.65
1:A:60:LYS:O	1:A:64:GLU:HG2	1.97	0.65
1:A:139:GLY:O	1:A:140:LEU:HD23	1.97	0.65
1:B:207:ILE:HG12	1:B:249:ILE:CD1	2.26	0.64
1:A:106:THR:O	1:A:108:THR:HG22	1.97	0.64
1:A:126:GLN:NE2	1:A:161:MET:SD	2.72	0.63
1:A:169:ILE:HG12	1:A:170:ASP:H	1.63	0.63
1:A:185:ASP:OD1	1:B:41:VAL:HG21	1.99	0.62
1:A:192:ASP:O	1:A:195:GLN:HG2	1.99	0.62
1:A:88:LYS:HE2	1:A:105:GLU:CG	2.29	0.62
1:B:95:ALA:HB1	1:B:310:VAL:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:HB1	1:B:310:VAL:HG21	1.82	0.62
1:A:205:LYS:HA	1:A:249:ILE:CG2	2.30	0.62
1:A:13:THR:CG2	1:A:15:ASN:HD22	2.13	0.62
1:A:195:GLN:HA	1:A:243:LEU:HD21	1.81	0.62
1:B:220:TYR:OH	1:B:232:LYS:HE3	2.00	0.62
1:A:113:PHE:HZ	1:A:300:VAL:HG21	1.63	0.61
1:A:179:ILE:HD11	1:A:190:ILE:HG12	1.83	0.61
1:B:133:LEU:HD21	1:B:167:LEU:HD11	1.82	0.61
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.66	0.61
1:B:177:TYR:CE1	1:B:204:ILE:HD11	2.36	0.60
1:A:169:ILE:HG12	1:A:170:ASP:N	2.16	0.60
1:A:197:LEU:HD22	1:B:73:PHE:CD1	2.37	0.60
1:B:126:GLN:HE21	1:B:161:MET:CE	2.15	0.60
1:B:115:GLU:HG2	1:B:116:PHE:N	2.17	0.59
1:A:20:ILE:HG23	1:A:25:ILE:HD11	1.84	0.59
1:A:169:ILE:HD13	1:A:169:ILE:H	1.68	0.59
1:B:186:HIS:O	1:B:190:ILE:HG13	2.02	0.59
1:B:83:ARG:HH11	1:B:83:ARG:CG	2.10	0.59
1:B:310:VAL:CG2	1:B:311:VAL:N	2.66	0.59
1:A:206:LEU:HD11	1:A:252:ILE:HD12	1.85	0.58
1:A:88:LYS:HE2	1:A:105:GLU:HG3	1.84	0.58
1:B:113:PHE:CZ	1:B:286:GLN:HB2	2.38	0.58
1:B:258:MET:O	1:B:259:ALA:HB2	2.04	0.58
1:A:298:ARG:HB2	1:A:309:GLU:HB3	1.84	0.57
1:A:159:GLU:O	1:A:162:ALA:HB3	2.04	0.57
1:B:122:GLN:HB3	1:B:319:ILE:HD11	1.86	0.57
1:A:35:SER:HB3	1:A:298:ARG:NH2	2.17	0.57
1:A:13:THR:HG21	1:A:15:ASN:HD22	1.69	0.57
1:B:242:ARG:HG2	1:B:242:ARG:HH11	1.70	0.57
1:A:43:SER:OG	1:A:46:ASP:HB2	2.05	0.57
1:B:132:GLN:HE22	1:B:172:VAL:HA	1.68	0.56
1:A:213:THR:HG22	1:A:233:LEU:HD21	1.86	0.56
1:B:159:GLU:O	1:B:162:ALA:HB3	2.05	0.56
1:A:109:MET:CE	1:A:281:PRO:HA	2.35	0.56
1:B:26:ASN:O	1:B:30:GLU:HG2	2.06	0.56
1:A:113:PHE:CZ	1:A:300:VAL:HG21	2.40	0.56
1:B:133:LEU:O	1:B:139:GLY:HA3	2.07	0.55
1:A:178:TYR:CD2	1:A:179:ILE:N	2.74	0.55
1:A:157:ARG:HG2	1:A:161:MET:HE3	1.88	0.55
1:A:295:ARG:HE	1:A:314:LEU:HD11	1.71	0.55
1:B:225:ASN:O	1:B:227:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:HG23	1:B:20:ILE:O	2.06	0.55
1:B:212:VAL:HG21	1:B:253:ILE:HB	1.88	0.55
1:B:149:THR:CG2	1:B:150:GLU:HG3	2.36	0.55
1:A:173:MET:O	1:B:76:ALA:HB3	2.07	0.55
1:B:225:ASN:O	1:B:228:VAL:HG22	2.07	0.55
1:A:126:GLN:HE22	1:A:161:MET:CG	2.19	0.55
1:B:28:LEU:CD2	1:B:47:LEU:HD11	2.37	0.55
1:B:163:LYS:O	1:B:166:GLY:N	2.24	0.55
1:A:310:VAL:HG22	1:A:311:VAL:N	2.20	0.55
1:A:78:GLU:O	1:A:82:GLU:HG3	2.06	0.54
1:A:229:ARG:O	1:A:233:LEU:HB2	2.08	0.54
1:B:163:LYS:O	1:B:165:LEU:N	2.41	0.54
1:A:94:GLN:N	1:A:321:ASP:OD1	2.40	0.54
1:B:209:VAL:HG11	1:B:212:VAL:HG13	1.89	0.54
1:A:187:GLN:HE21	1:A:236:HIS:CE1	2.25	0.54
1:B:88:LYS:HE2	1:B:105:GLU:HG2	1.88	0.54
1:A:169:ILE:CD1	1:A:169:ILE:H	2.20	0.54
1:B:40:ALA:HB2	1:B:69:LEU:CD2	2.35	0.54
1:B:151:GLY:H	1:B:180:ARG:HH11	1.56	0.54
1:A:187:GLN:NE2	1:A:236:HIS:HE1	2.06	0.54
1:A:194:LEU:O	1:A:198:VAL:HG22	2.07	0.54
1:B:139:GLY:O	1:B:140:LEU:HD23	2.07	0.54
1:A:109:MET:HE2	1:A:281:PRO:HA	1.89	0.53
1:A:212:VAL:HG23	1:A:213:THR:HG23	1.90	0.53
1:A:217:ARG:HH22	1:A:255:ASN:ND2	1.98	0.53
1:A:225:ASN:O	1:A:226:LEU:C	2.46	0.53
1:A:244:ALA:HB2	1:A:251:VAL:CG2	2.38	0.53
1:B:17:LEU:O	1:B:20:ILE:HG22	2.09	0.53
1:B:60:LYS:O	1:B:64:GLU:HG3	2.08	0.53
1:A:28:LEU:CD2	1:A:47:LEU:HD11	2.37	0.53
1:A:106:THR:O	1:A:108:THR:N	2.41	0.53
1:A:143:LYS:HD2	1:A:203:SER:HB3	1.90	0.53
1:A:177:TYR:HE2	1:A:197:LEU:HD11	1.74	0.52
1:B:94:GLN:N	1:B:321:ASP:OD1	2.43	0.52
1:B:149:THR:HB	1:B:210:ASP:O	2.09	0.52
1:A:244:ALA:HB2	1:A:251:VAL:HG23	1.91	0.52
1:B:212:VAL:CG2	1:B:253:ILE:HB	2.40	0.52
1:A:131:VAL:HG21	1:A:206:LEU:CB	2.40	0.52
1:B:22:GLN:O	1:B:22:GLN:HG3	2.10	0.52
1:A:95:ALA:HB2	1:A:321:ASP:OD2	2.10	0.52
1:A:322:ALA:O	1:A:323:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:HE21	1:B:236:HIS:HE1	1.57	0.51
1:A:33:TYR:CE2	1:A:47:LEU:HD13	2.44	0.51
1:B:57:THR:O	1:B:61:ILE:HG13	2.11	0.51
1:A:283:ILE:HD13	1:A:303:PRO:HD2	1.93	0.51
1:B:122:GLN:NE2	1:B:122:GLN:H	2.09	0.51
1:A:122:GLN:CG	1:A:314:LEU:HD22	2.37	0.51
1:A:298:ARG:CB	1:A:309:GLU:HB3	2.40	0.51
1:B:151:GLY:N	1:B:180:ARG:NH1	2.59	0.51
1:A:20:ILE:CG2	1:A:25:ILE:HD11	2.41	0.51
1:B:149:THR:HG22	1:B:150:GLU:HG3	1.93	0.51
1:A:99:LEU:CD1	1:A:299:VAL:HG23	2.41	0.51
1:A:297:ALA:HB2	1:A:312:PHE:HE2	1.77	0.50
1:B:107:ARG:NH1	1:B:248:ASP:OD1	2.44	0.50
1:A:255:ASN:ND2	1:A:256:GLN:N	2.59	0.50
1:A:322:ALA:O	1:A:323:GLU:CB	2.59	0.50
1:A:106:THR:C	1:A:108:THR:H	2.15	0.50
1:B:116:PHE:C	1:B:116:PHE:CD2	2.85	0.50
1:A:99:LEU:O	1:A:305:LEU:HD22	2.12	0.50
1:A:122:GLN:H	1:A:122:GLN:CD	2.12	0.50
1:A:191:VAL:HG21	1:A:236:HIS:NE2	2.27	0.50
1:B:127:LEU:HD12	1:B:252:ILE:CD1	2.41	0.50
1:A:168:ASP:O	1:A:169:ILE:C	2.51	0.49
1:A:255:ASN:HD22	1:A:256:GLN:H	1.60	0.49
1:B:70:ASP:OD1	1:B:70:ASP:O	2.30	0.49
1:A:17:LEU:HD22	1:A:64:GLU:CB	2.43	0.49
1:B:122:GLN:CB	1:B:319:ILE:HD11	2.42	0.49
1:A:323:GLU:O	1:A:323:GLU:HG2	2.12	0.49
1:B:44:PRO:HA	1:B:62:ILE:HD12	1.94	0.49
1:A:23:THR:O	1:A:27:LYS:HG3	2.13	0.49
1:A:236:HIS:O	1:A:239:GLN:HB3	2.12	0.49
1:A:225:ASN:O	1:A:228:VAL:HG22	2.13	0.49
1:B:225:ASN:O	1:B:226:LEU:C	2.52	0.49
1:A:17:LEU:HD22	1:A:64:GLU:HB2	1.95	0.49
1:A:13:THR:HG23	1:A:15:ASN:H	1.78	0.48
1:A:42:ALA:O	1:A:62:ILE:HD13	2.12	0.48
1:B:27:LYS:HE2	1:B:51:ALA:O	2.13	0.48
1:A:132:GLN:NE2	1:A:172:VAL:HA	2.08	0.48
1:A:170:ASP:OD1	1:B:77:LEU:HD11	2.13	0.48
1:B:87:LYS:HG3	1:B:140:LEU:CD2	2.44	0.48
1:A:155:TRP:CE3	1:B:80:LYS:NZ	2.81	0.48
1:A:176:ILE:HB	1:B:76:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:NZ	1:B:72:ARG:HH22	2.11	0.48
1:B:112:PHE:O	1:B:254:THR:HA	2.14	0.48
1:A:238:HIS:O	1:A:242:ARG:HG3	2.13	0.48
1:A:284:ARG:HB2	1:A:301:ASP:HB2	1.94	0.48
1:B:294:ARG:O	1:B:295:ARG:NH1	2.41	0.48
1:B:310:VAL:CG2	1:B:311:VAL:H	2.27	0.48
1:A:283:ILE:CD1	1:A:303:PRO:HD2	2.44	0.48
1:B:149:THR:HG22	1:B:150:GLU:N	2.29	0.48
1:A:200:LYS:HZ3	1:B:72:ARG:HH22	1.60	0.48
1:B:184:THR:O	1:B:188:ILE:HG12	2.13	0.48
1:B:187:GLN:HE21	1:B:236:HIS:CE1	2.31	0.48
1:B:194:LEU:O	1:B:198:VAL:HG23	2.14	0.48
1:B:298:ARG:HG3	1:B:298:ARG:NH1	2.24	0.48
1:A:200:LYS:NZ	1:B:72:ARG:NH2	2.62	0.47
1:A:89:ILE:HG21	1:A:131:VAL:HG23	1.95	0.47
1:B:107:ARG:HD2	1:B:245:GLU:HA	1.96	0.47
1:A:187:GLN:O	1:A:191:VAL:HG23	2.14	0.47
1:B:88:LYS:HE2	1:B:105:GLU:CG	2.45	0.47
1:A:126:GLN:HE21	1:A:161:MET:CE	2.28	0.47
1:A:155:TRP:CE3	1:B:80:LYS:CE	2.98	0.47
1:A:53:ILE:HG23	1:A:54:PRO:HD2	1.95	0.47
1:B:53:ILE:CG2	1:B:57:THR:HB	2.41	0.47
1:A:99:LEU:CD1	1:A:308:GLY:O	2.62	0.47
1:A:101:ALA:HB2	1:A:305:LEU:CD2	2.45	0.47
1:A:195:GLN:O	1:A:198:VAL:HG23	2.14	0.47
1:A:99:LEU:HD11	1:A:308:GLY:O	2.14	0.47
1:B:322:ALA:O	1:B:323:GLU:HB3	2.14	0.47
1:B:288:LYS:HE3	1:B:298:ARG:HD2	1.96	0.47
1:A:176:ILE:O	1:B:76:ALA:N	2.42	0.46
1:A:194:LEU:HB3	1:A:243:LEU:HD11	1.96	0.46
1:A:14:ILE:H	1:A:14:ILE:HG12	1.51	0.46
1:A:147:ILE:HA	1:A:179:ILE:HG23	1.97	0.46
1:A:133:LEU:O	1:A:140:LEU:N	2.48	0.46
1:A:155:TRP:CZ3	1:B:80:LYS:HE3	2.50	0.46
1:B:28:LEU:HD21	1:B:47:LEU:HD11	1.96	0.46
1:B:213:THR:O	1:B:216:PHE:HB2	2.14	0.46
1:A:13:THR:HG23	1:A:15:ASN:ND2	2.31	0.46
1:A:113:PHE:CZ	1:A:286:GLN:HB2	2.51	0.46
1:B:244:ALA:HB2	1:B:251:VAL:CG2	2.45	0.46
1:A:89:ILE:HD13	1:A:131:VAL:HG23	1.96	0.46
1:A:212:VAL:CG2	1:A:213:THR:H	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLN:NE2	1:B:161:MET:CE	2.78	0.46
1:B:126:GLN:HB2	1:B:161:MET:HE1	1.96	0.46
1:A:126:GLN:HE21	1:A:161:MET:HE1	1.81	0.46
1:A:133:LEU:O	1:A:139:GLY:CA	2.63	0.46
1:A:192:ASP:O	1:A:195:GLN:CG	2.64	0.46
1:B:72:ARG:HD2	1:B:72:ARG:HA	1.75	0.46
1:B:126:GLN:HE21	1:B:161:MET:HE1	1.81	0.45
1:B:298:ARG:NH1	1:B:298:ARG:CG	2.78	0.45
1:A:186:HIS:NE2	1:B:37:GLU:OE1	2.49	0.45
1:A:195:GLN:HG2	1:A:195:GLN:H	1.51	0.45
1:B:260:ARG:HA	1:B:261:PRO:HD2	1.60	0.45
1:A:255:ASN:HD22	1:A:256:GLN:N	2.14	0.45
1:A:253:ILE:HG13	1:A:253:ILE:O	2.16	0.45
1:B:298:ARG:CB	1:B:309:GLU:HB3	2.46	0.45
1:A:220:TYR:HB3	1:A:225:ASN:HB3	1.99	0.45
1:A:99:LEU:HD22	1:A:310:VAL:CG1	2.44	0.44
1:B:151:GLY:N	1:B:180:ARG:HH11	2.13	0.44
1:B:194:LEU:HA	1:B:194:LEU:HD12	1.71	0.44
1:B:244:ALA:HB2	1:B:251:VAL:HG23	1.99	0.44
1:A:127:LEU:HD13	1:A:252:ILE:HD13	1.99	0.44
1:A:101:ALA:CB	1:A:305:LEU:HD21	2.48	0.44
1:A:106:THR:C	1:A:108:THR:N	2.71	0.44
1:A:128:SER:HA	1:A:206:LEU:HD23	2.00	0.44
1:B:297:ALA:HB2	1:B:312:PHE:HE2	1.81	0.44
1:A:20:ILE:HG23	1:A:20:ILE:O	2.17	0.43
1:B:210:ASP:O	1:B:211:SER:HB2	2.18	0.43
1:A:60:LYS:HE3	1:A:60:LYS:HB2	1.77	0.43
1:A:126:GLN:NE2	1:A:126:GLN:HA	2.33	0.43
1:A:149:THR:HG21	1:A:211:SER:O	2.19	0.43
1:B:20:ILE:O	1:B:20:ILE:CG2	2.66	0.43
1:B:284:ARG:HD3	1:B:301:ASP:OD2	2.19	0.43
1:A:280:VAL:N	1:A:281:PRO:CD	2.81	0.43
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.21	0.43
1:B:115:GLU:CG	1:B:116:PHE:N	2.80	0.43
1:A:12:LYS:HE2	1:A:12:LYS:HB2	1.89	0.43
1:A:149:THR:HG22	1:A:150:GLU:N	2.34	0.43
1:A:209:VAL:HG11	1:A:212:VAL:HG12	2.01	0.43
1:A:310:VAL:CG2	1:A:311:VAL:N	2.81	0.43
1:A:179:ILE:HD13	1:A:190:ILE:HG23	2.00	0.43
1:A:297:ALA:HB2	1:A:312:PHE:CE2	2.54	0.43
1:B:65:ALA:O	1:B:69:LEU:CD2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG12	1:A:140:LEU:HG	2.00	0.42
1:A:126:GLN:HG2	1:A:319:ILE:HB	2.00	0.42
1:A:226:LEU:HD12	1:A:230:GLN:HG3	2.01	0.42
1:A:178:TYR:CG	1:A:179:ILE:N	2.87	0.42
1:B:83:ARG:CG	1:B:83:ARG:NH1	2.74	0.42
1:B:37:GLU:O	1:B:41:VAL:HG22	2.19	0.42
1:B:118:SER:O	1:B:295:ARG:HD2	2.20	0.42
1:A:48:SER:CB	1:A:55:LEU:HD12	2.49	0.42
1:A:115:GLU:CG	1:A:116:PHE:N	2.82	0.42
1:B:206:LEU:HD11	1:B:252:ILE:CD1	2.45	0.42
1:A:225:ASN:O	1:A:228:VAL:N	2.52	0.42
1:B:99:LEU:HD11	1:B:299:VAL:CG2	2.44	0.42
1:A:119:GLY:HA2	1:A:122:GLN:NE2	2.34	0.42
1:A:48:SER:HB2	1:A:55:LEU:HD12	2.02	0.42
1:B:89:ILE:HD13	1:B:131:VAL:HG23	2.01	0.42
1:A:155:TRP:CE3	1:B:80:LYS:HE3	2.55	0.42
1:B:17:LEU:HA	1:B:18:PRO:HD3	1.91	0.42
1:B:280:VAL:HB	1:B:281:PRO:CD	2.48	0.42
1:B:94:GLN:HB2	1:B:321:ASP:OD1	2.20	0.41
1:B:157:ARG:O	1:B:161:MET:HG3	2.20	0.41
1:A:13:THR:HG23	1:A:15:ASN:HD22	1.83	0.41
1:A:122:GLN:H	1:A:122:GLN:HE21	1.60	0.41
1:A:183:ASN:HA	1:A:215:HIS:CD2	2.55	0.41
1:B:168:ASP:O	1:B:169:ILE:C	2.58	0.41
1:A:20:ILE:CG2	1:A:20:ILE:O	2.68	0.41
1:B:258:MET:O	1:B:259:ALA:CB	2.67	0.41
1:B:298:ARG:HB3	1:B:309:GLU:HB3	2.02	0.41
1:B:284:ARG:NH1	1:B:301:ASP:OD2	2.53	0.41
1:A:107:ARG:HG2	1:A:245:GLU:HA	2.01	0.41
1:A:153:PHE:HB2	1:A:178:TYR:HE1	1.85	0.41
1:A:13:THR:CG2	1:A:15:ASN:H	2.34	0.41
1:A:169:ILE:CG1	1:A:170:ASP:N	2.84	0.41
1:B:81:LYS:HB3	1:B:81:LYS:HE3	1.85	0.41
1:B:284:ARG:HD3	1:B:301:ASP:HB2	2.02	0.41
1:A:35:SER:CB	1:A:298:ARG:HH22	2.28	0.41
1:A:307:GLU:CD	1:A:308:GLY:N	2.74	0.41
1:B:93:SER:HB2	1:B:320:ARG:C	2.41	0.41
1:B:280:VAL:N	1:B:281:PRO:CD	2.84	0.41
1:A:179:ILE:HD13	1:A:190:ILE:CG2	2.50	0.41
1:A:168:ASP:HB3	1:A:171:ASN:CB	2.49	0.40
1:A:113:PHE:HA	1:A:255:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HG2	1:A:116:PHE:N	2.36	0.40
1:B:126:GLN:HG2	1:B:319:ILE:HB	2.04	0.40
1:B:201:ASP:N	1:B:202:PRO:HD3	2.36	0.40
1:B:127:LEU:CD1	1:B:252:ILE:CD1	2.99	0.40
1:B:144:ALA:CB	1:B:206:LEU:HD23	2.52	0.40
1:B:238:HIS:O	1:B:241:THR:HB	2.22	0.40
1:B:116:PHE:C	1:B:116:PHE:HD2	2.23	0.40
1:B:145:VAL:HB	1:B:207:ILE:HD12	2.04	0.40
1:A:112:PHE:HB2	1:A:254:THR:HG22	2.03	0.40
1:B:57:THR:HG22	1:B:61:ILE:HD11	2.03	0.40
1:B:178:TYR:OH	1:B:180:ARG:HG2	2.22	0.40
1:B:183:ASN:ND2	1:B:186:HIS:HD2	2.20	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	293/324 (90%)	261 (89%)	23 (8%)	9 (3%)	4	23
1	B	297/324 (92%)	262 (88%)	23 (8%)	12 (4%)	3	18
All	All	590/648 (91%)	523 (89%)	46 (8%)	21 (4%)	3	20

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	226	LEU
1	B	13	THR
1	B	226	LEU
1	B	259	ALA
1	B	261	PRO

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Mol	Chain	Res	Type
1	A	13	THR
1	B	164	ALA
1	B	262	ASP
1	B	291	ARG
1	B	292	GLY
1	A	164	ALA
1	A	281	PRO
1	B	202	PRO
1	B	276	THR
1	B	107	ARG
1	A	169	ILE
1	A	135	PRO
1	A	212	VAL
1	A	282	GLY
1	B	281	PRO

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	253/275 (92%)	236 (93%)	17 (7%)	16	45
1	B	256/275 (93%)	239 (93%)	17 (7%)	16	46
All	All	509/550 (92%)	475 (93%)	34 (7%)	16	45

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	14	ILE
1	A	21	SER
1	A	24	VAL
1	A	86	VAL
1	A	93	SER
1	A	122	GLN
1	A	149	THR

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Mol	Chain	Res	Type
1	A	169	ILE
1	A	195	GLN
1	A	241	THR
1	A	288	LYS
1	A	298	ARG
1	A	301	ASP
1	A	311	VAL
1	A	316	GLU
1	A	321	ASP
1	B	13	THR
1	B	16	ASP
1	B	21	SER
1	B	38	THR
1	B	72	ARG
1	B	90	SER
1	B	93	SER
1	B	96	LEU
1	B	97	ASP
1	B	116	PHE
1	B	136	GLU
1	B	149	THR
1	B	170	ASP
1	B	171	ASN
1	B	212	VAL
1	B	298	ARG
1	B	316	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	22	GLN
1	A	26	ASN
1	A	85	ASN
1	A	122	GLN
1	A	126	GLN
1	A	132	GLN
1	A	187	GLN
1	A	195	GLN
1	A	225	ASN
1	A	234	ASN
1	A	255	ASN

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Mol	Chain	Res	Type
1	A	293	ASN
1	B	122	GLN
1	B	126	GLN
1	B	132	GLN
1	B	171	ASN
1	B	175	ASN
1	B	186	HIS
1	B	230	GLN
1	B	234	ASN
1	B	236	HIS

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 monosaccharides 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	297/324 (91%)	0.14	11 (3%)	41	38	44, 85, 123, 164	0
1	B	301/324 (92%)	0.26	26 (8%)	10	10	31, 68, 151, 154	0
All	All	598/648 (92%)	0.20	37 (6%)	20	20	31, 78, 149, 164	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LYS	5.9
1	B	23	THR	5.5
1	B	276	THR	5.4
1	B	31	ALA	5.2
1	B	30	GLU	5.1
1	B	19	GLY	4.7
1	B	262	ASP	4.7
1	B	29	ILE	4.6
1	B	48	SER	3.5
1	B	52	GLY	3.5
1	B	24	VAL	3.5
1	B	28	LEU	3.5
1	A	275	HIS	3.4
1	A	128	SER	3.4
1	B	53	ILE	3.4
1	B	263	MET	3.3
1	A	30	GLU	3.2
1	A	81	LYS	2.9
1	B	124	CYS	2.9
1	A	124	CYS	2.9
1	B	26	ASN	2.9
1	A	33	TYR	2.8
1	B	51	ALA	2.8
1	A	278	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	2.7
1	A	85	ASN	2.6
1	B	70	ASP	2.6
1	B	261	PRO	2.5
1	B	18	PRO	2.3
1	B	317	GLU	2.3
1	B	15	ASN	2.2
1	B	49	VAL	2.2
1	A	55	LEU	2.2
1	B	59	GLN	2.1
1	B	56	SER	2.1
1	A	136	GLU	2.1
1	A	245	GLU	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 monosaccharides 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.