Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 01:45 AM EDT

PDB ID	:	2CVH
Title	:	Crystal structure of the RadB recombinase
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Deposited on	:	2005-06-03
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

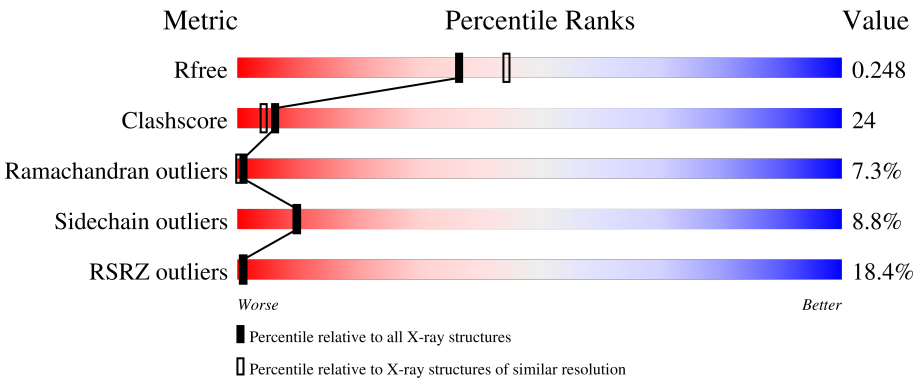
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	220	18% 55% 36% 7% •
1	B	220	19% 54% 36% 9% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3755 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 radB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	220	1729	1097	308	319	5	0	0	0
1	B	220	1729	1097	308	319	5	0	0	0

- Molecule 2 is water.

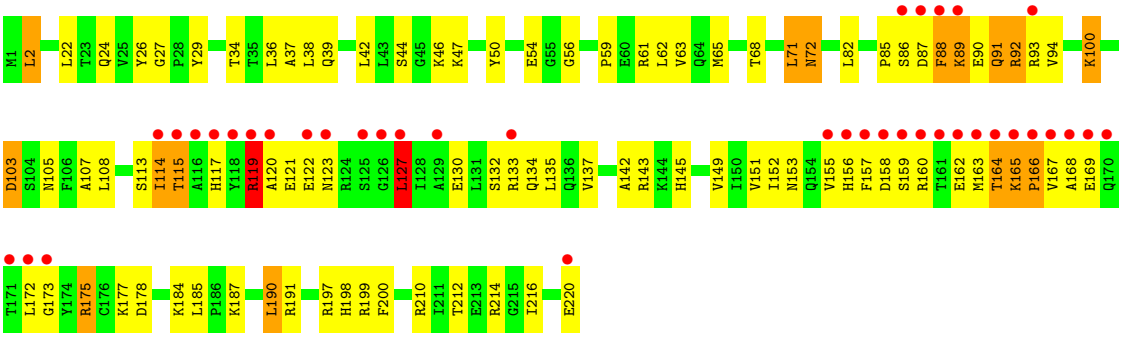
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	147	147	147	0	0
2	B	150	150	150	0	0

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.

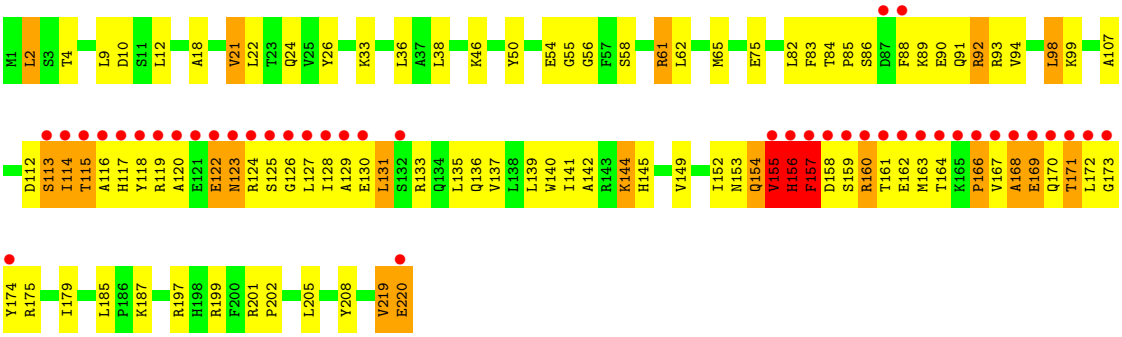
- Molecule 1: DNA repair and recombination protein radB

Chain A:



- Molecule 1: DNA repair and recombination protein radB

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.73Å 82.87Å 96.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 6.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 96.3 (6.01-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	19.32 (at 2.20Å)	Xtriage
Refinement program	CNS, X-PLOR	Depositor
R, R_{free}	0.193 , 0.253 0.192 , 0.248	Depositor DCC
R_{free} test set	2303 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 148.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3755	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.08% 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 (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	0.52	0/1759	0.80	2/2374 (0.1%)
1	B	0.54	0/1759	0.80	3/2374 (0.1%)
All	All	0.53	0/3518	0.80	5/4748 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	219	VAL	N-CA-C	-7.20	91.56	111.00
1	A	71	LEU	N-CA-C	5.71	126.42	111.00
1	B	2	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	165	LYS	C-N-CD	-5.19	109.19	120.60
1	B	156	HIS	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1729	0	1781	74	0
1	B	1729	0	1781	97	0
2	A	147	0	0	5	0
2	B	150	0	0	4	0
All	All	3755	0	3562	171	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 24.

All (171) 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:B:112:ASP:HA	1:B:113:SER:CB	1.99	0.93
1:A:177:LYS:HB3	1:A:199:ARG:HD2	1.53	0.90
1:B:112:ASP:HA	1:B:113:SER:HB3	1.59	0.85
1:B:114:ILE:HG21	1:B:154:GLN:HG2	1.66	0.78
1:B:114:ILE:HG13	1:B:115:THR:H	1.49	0.77
1:B:112:ASP:HA	1:B:113:SER:OG	1.86	0.75
1:B:33:LYS:NZ	1:B:154:GLN:HE22	1.87	0.73
1:B:33:LYS:HZ1	1:B:154:GLN:HE22	1.34	0.72
1:B:169:GLU:H	1:B:173:GLY:HA3	1.55	0.72
1:A:122:GLU:O	1:A:127:LEU:HD21	1.90	0.71
1:A:158:ASP:HB3	1:A:169:GLU:HB3	1.73	0.70
1:A:38:LEU:HD22	1:A:62:LEU:HD13	1.74	0.69
1:B:26:TYR:OH	1:B:166:PRO:HD2	1.91	0.69
1:B:136:GLN:HG3	2:B:704:HOH:O	1.90	0.69
1:B:4:THR:HG21	1:B:9:LEU:HB2	1.73	0.69
1:A:178:ASP:OD1	1:A:199:ARG:HD3	1.95	0.67
1:B:124:ARG:HB3	1:B:127:LEU:HD13	1.76	0.67
1:A:185:LEU:HB2	1:A:190:LEU:HB3	1.75	0.67
1:B:219:VAL:HG13	1:B:220:GLU:HG2	1.77	0.67
1:A:145:HIS:HD2	2:A:616:HOH:O	1.78	0.66
1:B:112:ASP:CA	1:B:113:SER:HB3	2.26	0.65
1:A:87:ASP:O	1:A:89:LYS:HE3	1.97	0.64
1:B:219:VAL:HG13	1:B:220:GLU:H	1.61	0.64
1:A:39:GLN:HE22	1:A:216:ILE:H	1.45	0.64
1:A:92:ARG:HH21	1:A:134:GLN:HA	1.63	0.62
1:A:113:SER:O	1:A:114:ILE:HG22	1.99	0.62
1:A:187:LYS:HD3	1:A:190:LEU:HD12	1.82	0.62
1:B:124:ARG:HG3	1:B:126:GLY:H	1.65	0.61
1:B:33:LYS:NZ	1:B:154:GLN:NE2	2.47	0.61
1:A:177:LYS:HB3	1:A:199:ARG:CD	2.29	0.60
1:A:68:THR:HG21	1:A:214:ARG:HG2	1.83	0.60
1:A:172:LEU:O	1:A:175:ARG:HB2	2.01	0.60
1:A:113:SER:HB2	1:A:152:ILE:O	2.01	0.60
1:A:114:ILE:HG23	1:A:114:ILE:O	2.03	0.59
1:B:54:GLU:HG3	1:B:114:ILE:HG22	1.84	0.59
1:A:22:LEU:HD22	1:A:149:VAL:HB	1.85	0.59
1:A:59:PRO:O	1:A:63:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:HG13	1:B:220:GLU:N	2.18	0.58
1:A:2:LEU:CD1	1:A:108:LEU:HD13	2.33	0.58
1:A:127:LEU:H	1:A:127:LEU:HD23	1.69	0.58
1:A:103:ASP:OD2	1:A:105:ASN:HB2	2.04	0.57
1:B:114:ILE:HG23	1:B:115:THR:N	2.20	0.56
1:A:155:VAL:HG22	1:A:156:HIS:N	2.20	0.56
1:A:68:THR:CG2	1:A:214:ARG:HG2	2.36	0.56
1:B:140:TRP:HB2	2:B:831:HOH:O	2.06	0.56
1:B:168:ALA:O	1:B:169:GLU:HB2	2.04	0.56
1:A:91:GLN:NE2	1:A:114:ILE:HD12	2.21	0.56
1:A:169:GLU:HG3	1:A:172:LEU:HB2	1.88	0.56
1:B:158:ASP:HA	1:B:160:ARG:NH2	2.21	0.55
1:B:135:LEU:HD11	1:B:172:LEU:HA	1.88	0.55
1:A:177:LYS:CB	1:A:199:ARG:HD2	2.32	0.55
1:B:168:ALA:HB1	1:B:197:ARG:NH2	2.22	0.55
1:B:38:LEU:HD23	1:B:65:MET:CE	2.36	0.55
1:B:161:THR:O	1:B:162:GLU:HB2	2.07	0.55
1:B:158:ASP:HA	1:B:160:ARG:HH21	1.72	0.55
1:A:100:LYS:HE3	1:A:100:LYS:HA	1.89	0.55
1:B:219:VAL:CG1	1:B:220:GLU:H	2.20	0.54
1:B:54:GLU:O	1:B:56:GLY:N	2.40	0.54
1:B:61:ARG:HB3	1:B:65:MET:HE3	1.90	0.54
1:A:113:SER:CB	1:A:152:ILE:O	2.56	0.53
1:B:90:GLU:O	1:B:94:VAL:HG23	2.08	0.53
1:B:50:TYR:HB3	1:B:82:LEU:HD22	1.90	0.53
1:B:118:TYR:O	1:B:120:ALA:N	2.42	0.53
1:A:46:LYS:HB2	1:A:107:ALA:HB2	1.90	0.53
1:B:208:TYR:HB2	1:B:220:GLU:HG2	1.90	0.53
1:A:91:GLN:HE21	1:A:114:ILE:HB	1.74	0.53
1:B:113:SER:CB	1:B:152:ILE:O	2.57	0.53
1:A:26:TYR:HE2	1:A:155:VAL:HG23	1.73	0.52
1:A:184:LYS:HA	1:A:191:ARG:HD3	1.90	0.52
1:B:4:THR:HG21	1:B:9:LEU:CB	2.39	0.52
1:B:135:LEU:HD13	1:B:175:ARG:HB2	1.91	0.52
1:B:140:TRP:O	1:B:144:LYS:HB2	2.10	0.52
1:B:113:SER:OG	1:B:152:ILE:O	2.28	0.52
1:A:27:GLY:HA2	1:A:155:VAL:HB	1.91	0.52
1:B:4:THR:HB	1:B:10:ASP:OD1	2.10	0.52
1:B:46:LYS:HB2	1:B:107:ALA:HB2	1.91	0.52
1:A:2:LEU:HD21	1:A:44:SER:HB3	1.91	0.51
1:B:24:GLN:NE2	1:B:172:LEU:HD11	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HG21	1:A:56:GLY:O	2.11	0.50
1:B:122:GLU:HG3	1:B:123:ASN:N	2.27	0.50
1:A:142:ALA:HB2	1:A:149:VAL:HG23	1.92	0.50
1:A:155:VAL:HG22	1:A:156:HIS:H	1.76	0.50
1:B:113:SER:HB2	1:B:152:ILE:O	2.12	0.50
1:A:151:VAL:HG12	1:A:153:ASN:HD21	1.76	0.50
1:A:173:GLY:C	1:A:197:ARG:NH2	2.65	0.50
1:B:127:LEU:HA	1:B:130:GLU:HB3	1.94	0.49
1:A:2:LEU:HD23	2:A:753:HOH:O	2.12	0.49
1:A:90:GLU:HA	1:A:93:ARG:CD	2.42	0.49
1:B:114:ILE:HG12	1:B:154:GLN:HB2	1.95	0.49
1:A:132:SER:HB3	1:A:175:ARG:NH2	2.28	0.49
1:B:208:TYR:HB2	1:B:220:GLU:CG	2.42	0.49
1:A:85:PRO:O	1:A:87:ASP:N	2.45	0.49
1:B:33:LYS:HZ1	1:B:154:GLN:NE2	2.05	0.48
1:B:61:ARG:O	1:B:65:MET:HG3	2.14	0.48
1:B:163:MET:SD	1:B:163:MET:N	2.86	0.48
1:B:38:LEU:HD23	1:B:65:MET:HE1	1.95	0.48
1:B:125:SER:HA	1:B:128:ILE:HG12	1.95	0.48
1:B:114:ILE:HG12	1:B:154:GLN:H	1.79	0.48
1:B:12:LEU:O	1:B:201:ARG:HD3	2.14	0.48
1:B:83:PHE:C	1:B:85:PRO:HD3	2.33	0.48
1:B:164:THR:HG22	1:B:166:PRO:HA	1.95	0.48
1:B:98:LEU:HB3	1:B:141:ILE:CD1	2.43	0.47
1:A:92:ARG:NH2	1:A:137:VAL:HG21	2.29	0.47
1:A:92:ARG:HD2	1:A:130:GLU:OE2	2.15	0.47
1:B:136:GLN:HG2	1:B:140:TRP:CE2	2.49	0.47
1:A:26:TYR:CE2	1:A:155:VAL:HG23	2.49	0.47
1:A:92:ARG:HH22	1:A:137:VAL:HG21	1.80	0.47
1:B:133:ARG:O	1:B:137:VAL:HG23	2.14	0.46
1:B:158:ASP:O	1:B:160:ARG:N	2.47	0.46
1:A:91:GLN:NE2	1:A:114:ILE:HB	2.30	0.46
1:B:129:ALA:O	1:B:133:ARG:HG3	2.14	0.46
1:B:85:PRO:HB3	1:B:91:GLN:HA	1.98	0.46
1:B:116:ALA:HA	1:B:122:GLU:CG	2.46	0.46
1:A:90:GLU:O	1:A:94:VAL:HG23	2.15	0.46
1:A:117:HIS:HB2	1:A:122:GLU:OE1	2.15	0.46
1:A:163:MET:O	1:A:165:LYS:N	2.49	0.46
1:B:85:PRO:HG3	1:B:94:VAL:HG21	1.98	0.46
1:A:37:ALA:HB2	1:A:152:ILE:HD11	1.98	0.45
1:B:170:GLN:HG2	1:B:171:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:NH2	2:A:649:HOH:O	2.46	0.45
1:B:89:LYS:HG2	1:B:93:ARG:HH22	1.82	0.45
1:A:71:LEU:O	1:A:72:ASN:HB3	2.16	0.45
1:A:163:MET:HG2	1:A:165:LYS:HB2	1.98	0.45
1:B:99:LYS:HE3	2:B:831:HOH:O	2.17	0.45
1:B:170:GLN:HA	1:B:174:TYR:CE1	2.51	0.45
1:A:135:LEU:HB3	1:A:175:ARG:HG2	1.97	0.45
1:B:124:ARG:O	1:B:128:ILE:HG23	2.17	0.44
1:B:114:ILE:HD13	1:B:153:ASN:HD22	1.82	0.44
1:A:163:MET:SD	1:A:165:LYS:HB2	2.57	0.44
1:B:155:VAL:HB	1:B:156:HIS:H	1.54	0.44
1:B:116:ALA:HA	1:B:122:GLU:HG2	1.98	0.44
1:B:124:ARG:HG3	1:B:126:GLY:N	2.31	0.44
1:B:114:ILE:HG13	1:B:115:THR:N	2.25	0.44
1:A:61:ARG:O	1:A:65:MET:HG3	2.17	0.44
1:A:166:PRO:O	1:A:167:VAL:HG23	2.18	0.44
1:B:22:LEU:HD23	1:B:135:LEU:HD22	1.99	0.44
1:B:142:ALA:HB2	1:B:149:VAL:HG23	1.99	0.44
1:A:159:SER:O	1:A:164:THR:HA	2.18	0.44
1:B:18:ALA:HB3	1:B:21:VAL:HG11	2.00	0.44
1:A:198:HIS:HE1	1:A:200:PHE:CE2	2.35	0.43
1:B:113:SER:O	1:B:114:ILE:HB	2.18	0.43
1:B:145:HIS:HB3	2:B:656:HOH:O	2.19	0.43
1:B:137:VAL:HG22	1:B:140:TRP:CZ3	2.53	0.43
1:A:47:LYS:HD2	1:A:105:ASN:HB3	2.01	0.43
1:A:133:ARG:O	1:A:137:VAL:HG23	2.18	0.43
1:A:212:THR:HB	2:A:835:HOH:O	2.19	0.43
1:B:127:LEU:O	1:B:130:GLU:HB3	2.18	0.43
1:B:167:VAL:O	1:B:168:ALA:HB2	2.19	0.43
1:A:24:GLN:HG3	1:A:153:ASN:HD22	1.84	0.43
1:B:117:HIS:O	1:B:117:HIS:ND1	2.51	0.43
1:A:88:PHE:HB2	1:A:117:HIS:CE1	2.53	0.43
1:A:119:ARG:O	1:A:121:GLU:N	2.52	0.43
1:A:220:GLU:HG3	2:A:854:HOH:O	2.19	0.43
1:B:202:PRO:HB2	1:B:205:LEU:HD22	2.01	0.42
1:A:22:LEU:CD2	1:A:149:VAL:HB	2.48	0.42
1:B:18:ALA:HB3	1:B:21:VAL:CG1	2.50	0.42
1:B:92:ARG:HH22	1:B:137:VAL:HG21	1.84	0.42
1:A:90:GLU:HA	1:A:93:ARG:HD2	2.01	0.42
1:B:38:LEU:HD23	1:B:65:MET:HE3	1.99	0.42
1:B:156:HIS:O	1:B:156:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:HD12	1:A:108:LEU:HD13	2.00	0.41
1:A:50:TYR:HB3	1:A:82:LEU:HD23	2.02	0.41
1:B:156:HIS:O	1:B:157:PHE:HB2	2.20	0.41
1:B:18:ALA:O	1:B:21:VAL:HG13	2.20	0.41
1:A:29:TYR:HE2	1:A:54:GLU:OE1	2.03	0.41
1:B:164:THR:C	1:B:166:PRO:HA	2.41	0.41
1:B:4:THR:HG23	1:B:36:LEU:HD11	2.03	0.41
1:B:168:ALA:HB2	1:B:179:ILE:HD13	2.02	0.41
1:B:4:THR:HG23	1:B:36:LEU:CD1	2.51	0.40
1:B:58:SER:HB3	1:B:61:ARG:HB2	2.03	0.40
1:B:127:LEU:O	1:B:131:LEU:N	2.53	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	218/220 (99%)	187 (86%)	16 (7%)	15 (7%)	1 0
1	B	218/220 (99%)	187 (86%)	14 (6%)	17 (8%)	1 0
All	All	436/440 (99%)	374 (86%)	30 (7%)	32 (7%)	1 0

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	88	PHE
1	A	114	ILE
1	A	120	ALA
1	A	123	ASN
1	A	160	ARG
1	A	162	GLU

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Mol	Chain	Res	Type
1	A	166	PRO
1	B	55	GLY
1	B	113	SER
1	B	114	ILE
1	B	115	THR
1	B	119	ARG
1	B	155	VAL
1	B	157	PHE
1	B	159	SER
1	B	169	GLU
1	A	127	LEU
1	A	157	PHE
1	B	123	ASN
1	B	168	ALA
1	B	171	THR
1	B	122	GLU
1	B	154	GLN
1	A	115	THR
1	A	119	ARG
1	B	86	SER
1	B	166	PRO
1	A	164	THR
1	A	168	ALA
1	B	156	HIS
1	A	72	ASN

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	188/188 (100%)	174 (93%)	14 (7%)	13 14
1	B	188/188 (100%)	169 (90%)	19 (10%)	7 7
All	All	376/376 (100%)	343 (91%)	33 (9%)	10 10

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

Mol	Chain	Res	Type
1	A	2	LEU
1	A	36	LEU
1	A	42	LEU
1	A	89	LYS
1	A	91	GLN
1	A	92	ARG
1	A	100	LYS
1	A	103	ASP
1	A	115	THR
1	A	119	ARG
1	A	127	LEU
1	A	143	ARG
1	A	175	ARG
1	A	190	LEU
1	B	2	LEU
1	B	21	VAL
1	B	61	ARG
1	B	62	LEU
1	B	75	GLU
1	B	84	THR
1	B	88	PHE
1	B	92	ARG
1	B	98	LEU
1	B	131	LEU
1	B	139	LEU
1	B	144	LYS
1	B	155	VAL
1	B	157	PHE
1	B	160	ARG
1	B	185	LEU
1	B	187	LYS
1	B	199	ARG
1	B	220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	91	GLN
1	A	105	ASN
1	A	117	HIS
1	A	145	HIS
1	A	153	ASN

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Mol	Chain	Res	Type
1	B	24	GLN
1	B	136	GLN
1	B	153	ASN
1	B	154	GLN
1	B	170	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	220/220 (100%)	0.32	39 (17%)	1	1	10, 26, 103, 113	0
1	B	220/220 (100%)	0.48	42 (19%)	1	1	12, 26, 108, 120	0
All	All	440/440 (100%)	0.40	81 (18%)	1	1	10, 26, 106, 120	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	ILE	12.6
1	B	120	ALA	10.8
1	B	125	SER	9.0
1	B	126	GLY	8.6
1	B	174	TYR	8.4
1	B	117	HIS	7.9
1	B	118	TYR	7.8
1	A	171	THR	7.2
1	B	128	ILE	7.1
1	A	160	ARG	7.0
1	A	117	HIS	6.9
1	B	157	PHE	6.9
1	A	168	ALA	6.9
1	B	161	THR	6.6
1	B	158	ASP	6.2
1	B	164	THR	6.1
1	A	159	SER	6.0
1	A	157	PHE	5.8
1	A	163	MET	5.8
1	B	167	VAL	5.7
1	B	168	ALA	5.6
1	A	116	ALA	5.6
1	B	122	GLU	5.5
1	B	119	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	5.4
1	A	164	THR	5.3
1	A	115	THR	5.3
1	A	120	ALA	5.2
1	B	114	ILE	5.2
1	A	156	HIS	5.2
1	B	171	THR	5.1
1	B	172	LEU	5.0
1	B	156	HIS	5.0
1	A	118	TYR	4.9
1	A	88	PHE	4.8
1	B	116	ALA	4.7
1	A	169	GLU	4.7
1	B	165	LYS	4.7
1	A	125	SER	4.6
1	B	160	ARG	4.5
1	B	155	VAL	4.4
1	B	121	GLU	4.3
1	B	159	SER	4.2
1	B	88	PHE	4.1
1	A	126	GLY	4.0
1	A	86	SER	3.9
1	A	127	LEU	3.9
1	A	89	LYS	3.8
1	B	163	MET	3.7
1	B	166	PRO	3.6
1	A	158	ASP	3.6
1	B	162	GLU	3.5
1	B	123	ASN	3.5
1	B	173	GLY	3.5
1	A	172	LEU	3.5
1	A	123	ASN	3.4
1	B	130	GLU	3.4
1	A	119	ARG	3.4
1	B	169	GLU	3.3
1	B	115	THR	3.3
1	A	129	ALA	3.2
1	B	170	GLN	3.1
1	A	161	THR	3.0
1	B	129	ALA	3.0
1	A	166	PRO	3.0
1	A	173	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	162	GLU	2.9
1	A	93	ARG	2.9
1	A	167	VAL	2.8
1	A	170	GLN	2.8
1	A	155	VAL	2.7
1	B	132	SER	2.7
1	B	124	ARG	2.5
1	A	165	LYS	2.5
1	B	87	ASP	2.5
1	B	113	SER	2.4
1	A	220	GLU	2.4
1	A	87	ASP	2.3
1	A	133	ARG	2.3
1	B	220	GLU	2.0
1	A	122	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.