Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2023 – 03:18 pm GMT

PDB ID	:	8ARK
Title	:	Crystal structure of DEAD-box protein Dbp2 in apo form
Authors	:	Rety, S.; Xi, X.G.
Deposited on	:	2022-08-17
Resolution	:	3.22 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 (i)) were used in the production of this report:

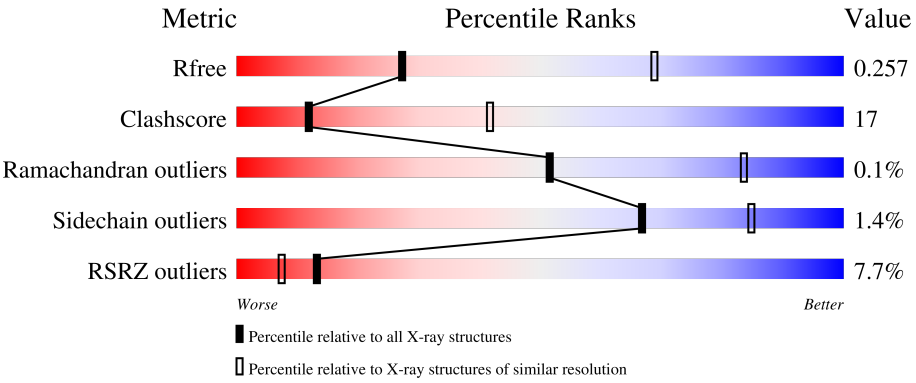
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	546	6% 52% 27% · 19%
1	B	546	8% 47% 32% · 19%
1	C	546	% 35% 14% · 51%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9085 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.

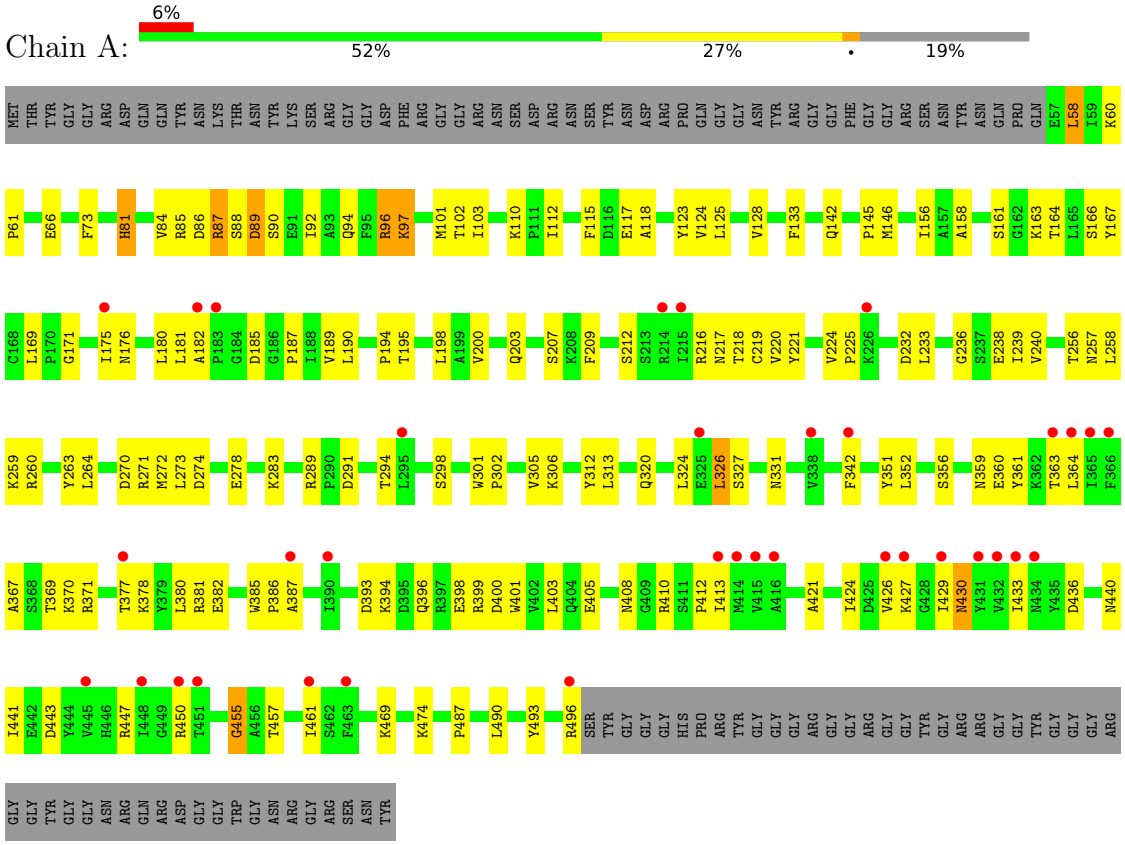
- Molecule 1 is a protein called ATP-dependent RNA helicase DBP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3483	2189	613	665	16			
1	B	440	Total	C	N	O	S	0	0	0
			3483	2189	613	665	16			
1	C	270	Total	C	N	O	S	0	0	0
			2119	1340	364	404	11			

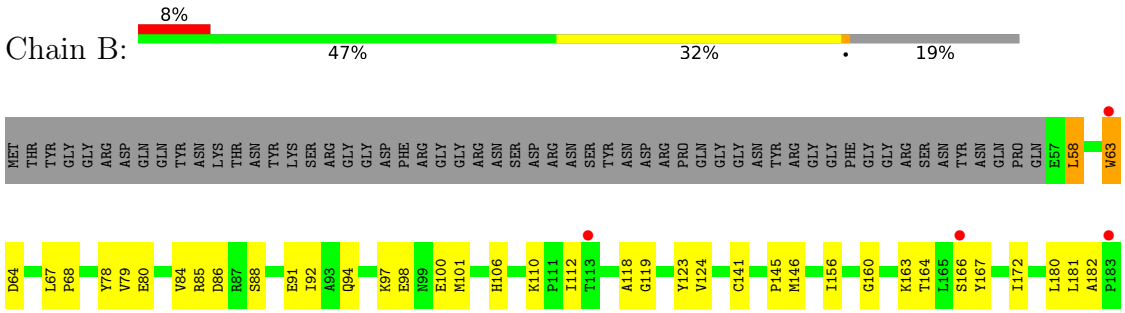
3 Residue-property plots (i)

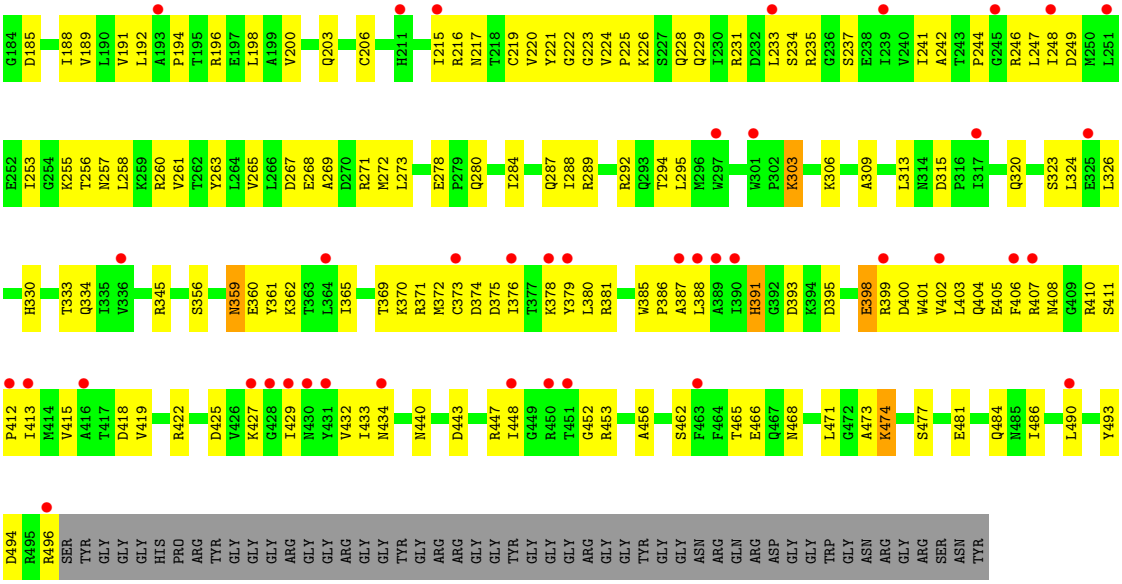
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-dependent RNA helicase DBP2



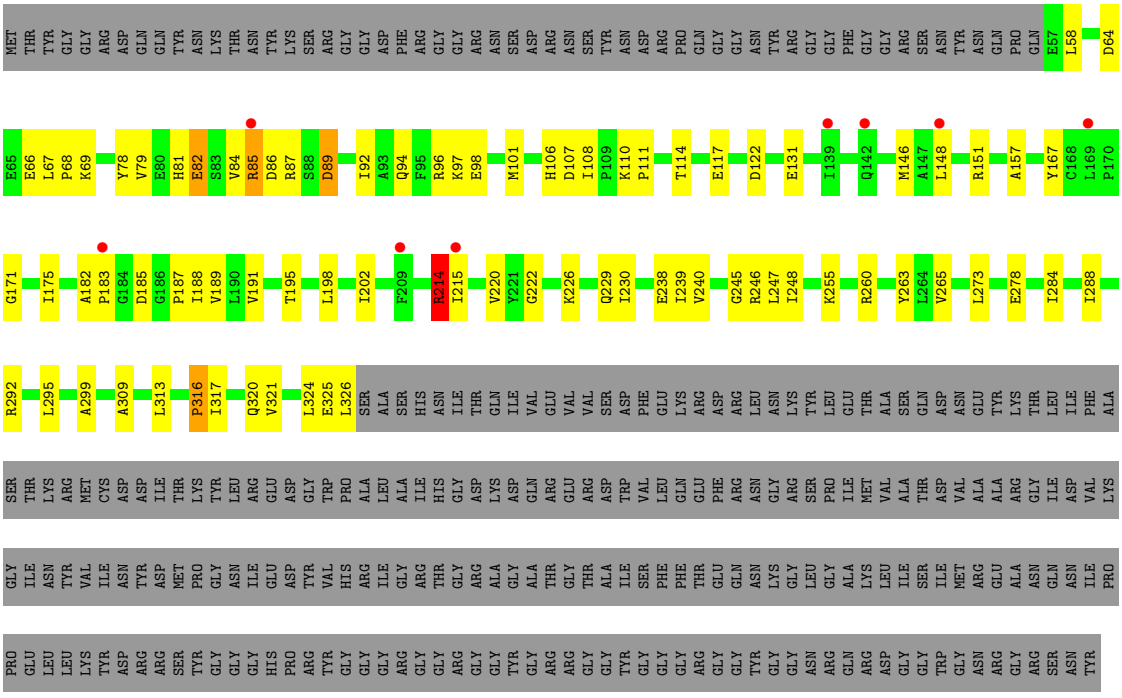
• Molecule 1: ATP-dependent RNA helicase DBP2





• Molecule 1: ATP-dependent RNA helicase DBP2

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.10Å 115.12Å 81.41Å 90.00° 101.92° 90.00°	Depositor
Resolution (Å)	38.85 – 3.22 99.85 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.5 (38.85-3.22) 94.9 (99.85-3.22)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.253 0.226 , 0.257	Depositor DCC
R_{free} test set	1438 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	97.1	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 94.7	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	0.93	EDS
Total number of atoms	9085	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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	0.30	0/3551	0.62	2/4807 (0.0%)
1	B	0.30	0/3551	0.63	1/4807 (0.0%)
1	C	0.32	0/2163	0.60	1/2934 (0.0%)
All	All	0.30	0/9265	0.62	4/12548 (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	7
1	B	0	7
1	C	0	4
All	All	0	18

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	ARG	CG-CD-NE	-8.24	94.50	111.80
1	B	359	ASN	C-N-CA	6.62	138.26	121.70
1	A	326	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	87	ARG	C-N-CA	5.77	136.13	121.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	ASN	Peptide
1	A	182	ALA	Peptide
1	A	394	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	455	GLY	Peptide
1	A	58	LEU	Peptide
1	A	96	ARG	Sidechain
1	A	97	LYS	Peptide
1	B	235	ARG	Peptide
1	B	356	SER	Peptide
1	B	379	TYR	Peptide
1	B	474	LYS	Peptide
1	B	58	LEU	Peptide
1	B	63	TRP	Peptide
1	B	79	VAL	Peptide
1	C	214	ARG	Sidechain
1	C	316	PRO	Peptide
1	C	58	LEU	Peptide
1	C	89	ASP	Peptide

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	3483	0	3470	111	0
1	B	3483	0	3470	147	0
1	C	2119	0	2123	59	0
All	All	9085	0	9063	313	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 17.

All (313) 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:398:GLU:HB2	1:A:401:TRP:HE1	1.21	1.04
1:B:248:ILE:HD12	1:B:284:ILE:HG21	1.46	0.97
1:B:386:PRO:HB2	1:B:411:SER:HA	1.57	0.85
1:B:334:GLN:H	1:B:484:GLN:HG2	1.39	0.84
1:B:365:ILE:HB	1:B:415:VAL:HG12	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:HD12	1:B:256:THR:HG21	1.60	0.81
1:B:196:ARG:HB2	1:B:221:TYR:HB2	1.66	0.77
1:B:222:GLY:HA2	1:B:246:ARG:HE	1.51	0.76
1:C:222:GLY:HA2	1:C:246:ARG:HE	1.49	0.76
1:B:112:ILE:HD13	1:B:118:ALA:HB2	1.69	0.74
1:A:87:ARG:N	1:A:88:SER:OG	2.14	0.74
1:B:222:GLY:HA2	1:B:246:ARG:NE	2.04	0.73
1:A:326:LEU:HD13	1:A:327:SER:H	1.54	0.72
1:B:361:TYR:HA	1:B:412:PRO:HB3	1.71	0.72
1:B:370:LYS:HD3	1:B:391:HIS:HB2	1.72	0.72
1:B:196:ARG:HH12	1:B:224:VAL:HG23	1.54	0.72
1:C:85:ARG:HG2	1:C:87:ARG:HB3	1.72	0.72
1:B:381:ARG:HD2	1:B:387:ALA:H	1.54	0.71
1:B:359:ASN:H	1:B:360:GLU:HA	1.56	0.70
1:B:219:CYS:HG	1:B:221:TYR:HE2	1.40	0.70
1:B:58:LEU:O	1:B:287:GLN:NE2	2.25	0.69
1:B:403:LEU:HD12	1:B:406:PHE:HB3	1.73	0.69
1:B:163:LYS:O	1:B:166:SER:HB3	1.94	0.68
1:B:80:GLU:HB3	1:B:85:ARG:CZ	2.24	0.68
1:A:115:PHE:HE1	1:A:496:ARG:HH21	1.43	0.67
1:A:369:THR:HG22	1:A:371:ARG:H	1.58	0.67
1:C:84:VAL:O	1:C:85:ARG:HG3	1.95	0.66
1:C:78:TYR:HB2	1:C:148:LEU:HB3	1.78	0.66
1:C:313:LEU:HB3	1:C:316:PRO:HG3	1.77	0.66
1:B:419:VAL:O	1:B:422:ARG:HG3	1.94	0.66
1:B:244:PRO:O	1:B:248:ILE:HG12	1.94	0.66
1:A:181:LEU:HD23	1:A:260:ARG:HH21	1.61	0.66
1:B:194:PRO:HD2	1:B:198:LEU:HD23	1.78	0.66
1:A:96:ARG:NH1	1:A:103:ILE:HD12	2.10	0.66
1:A:161:SER:HB2	1:A:163:LYS:HG3	1.76	0.66
1:C:81:HIS:HB2	1:C:84:VAL:HG12	1.78	0.66
1:B:78:TYR:HD1	1:B:119:GLY:H	1.43	0.65
1:B:222:GLY:HA2	1:B:246:ARG:CD	2.27	0.65
1:B:222:GLY:HA2	1:B:246:ARG:HD2	1.79	0.64
1:B:432:VAL:HG11	1:B:448:ILE:HA	1.78	0.64
1:B:242:ALA:HB1	1:B:247:LEU:HB2	1.80	0.64
1:A:163:LYS:O	1:A:166:SER:HB3	1.99	0.63
1:B:261:VAL:HG23	1:B:288:ILE:HG23	1.81	0.63
1:B:91:GLU:HA	1:B:94:GLN:HB3	1.80	0.62
1:B:369:THR:HG23	1:B:372:MET:H	1.65	0.62
1:A:426:VAL:HG23	1:A:429:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:NE	1:B:221:TYR:HD1	1.98	0.62
1:A:220:VAL:HG11	1:A:233:LEU:HD11	1.82	0.61
1:B:362:LYS:NZ	1:B:427:LYS:O	2.29	0.61
1:A:352:LEU:HD11	1:A:380:LEU:HD21	1.82	0.61
1:A:398:GLU:CB	1:A:401:TRP:HE1	2.04	0.61
1:A:469:LYS:HG2	1:A:493:TYR:HE2	1.65	0.61
1:A:128:VAL:HG22	1:A:496:ARG:HH22	1.65	0.61
1:C:85:ARG:HB3	1:C:86:ASP:HA	1.81	0.61
1:A:112:ILE:HD13	1:A:118:ALA:HB2	1.82	0.61
1:B:365:ILE:HG12	1:B:433:ILE:HB	1.82	0.61
1:B:474:LYS:HE2	1:B:494:ASP:O	2.00	0.61
1:C:247:LEU:HD23	1:C:284:ILE:HD13	1.83	0.61
1:A:85:ARG:HB2	1:A:110:LYS:HD2	1.82	0.60
1:B:405:GLU:HB3	1:B:408:ASN:HD21	1.66	0.60
1:A:264:LEU:HD23	1:A:294:THR:HG23	1.83	0.60
1:B:405:GLU:HB2	1:B:410:ARG:HH11	1.67	0.60
1:C:151:ARG:HE	1:C:317:ILE:HD11	1.66	0.59
1:B:361:TYR:CD2	1:B:362:LYS:HG2	2.37	0.59
1:A:405:GLU:HG2	1:A:410:ARG:HH11	1.67	0.59
1:B:231:ARG:HA	1:B:234:SER:HB2	1.85	0.59
1:B:191:VAL:HB	1:B:241:ILE:HG22	1.85	0.58
1:C:273:LEU:HD22	1:C:278:GLU:HB2	1.84	0.58
1:B:203:GLN:HB3	1:B:241:ILE:HD11	1.85	0.58
1:B:452:GLY:HA2	1:B:456:ALA:O	2.02	0.58
1:B:359:ASN:N	1:B:360:GLU:HA	2.18	0.58
1:C:222:GLY:HA2	1:C:246:ARG:NE	2.18	0.58
1:B:405:GLU:HG3	1:B:410:ARG:HD3	1.84	0.58
1:B:362:LYS:HB3	1:B:429:ILE:HA	1.85	0.57
1:B:330:HIS:NE2	1:B:481:GLU:OE2	2.35	0.57
1:B:191:VAL:HG22	1:B:265:VAL:HG22	1.87	0.57
1:A:112:ILE:HG23	1:A:145:PRO:HG3	1.86	0.57
1:C:108:ILE:HG22	1:C:317:ILE:HD12	1.87	0.57
1:C:175:ILE:HG23	1:C:188:ILE:HD12	1.86	0.57
1:A:385:TRP:HB3	1:A:413:ILE:HD11	1.87	0.56
1:B:100:GLU:OE1	1:B:323:SER:OG	2.23	0.56
1:A:367:ALA:HA	1:A:436:ASP:HB2	1.86	0.56
1:A:405:GLU:HG2	1:A:410:ARG:HD2	1.86	0.56
1:A:326:LEU:HD13	1:A:327:SER:N	2.20	0.56
1:B:220:VAL:HB	1:B:233:LEU:HD21	1.88	0.56
1:B:465:THR:HG22	1:B:466:GLU:H	1.71	0.56
1:B:257:ASN:OD1	1:B:258:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PRO:HG2	1:A:412:PRO:HD2	1.88	0.55
1:C:92:ILE:O	1:C:96:ARG:HG2	2.06	0.55
1:A:158:ALA:O	1:A:161:SER:OG	2.21	0.55
1:B:399:ARG:NH1	1:B:400:ASP:OD1	2.38	0.55
1:B:289:ARG:O	1:B:292:ARG:HG2	2.06	0.55
1:A:123:TYR:CD2	1:A:124:VAL:HG13	2.42	0.55
1:A:370:LYS:HD3	1:A:393:ASP:HB2	1.89	0.55
1:A:403:LEU:HD21	1:A:424:ILE:HD13	1.89	0.55
1:A:87:ARG:NH2	1:A:117:GLU:OE1	2.39	0.54
1:A:133:PHE:HB3	1:A:496:ARG:HG2	1.89	0.54
1:A:195:THR:HG23	1:A:198:LEU:H	1.72	0.54
1:B:80:GLU:HG2	1:B:84:VAL:HG23	1.89	0.54
1:A:302:PRO:HD2	1:A:305:VAL:HB	1.90	0.54
1:B:222:GLY:CA	1:B:246:ARG:HE	2.17	0.54
1:B:203:GLN:HA	1:B:206:CYS:HB2	1.90	0.54
1:C:66:GLU:HA	1:C:69:LYS:HD2	1.89	0.54
1:A:324:LEU:HD21	1:C:324:LEU:HD11	1.89	0.53
1:C:189:VAL:HB	1:C:239:ILE:HG12	1.91	0.53
1:C:106:HIS:ND1	1:C:107:ASP:OD1	2.33	0.53
1:A:219:CYS:HG	1:A:221:TYR:HE2	1.57	0.53
1:A:181:LEU:O	1:A:185:ASP:HB2	2.09	0.53
1:A:405:GLU:HB3	1:A:410:ARG:HB2	1.89	0.53
1:C:89:ASP:OD1	1:C:89:ASP:N	2.41	0.53
1:B:194:PRO:HB3	1:B:272:MET:HG2	1.89	0.53
1:B:418:ASP:OD2	1:B:447:ARG:NH2	2.32	0.53
1:B:226:LYS:HD2	1:B:246:ARG:HH12	1.73	0.53
1:C:185:ASP:OD2	1:C:260:ARG:HD2	2.08	0.53
1:C:82:GLU:HA	1:C:85:ARG:O	2.09	0.53
1:A:58:LEU:HD13	1:A:283:LYS:HE3	1.89	0.53
1:B:248:ILE:HG13	1:B:280:GLN:HB3	1.90	0.52
1:B:226:LYS:HD2	1:B:246:ARG:NH1	2.24	0.52
1:B:387:ALA:HA	1:B:413:ILE:O	2.09	0.52
1:C:189:VAL:HG22	1:C:263:TYR:HB3	1.90	0.52
1:A:216:ARG:NH2	1:A:236:GLY:O	2.42	0.52
1:B:267:ASP:OD1	1:B:268:GLU:N	2.43	0.52
1:C:182:ALA:HB1	1:C:183:PRO:HD2	1.91	0.52
1:C:214:ARG:NH2	1:C:238:GLU:HG2	2.25	0.52
1:A:190:LEU:HD22	1:A:258:LEU:HD22	1.91	0.52
1:B:410:ARG:NH1	1:B:411:SER:OG	2.43	0.51
1:A:396:GLN:HA	1:A:399:ARG:HB3	1.91	0.51
1:B:371:ARG:NH1	1:B:375:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:O	1:B:385:TRP:HD1	1.94	0.51
1:C:288:ILE:HG22	1:C:292:ARG:HD3	1.91	0.51
1:C:198:LEU:O	1:C:202:ILE:HG12	2.09	0.51
1:A:447:ARG:HA	1:A:450:ARG:HH12	1.74	0.51
1:B:192:LEU:HD11	1:B:284:ILE:HD11	1.93	0.51
1:B:474:LYS:HD2	1:B:477:SER:OG	2.10	0.51
1:A:128:VAL:HG22	1:A:496:ARG:NH2	2.24	0.51
1:A:189:VAL:HG12	1:A:263:TYR:HB3	1.93	0.51
1:B:486:ILE:HG23	1:B:490:LEU:HD23	1.93	0.51
1:A:455:GLY:O	1:A:457:THR:N	2.43	0.50
1:B:401:TRP:HA	1:B:404:GLN:HB2	1.94	0.50
1:A:398:GLU:HB2	1:A:401:TRP:NE1	2.06	0.50
1:B:112:ILE:O	1:B:141:CYS:HB3	2.11	0.50
1:C:96:ARG:NH2	1:C:111:PRO:HD3	2.27	0.50
1:C:101:MET:HG2	1:C:321:VAL:HG12	1.93	0.50
1:B:273:LEU:HD23	1:B:278:GLU:HB2	1.94	0.50
1:B:473:ALA:HA	1:B:493:TYR:O	2.12	0.50
1:A:377:THR:O	1:A:381:ARG:HG2	2.11	0.50
1:B:395:ASP:O	1:B:398:GLU:HG3	2.12	0.50
1:A:331:ASN:O	1:A:457:THR:HA	2.12	0.50
1:C:230:ILE:HG23	1:C:255:LYS:HG3	1.94	0.49
1:B:123:TYR:CD2	1:B:124:VAL:HG13	2.47	0.49
1:B:228:GLN:O	1:B:228:GLN:HG3	2.12	0.49
1:A:142:GLN:HG3	1:A:146:MET:HE1	1.94	0.49
1:B:189:VAL:HG22	1:B:263:TYR:HB3	1.93	0.49
1:B:200:VAL:HA	1:B:203:GLN:HG2	1.93	0.49
1:B:224:VAL:HG13	1:B:225:PRO:HD2	1.95	0.49
1:A:405:GLU:HA	1:A:408:ASN:HD21	1.78	0.49
1:B:261:VAL:HG21	1:B:288:ILE:HG12	1.94	0.49
1:A:400:ASP:OD1	1:A:400:ASP:N	2.44	0.48
1:C:114:THR:HG22	1:C:117:GLU:HG3	1.95	0.48
1:B:106:HIS:NE2	1:B:315:ASP:OD2	2.41	0.48
1:A:92:ILE:O	1:A:96:ARG:HB2	2.14	0.48
1:B:369:THR:CG2	1:B:372:MET:H	2.26	0.48
1:C:97:LYS:HA	1:C:97:LYS:HD3	1.53	0.48
1:C:309:ALA:HA	1:C:313:LEU:HD13	1.95	0.48
1:A:156:ILE:HD11	1:A:301:TRP:CE3	2.49	0.48
1:B:388:LEU:HD22	1:B:402:VAL:HA	1.94	0.48
1:A:96:ARG:HG3	1:A:101:MET:HB2	1.95	0.48
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.71	0.48
1:C:101:MET:HA	1:C:320:GLN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:TYR:CE1	1:C:265:VAL:HG11	2.49	0.48
1:A:200:VAL:HA	1:A:203:GLN:HG2	1.95	0.48
1:B:216:ARG:O	1:B:237:SER:HB3	2.14	0.47
1:A:90:SER:O	1:A:94:GLN:HB2	2.14	0.47
1:A:97:LYS:CG	1:C:97:LYS:HD2	2.44	0.47
1:B:85:ARG:HA	1:B:86:ASP:HA	1.41	0.47
1:B:265:VAL:HA	1:B:295:LEU:O	2.15	0.47
1:B:333:THR:HG22	1:B:484:GLN:HE21	1.79	0.47
1:A:224:VAL:HB	1:A:225:PRO:HD2	1.97	0.47
1:C:84:VAL:HG22	1:C:85:ARG:NH2	2.30	0.47
1:B:156:ILE:HB	1:B:320:GLN:HG3	1.96	0.47
1:B:391:HIS:CE1	1:B:393:ASP:HB3	2.50	0.47
1:A:97:LYS:HD3	1:A:101:MET:O	2.15	0.47
1:A:312:TYR:O	1:A:313:LEU:HD23	2.14	0.47
1:B:196:ARG:NH1	1:B:224:VAL:HG23	2.27	0.47
1:B:64:ASP:OD1	1:B:64:ASP:N	2.47	0.47
1:B:376:ILE:O	1:B:380:LEU:HG	2.15	0.47
1:A:187:PRO:HB3	1:A:240:VAL:HG23	1.97	0.47
1:A:207:SER:HB3	1:A:217:ASN:HD21	1.80	0.47
1:B:63:TRP:CH2	1:B:289:ARG:HG2	2.51	0.47
1:C:171:GLY:O	1:C:175:ILE:HG13	2.15	0.47
1:A:364:LEU:HB2	1:A:429:ILE:HG21	1.97	0.46
1:B:58:LEU:HD23	1:B:58:LEU:H	1.80	0.46
1:C:182:ALA:HB3	1:C:185:ASP:OD2	2.15	0.46
1:A:433:ILE:HG12	1:A:461:ILE:HB	1.96	0.46
1:A:440:ASN:OD1	1:A:443:ASP:N	2.49	0.46
1:B:374:ASP:O	1:B:378:LYS:N	2.36	0.46
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.75	0.46
1:B:373:CYS:HB3	1:B:415:VAL:HG23	1.97	0.46
1:A:87:ARG:H	1:A:88:SER:HG	1.52	0.46
1:B:408:ASN:HD21	1:B:410:ARG:HB3	1.81	0.46
1:B:425:ASP:OD2	1:B:453:ARG:NH1	2.49	0.46
1:A:306:LYS:HE3	1:C:326:LEU:HD12	1.97	0.46
1:B:67:LEU:HB3	1:B:68:PRO:HD3	1.96	0.46
1:A:294:THR:HB	1:A:313:LEU:HD22	1.98	0.46
1:A:270:ASP:HB3	1:A:298:SER:OG	2.15	0.46
1:C:187:PRO:HB3	1:C:240:VAL:HG23	1.98	0.46
1:A:60:LYS:HE3	1:A:60:LYS:HB3	1.76	0.45
1:A:380:LEU:O	1:A:385:TRP:HB2	2.16	0.45
1:C:94:GLN:O	1:C:98:GLU:HB2	2.16	0.45
1:A:427:LYS:HE2	1:A:450:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:O	1:B:92:ILE:HG12	2.15	0.45
1:B:223:GLY:H	1:B:246:ARG:NE	2.15	0.45
1:B:303:LYS:HD3	1:B:306:LYS:HD3	1.99	0.45
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.64	0.45
1:B:196:ARG:HE	1:B:221:TYR:HD1	1.63	0.45
1:C:96:ARG:HH21	1:C:111:PRO:HD3	1.81	0.45
1:B:309:ALA:O	1:B:313:LEU:HB2	2.17	0.45
1:B:188:ILE:HA	1:B:260:ARG:O	2.16	0.45
1:B:253:ILE:HG22	1:B:255:LYS:HD3	1.99	0.45
1:C:67:LEU:HB3	1:C:68:PRO:HD3	1.99	0.45
1:A:101:MET:HA	1:A:320:GLN:O	2.15	0.44
1:B:78:TYR:CZ	1:B:80:GLU:HG3	2.52	0.44
1:B:223:GLY:H	1:B:246:ARG:HE	1.63	0.44
1:B:369:THR:HG23	1:B:371:ARG:N	2.32	0.44
1:C:191:VAL:HG22	1:C:265:VAL:HB	2.00	0.44
1:A:89:ASP:H	1:A:92:ILE:HG12	1.81	0.44
1:A:180:LEU:HD12	1:A:180:LEU:H	1.82	0.44
1:A:356:SER:O	1:A:356:SER:OG	2.33	0.44
1:B:172:ILE:HG23	1:B:215:ILE:HD13	1.98	0.44
1:B:468:ASN:HB3	1:B:471:LEU:HD21	1.99	0.44
1:B:88:SER:HB3	1:B:91:GLU:HG2	1.98	0.44
1:B:160:GLY:O	1:B:474:LYS:NZ	2.41	0.44
1:B:405:GLU:HB3	1:B:408:ASN:ND2	2.30	0.44
1:B:434:ASN:HB2	1:B:462:SER:HA	1.99	0.44
1:C:167:TYR:CD1	1:C:265:VAL:HG21	2.53	0.44
1:A:171:GLY:O	1:A:175:ILE:HG13	2.18	0.44
1:A:359:ASN:HA	1:A:360:GLU:HA	1.71	0.44
1:C:85:ARG:HG2	1:C:87:ARG:CB	2.45	0.44
1:C:226:LYS:O	1:C:230:ILE:HG12	2.18	0.44
1:B:164:THR:HA	1:B:167:TYR:CE2	2.53	0.44
1:A:85:ARG:HA	1:A:86:ASP:HA	1.50	0.43
1:B:146:MET:H	1:B:146:MET:HG2	1.61	0.43
1:C:195:THR:HG23	1:C:198:LEU:H	1.83	0.43
1:B:181:LEU:HD23	1:B:260:ARG:HH21	1.83	0.43
1:C:220:VAL:HG12	1:C:229:GLN:NE2	2.32	0.43
1:A:259:LYS:HE2	1:A:259:LYS:HB3	1.83	0.43
1:A:351:TYR:CG	1:A:461:ILE:HD13	2.54	0.43
1:A:363:THR:HA	1:A:430:ASN:O	2.18	0.43
1:A:273:LEU:HD22	1:A:278:GLU:HB2	2.00	0.43
1:A:387:ALA:HB2	1:A:413:ILE:HD11	2.00	0.43
1:B:86:ASP:HB3	1:B:110:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASP:O	1:B:253:ILE:HG13	2.18	0.43
1:B:294:THR:O	1:B:295:LEU:HD23	2.19	0.43
1:B:265:VAL:HG12	1:B:295:LEU:HB2	2.00	0.43
1:B:269:ALA:O	1:B:273:LEU:HD12	2.18	0.43
1:A:87:ARG:HB2	1:A:88:SER:HA	2.01	0.43
1:A:289:ARG:NH2	1:A:291:ASP:OD2	2.51	0.43
1:B:229:GLN:O	1:B:233:LEU:N	2.26	0.43
1:B:292:ARG:NH1	1:B:294:THR:OG1	2.52	0.43
1:B:440:ASN:ND2	1:B:443:ASP:OD2	2.42	0.43
1:A:441:ILE:HG13	1:A:474:LYS:HB3	2.01	0.43
1:B:196:ARG:CZ	1:B:222:GLY:O	2.67	0.43
1:A:164:THR:HA	1:A:167:TYR:CE2	2.54	0.42
1:A:218:THR:HG21	1:A:232:ASP:HB3	2.00	0.42
1:A:342:PHE:HZ	1:B:345:ARG:HH11	1.66	0.42
1:A:487:PRO:HB2	1:A:490:LEU:HB3	2.02	0.42
1:B:182:ALA:O	1:B:185:ASP:HB2	2.19	0.42
1:B:258:LEU:O	1:B:261:VAL:HG22	2.19	0.42
1:B:78:TYR:OH	1:B:80:GLU:HG3	2.20	0.42
1:B:465:THR:HG22	1:B:466:GLU:N	2.34	0.42
1:A:181:LEU:HD11	1:A:238:GLU:HG3	2.01	0.42
1:C:265:VAL:HA	1:C:295:LEU:O	2.19	0.42
1:A:85:ARG:HG3	1:A:86:ASP:OD1	2.19	0.42
1:B:88:SER:CB	1:B:91:GLU:HG2	2.50	0.42
1:B:112:ILE:HG23	1:B:145:PRO:HG3	2.02	0.42
1:B:268:GLU:OE2	1:B:271:ARG:NH2	2.53	0.42
1:C:79:VAL:O	1:C:79:VAL:HG23	2.20	0.42
1:A:194:PRO:HB3	1:A:272:MET:HG2	2.02	0.41
1:B:219:CYS:SG	1:B:221:TYR:HE2	2.40	0.41
1:A:61:PRO:HB3	1:A:66:GLU:OE1	2.21	0.41
1:A:169:LEU:HD21	1:A:209:PHE:CD1	2.55	0.41
1:A:361:TYR:HD2	1:A:363:THR:HG23	1.85	0.41
1:B:97:LYS:O	1:B:98:GLU:HG2	2.20	0.41
1:B:101:MET:HA	1:B:320:GLN:O	2.20	0.41
1:A:73:PHE:H	1:A:73:PHE:HD1	1.68	0.41
1:B:380:LEU:O	1:B:385:TRP:CD1	2.73	0.41
1:B:407:ARG:H	1:B:407:ARG:HG3	1.64	0.41
1:C:146:MET:HE2	1:C:146:MET:HB2	1.90	0.41
1:A:301:TRP:N	1:A:302:PRO:HD3	2.35	0.41
1:C:245:GLY:O	1:C:248:ILE:HG22	2.20	0.41
1:C:188:ILE:HD11	1:C:260:ARG:HH12	1.85	0.41
1:B:167:TYR:CD1	1:B:265:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:HE3	1:A:283:LYS:HB2	1.85	0.41
1:A:443:ASP:O	1:A:447:ARG:N	2.39	0.41
1:B:326:LEU:HD12	1:B:326:LEU:HA	1.86	0.41
1:A:125:LEU:O	1:A:128:VAL:HG12	2.19	0.41
1:A:271:ARG:HA	1:A:274:ASP:HB2	2.03	0.41
1:C:84:VAL:O	1:C:87:ARG:NH2	2.49	0.41
1:A:97:LYS:NZ	1:A:102:THR:HA	2.36	0.41
1:B:217:ASN:HA	1:B:237:SER:HB3	2.03	0.41
1:B:365:ILE:O	1:B:415:VAL:HA	2.21	0.41
1:C:85:ARG:NH2	1:C:110:LYS:C	2.75	0.41
1:A:81:HIS:O	1:A:84:VAL:HG22	2.21	0.41
1:C:325:GLU:HG3	1:C:326:LEU:HG	2.03	0.41
1:A:189:VAL:HG22	1:A:239:ILE:HG12	2.03	0.40
1:A:256:THR:HG22	1:A:257:ASN:H	1.86	0.40
1:C:157:ALA:O	1:C:299:ALA:HA	2.20	0.40
1:B:191:VAL:HG13	1:B:265:VAL:HG23	2.03	0.40
1:A:421:ALA:HB1	1:A:450:ARG:NH2	2.37	0.40
1:A:378:LYS:O	1:A:382:GLU:HB2	2.21	0.40
1:B:196:ARG:NE	1:B:222:GLY:O	2.55	0.40
1:B:196:ARG:CZ	1:B:221:TYR:HD1	2.34	0.40
1:C:255:LYS:HA	1:C:255:LYS:HD3	1.88	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	438/546 (80%)	434 (99%)	4 (1%)	0	100	100
1	B	438/546 (80%)	436 (100%)	2 (0%)	0	100	100
1	C	268/546 (49%)	266 (99%)	1 (0%)	1 (0%)	34	69
All	All	1144/1638 (70%)	1136 (99%)	7 (1%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	215	ILE

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	380/450 (84%)	376 (99%)	4 (1%)	73	88
1	B	380/450 (84%)	375 (99%)	5 (1%)	69	86
1	C	235/450 (52%)	230 (98%)	5 (2%)	53	79
All	All	995/1350 (74%)	981 (99%)	14 (1%)	67	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	89	ASP
1	A	212	SER
1	A	430	ASN
1	B	180	LEU
1	B	303	LYS
1	B	391	HIS
1	B	398	GLU
1	B	496	ARG
1	C	64	ASP
1	C	82	GLU
1	C	122	ASP
1	C	131	GLU
1	C	214	ARG

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

Mol	Chain	Res	Type
1	A	217	ASN

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Mol	Chain	Res	Type
1	C	229	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 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	440/546 (80%)	0.66	35 (7%) 12 7	76, 128, 184, 227	0
1	B	440/546 (80%)	0.68	45 (10%) 6 4	98, 142, 214, 266	0
1	C	270/546 (49%)	0.42	8 (2%) 50 36	79, 111, 177, 261	0
All	All	1150/1638 (70%)	0.61	88 (7%) 13 7	76, 131, 196, 266	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	TYR	6.8
1	B	430	ASN	5.4
1	A	365	ILE	5.2
1	B	387	ALA	4.9
1	A	416	ALA	4.9
1	A	433	ILE	4.4
1	B	406	PHE	4.4
1	C	183	PRO	4.2
1	B	388	LEU	4.1
1	A	390	ILE	4.0
1	A	366	PHE	4.0
1	A	182	ALA	3.9
1	A	414	MET	3.9
1	A	432	VAL	3.9
1	B	496	ARG	3.9
1	A	496	ARG	3.8
1	B	63	TRP	3.8
1	B	248	ILE	3.8
1	B	428	GLY	3.7
1	B	389	ALA	3.7
1	A	431	TYR	3.6
1	A	363	THR	3.6
1	B	364	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	426	VAL	3.3
1	A	451	THR	3.3
1	B	390	ILE	3.3
1	C	215	ILE	3.2
1	A	415	VAL	3.1
1	A	364	LEU	3.0
1	A	463	PHE	2.9
1	B	407	ARG	2.8
1	B	490	LEU	2.7
1	B	434	ASN	2.7
1	C	209	PHE	2.7
1	B	251	LEU	2.7
1	A	175	ILE	2.6
1	B	297	TRP	2.6
1	A	450	ARG	2.6
1	A	448	ILE	2.6
1	A	429	ILE	2.6
1	A	342	PHE	2.6
1	A	461	ILE	2.6
1	A	445	VAL	2.5
1	C	148	LEU	2.5
1	C	85	ARG	2.5
1	B	416	ALA	2.5
1	C	139	ILE	2.5
1	B	211	HIS	2.5
1	B	373	CYS	2.5
1	B	325	GLU	2.4
1	B	448	ILE	2.4
1	B	412	PRO	2.4
1	B	183	PRO	2.4
1	B	215	ILE	2.4
1	B	402	VAL	2.4
1	B	239	ILE	2.3
1	B	301	TRP	2.3
1	B	413	ILE	2.3
1	A	226	LYS	2.3
1	B	463	PHE	2.3
1	A	427	LYS	2.3
1	B	427	LYS	2.3
1	A	338	VAL	2.3
1	A	434	ASN	2.3
1	C	169	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	451	THR	2.3
1	B	245	GLY	2.3
1	B	431	TYR	2.3
1	A	377	THR	2.3
1	A	325	GLU	2.2
1	A	214	ARG	2.2
1	B	166	SER	2.2
1	B	113	THR	2.2
1	B	317	ILE	2.2
1	B	233	LEU	2.2
1	B	399	ARG	2.2
1	C	142	GLN	2.2
1	B	376	ILE	2.2
1	A	413	ILE	2.1
1	A	183	PRO	2.1
1	B	193	ALA	2.1
1	B	450	ARG	2.1
1	A	387	ALA	2.1
1	A	295	LEU	2.1
1	B	429	ILE	2.1
1	B	336	VAL	2.0
1	B	378	LYS	2.0
1	A	215	ILE	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.