



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 AM GMT

PDB ID : 2Z43
Title : Structure of a twinned crystal of RadA
Authors : Chen, L.T.; Ko, T.P.; Wang, A.H.J.; Wang, T.F.
Deposited on : 2007-06-12
Resolution : 1.93 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

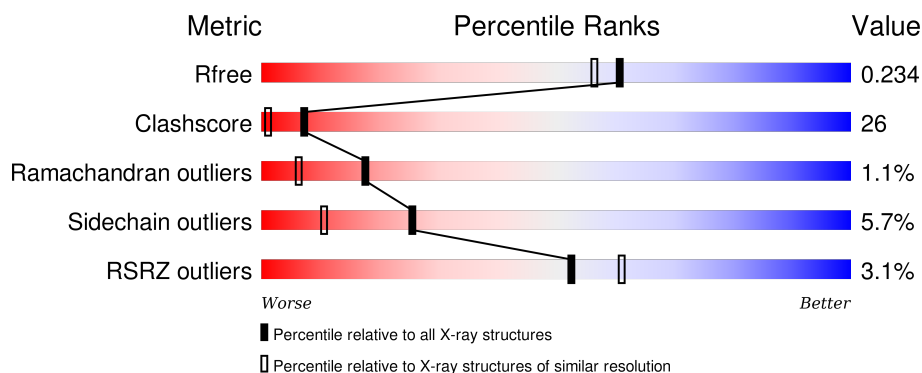
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	324	<div> <div>32%</div> <div>32%</div> <div>6%</div> <div>30%</div> </div>
1	B	324	<div> <div>4%</div> <div>60%</div> <div>26%</div> <div>10%</div> </div>
1	C	324	<div> <div>3%</div> <div>64%</div> <div>23%</div> <div>11%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7397 atoms, of which 0 are hydrogens and 0 are deuteriums.

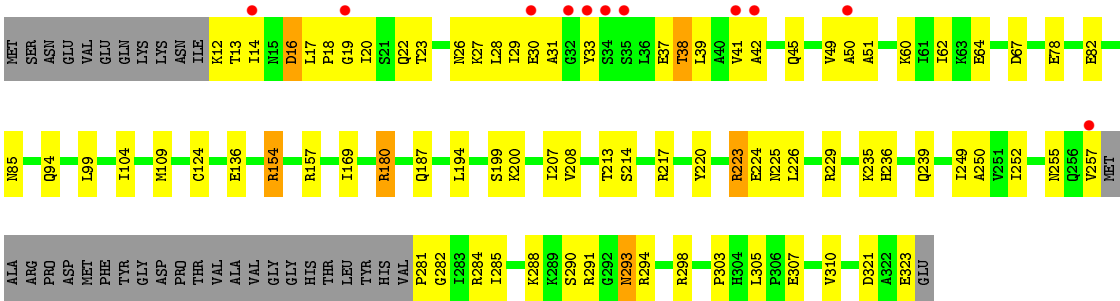
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA repair and recombination protein radA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1799	1130	326	338	5			
1	B	290	Total	C	N	O	S	0	0	0
			2254	1417	400	432	5			
1	C	289	Total	C	N	O	S	0	0	0
			2245	1412	399	429	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	347	Total	O	0	0
			347	347		
2	B	379	Total	O	0	0
			379	379		
2	C	373	Total	O	0	0
			373	373		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	99.55Å 99.55Å 99.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.93 27.61 – 1.93	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-1.93) 94.2 (27.61-1.93)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.93Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.241 0.192 , 0.234	Depositor DCC
R_{free} test set	3645 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.1	EDS
Estimated twinning fraction	0.038 for -h,-k,l 0.487 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 78018 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7397	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

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	0.78	0/1823	0.84	1/2456 (0.0%)
1	B	0.78	0/2283	0.82	2/3083 (0.1%)
1	C	0.82	0/2274	0.88	3/3071 (0.1%)
All	All	0.80	0/6380	0.85	6/8610 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	154	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	B	154	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	154	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	154	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	157	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	243	LEU	CB-CG-CD2	-5.07	102.38	111.00

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	1799	0	1837	170	0
1	B	2254	0	2315	98	0
1	C	2245	0	2309	67	0
2	A	347	0	0	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	379	0	0	16	0
2	C	373	0	0	14	0
All	All	7397	0	6461	332	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 26.

All (332) 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:181:ALA:HB3	2:A:441:HOH:O	1.47	1.12
1:B:85:ASN:HD21	1:B:87:LYS:HE2	1.23	1.00
1:A:85:ASN:HB3	2:A:357:HOH:O	1.59	1.00
1:A:129:VAL:HG23	2:A:518:HOH:O	1.62	0.99
1:A:123:LEU:HA	1:A:319:ILE:HD11	1.47	0.94
1:A:163:LYS:HG3	1:A:169:ILE:HD11	1.51	0.92
1:B:15:ASN:HB2	2:B:332:HOH:O	1.70	0.91
1:B:35:SER:OG	1:B:38:THR:HG23	1.69	0.90
1:B:194:LEU:HD13	1:B:207:ILE:HD13	1.54	0.89
1:A:187:GLN:HE21	1:A:236:HIS:CE1	1.93	0.87
1:A:151:GLY:N	1:A:180:ARG:HE	1.72	0.87
1:A:99:LEU:HD13	1:A:310:VAL:HG23	1.58	0.84
1:A:194:LEU:O	1:A:198:VAL:HG13	1.79	0.82
1:A:153:PHE:HB2	2:A:524:HOH:O	1.79	0.81
1:B:42:ALA:N	2:B:337:HOH:O	2.15	0.80
1:A:146:TYR:HA	1:A:208:VAL:HG22	1.63	0.80
1:A:79:VAL:O	1:A:83:ARG:HG3	1.82	0.80
1:B:85:ASN:ND2	1:B:87:LYS:HE2	1.97	0.80
1:A:158:ILE:HD13	2:A:518:HOH:O	1.82	0.79
1:A:83:ARG:HA	2:A:356:HOH:O	1.82	0.79
1:A:125:HIS:HE1	1:A:154:ARG:H	1.28	0.79
1:A:83:ARG:HH11	1:A:83:ARG:CB	1.97	0.76
1:A:83:ARG:NE	2:A:340:HOH:O	2.17	0.76
1:A:75:THR:HB	2:A:325:HOH:O	1.86	0.75
1:B:298:ARG:HB2	1:B:309:GLU:HG2	1.69	0.75
1:C:194:LEU:HD13	1:C:207:ILE:HD13	1.69	0.75
1:A:75:THR:HG23	1:A:78:GLU:H	1.52	0.74
1:A:143:LYS:HE3	1:A:175:ASN:HA	1.70	0.74
1:A:207:ILE:HD12	1:A:249:ILE:HG21	1.70	0.74
1:B:95:ALA:HB1	1:B:310:VAL:CG1	2.18	0.74
1:A:81:LYS:HD2	2:A:347:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:HD22	1:B:293:ASN:C	1.92	0.73
1:A:198:VAL:HG12	2:A:424:HOH:O	1.89	0.73
1:C:41:VAL:HG12	1:C:41:VAL:O	1.88	0.73
1:B:111:GLU:OE1	1:B:284:ARG:HD2	1.89	0.72
1:C:223:ARG:NE	1:C:223:ARG:H	1.86	0.72
1:A:79:VAL:HA	2:A:352:HOH:O	1.89	0.72
1:A:149:THR:HA	2:A:441:HOH:O	1.90	0.72
1:A:127:LEU:HD13	1:A:252:ILE:HD11	1.71	0.72
1:B:231:GLN:HE22	1:B:235:LYS:CE	2.03	0.72
1:A:148:ASP:O	1:A:180:ARG:HD3	1.90	0.71
1:A:178:TYR:CE2	2:A:442:HOH:O	2.43	0.71
1:B:22:GLN:HG3	1:B:26:ASN:HD21	1.56	0.71
1:A:148:ASP:CG	2:A:524:HOH:O	2.28	0.70
1:B:171:ASN:OD1	2:B:591:HOH:O	2.08	0.70
1:A:76:ALA:O	1:A:79:VAL:HG22	1.91	0.70
1:A:152:THR:HG21	2:A:407:HOH:O	1.92	0.70
1:A:211:SER:OG	2:A:406:HOH:O	2.09	0.70
1:B:48:SER:OG	1:B:55:LEU:HA	1.92	0.70
1:C:284:ARG:C	1:C:285:ILE:HD13	2.13	0.69
1:B:12:LYS:N	1:B:16:ASP:OD1	2.25	0.69
1:A:237:LEU:O	1:A:241:THR:HG23	1.93	0.69
1:B:12:LYS:HD2	2:B:327:HOH:O	1.93	0.69
1:A:160:ASN:ND2	2:A:445:HOH:O	2.27	0.68
1:A:123:LEU:HD22	1:A:127:LEU:HD11	1.77	0.67
1:A:186:HIS:O	1:A:190:ILE:HG13	1.95	0.67
1:B:281:PRO:HB3	2:B:421:HOH:O	1.95	0.66
1:C:291:ARG:O	1:C:294:ARG:HG3	1.95	0.66
1:A:168:ASP:OD1	2:A:452:HOH:O	2.13	0.66
1:C:12:LYS:N	1:C:16:ASP:OD2	2.29	0.66
1:A:91:THR:HG23	2:A:385:HOH:O	1.96	0.66
1:B:22:GLN:O	1:B:26:ASN:ND2	2.29	0.65
1:A:223:ARG:HG2	1:A:226:LEU:HD22	1.79	0.65
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.61	0.65
1:C:235:LYS:HE2	2:C:500:HOH:O	1.96	0.65
1:C:223:ARG:NH1	2:C:512:HOH:O	2.27	0.65
1:B:124:CYS:HB3	1:B:208:VAL:HG11	1.78	0.65
1:A:136:GLU:H	1:A:136:GLU:CD	2.00	0.64
1:B:21:SER:O	1:B:25:ILE:HG13	1.97	0.64
1:A:127:LEU:HD13	1:A:252:ILE:CD1	2.27	0.64
1:B:213:THR:HG23	1:B:255:ASN:OD1	1.97	0.64
1:C:288:LYS:HE3	2:C:524:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:CD1	2:B:610:HOH:O	2.44	0.64
1:B:236:HIS:HD2	2:B:478:HOH:O	1.80	0.64
1:A:207:ILE:CD1	1:A:249:ILE:HG21	2.27	0.63
1:C:13:THR:H	1:C:16:ASP:CG	2.02	0.63
1:A:100:LEU:HD21	1:A:285:ILE:HD11	1.79	0.63
1:A:151:GLY:CA	1:A:180:ARG:HE	2.12	0.63
1:A:289:LYS:HG2	1:A:295:ARG:HE	1.63	0.63
1:A:224:GLU:HG3	1:A:225:ASN:N	2.14	0.62
1:C:224:GLU:HG2	1:C:225:ASN:N	2.13	0.62
1:A:173:MET:CG	2:A:607:HOH:O	2.46	0.62
1:A:75:THR:CG2	1:A:78:GLU:H	2.12	0.62
1:A:99:LEU:HD13	1:A:310:VAL:CG2	2.27	0.62
1:B:293:ASN:ND2	1:B:293:ASN:C	2.54	0.61
1:B:85:ASN:OD1	2:B:371:HOH:O	2.16	0.61
1:A:208:VAL:HG23	2:A:413:HOH:O	2.01	0.61
1:B:298:ARG:HB2	1:B:309:GLU:CG	2.30	0.61
1:B:309:GLU:OE1	1:C:298:ARG:NH2	2.33	0.61
1:A:210:ASP:N	2:A:413:HOH:O	2.30	0.60
1:A:83:ARG:HH11	1:A:83:ARG:HB3	1.66	0.60
1:A:298:ARG:CD	1:A:309:GLU:HB3	2.32	0.60
1:B:85:ASN:O	1:B:85:ASN:ND2	2.35	0.59
1:B:35:SER:HB2	1:B:37:GLU:OE1	2.02	0.59
1:B:134:PRO:HG2	1:B:137:LYS:HG3	1.83	0.59
1:A:123:LEU:HG	1:A:319:ILE:CD1	2.33	0.59
1:B:16:ASP:OD2	1:B:16:ASP:N	2.35	0.59
1:A:298:ARG:HG3	1:A:308:GLY:O	2.03	0.59
1:B:231:GLN:HE22	1:B:235:LYS:HE2	1.66	0.59
1:C:290:SER:OG	1:C:291:ARG:N	2.35	0.59
1:A:75:THR:HG22	1:A:78:GLU:CG	2.33	0.58
1:A:74:LYS:HE2	2:A:329:HOH:O	2.02	0.58
1:B:28:LEU:O	1:B:31:ALA:HB3	2.03	0.58
1:A:289:LYS:HZ1	1:A:295:ARG:CZ	2.16	0.58
1:A:187:GLN:HE21	1:A:236:HIS:HE1	1.47	0.58
1:A:75:THR:HG23	1:A:77:LEU:N	2.19	0.58
1:A:125:HIS:CE1	1:A:154:ARG:H	2.16	0.58
1:C:31:ALA:HB1	1:C:50:ALA:O	2.03	0.58
1:C:37:GLU:H	1:C:37:GLU:CD	2.07	0.58
1:C:99:LEU:HD13	1:C:310:VAL:HG13	1.86	0.57
1:A:127:LEU:CD1	1:A:252:ILE:CD1	2.82	0.57
1:B:323:GLU:O	1:B:324:GLU:CB	2.52	0.57
1:B:21:SER:OG	1:B:23:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:HB2	1:A:178:TYR:CE1	2.39	0.57
1:A:213:THR:HG23	1:A:255:ASN:HD21	1.70	0.57
1:A:157:ARG:O	1:A:161:MET:HG3	2.05	0.57
1:B:194:LEU:O	1:B:198:VAL:HG22	2.05	0.57
1:A:75:THR:HG22	1:A:78:GLU:HG3	1.87	0.57
1:A:163:LYS:HG3	1:A:169:ILE:CD1	2.30	0.56
1:A:100:LEU:HD21	1:A:285:ILE:CD1	2.34	0.56
1:C:257:VAL:HG12	1:C:257:VAL:O	2.04	0.56
1:A:173:MET:HG2	2:A:607:HOH:O	2.05	0.56
1:A:289:LYS:HZ1	1:A:295:ARG:NH2	2.03	0.56
1:C:85:ASN:HD22	1:C:85:ASN:H	1.54	0.56
1:C:109:MET:CE	1:C:281:PRO:HB3	2.35	0.56
1:B:95:ALA:HB1	1:B:310:VAL:HG11	1.84	0.56
1:A:304:HIS:CE1	1:A:305:LEU:HG	2.40	0.56
1:A:319:ILE:O	1:A:320:ARG:HD3	2.05	0.56
1:A:123:LEU:HA	1:A:319:ILE:CD1	2.30	0.56
1:A:126:GLN:HB3	1:A:319:ILE:HD12	1.88	0.55
1:B:294:ARG:NH2	1:B:324:GLU:HB2	2.21	0.55
1:B:29:ILE:C	1:B:31:ALA:H	2.10	0.55
1:A:123:LEU:HG	1:A:319:ILE:HD13	1.87	0.55
1:A:316:GLU:HB2	1:A:317:GLU:OE2	2.07	0.55
1:A:157:ARG:NH2	2:A:411:HOH:O	2.40	0.55
1:B:281:PRO:HG3	2:B:413:HOH:O	2.07	0.55
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.19	0.54
1:A:99:LEU:HB2	1:A:310:VAL:HG21	1.89	0.54
1:C:281:PRO:HB3	2:C:564:HOH:O	2.07	0.54
1:A:110:THR:HG23	1:A:283:ILE:HB	1.90	0.54
1:B:37:GLU:CD	1:B:37:GLU:H	2.10	0.54
1:A:123:LEU:HD22	1:A:127:LEU:CD1	2.37	0.54
1:A:213:THR:CG2	1:A:255:ASN:HD21	2.21	0.53
1:C:187:GLN:HE21	1:C:236:HIS:CE1	2.27	0.53
1:A:149:THR:HG22	1:A:150:GLU:HG3	1.91	0.53
1:A:298:ARG:CG	1:A:309:GLU:HB3	2.39	0.53
1:C:281:PRO:HG3	2:C:428:HOH:O	2.08	0.53
1:C:85:ASN:ND2	1:C:85:ASN:H	2.07	0.53
1:C:293:ASN:HD22	1:C:293:ASN:C	2.10	0.53
1:C:136:GLU:HG3	2:C:469:HOH:O	2.09	0.53
1:C:213:THR:HG23	1:C:255:ASN:OD1	2.09	0.53
1:A:151:GLY:N	1:A:180:ARG:NE	2.50	0.53
1:B:226:LEU:HD12	2:B:610:HOH:O	2.05	0.53
1:A:123:LEU:CD2	1:A:127:LEU:HD11	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LYS:HE3	1:A:295:ARG:HH21	1.74	0.52
1:B:237:LEU:O	1:B:241:THR:HG23	2.09	0.52
1:A:298:ARG:HD2	1:A:309:GLU:OE1	2.08	0.52
1:A:158:ILE:HD12	1:A:176:ILE:HD13	1.91	0.52
1:C:78:GLU:O	1:C:82:GLU:HG3	2.09	0.52
1:A:173:MET:HG3	2:A:607:HOH:O	2.10	0.52
1:B:187:GLN:HE21	1:B:236:HIS:HE1	1.57	0.51
1:A:205:LYS:C	1:A:249:ILE:HG23	2.31	0.51
1:C:41:VAL:HG23	2:C:343:HOH:O	2.10	0.51
1:A:123:LEU:CA	1:A:319:ILE:HD11	2.31	0.51
1:A:75:THR:HG23	1:A:77:LEU:H	1.76	0.51
1:B:196:GLU:HG2	1:B:200:LYS:HD2	1.92	0.51
1:A:240:LEU:HD22	1:A:251:VAL:HG11	1.93	0.51
1:A:158:ILE:HD12	1:A:176:ILE:CD1	2.40	0.51
1:A:207:ILE:HD12	1:A:249:ILE:CG2	2.40	0.51
1:B:13:THR:OG1	1:B:16:ASP:OD2	2.24	0.51
1:A:198:VAL:CG1	2:A:424:HOH:O	2.51	0.51
1:A:289:LYS:NZ	1:A:295:ARG:NH2	2.58	0.51
1:C:27:LYS:HE2	1:C:51:ALA:O	2.11	0.51
1:C:94:GLN:HB2	1:C:321:ASP:OD1	2.10	0.51
1:C:213:THR:OG1	1:C:217:ARG:NH2	2.43	0.51
1:C:60:LYS:HE2	2:C:651:HOH:O	2.11	0.50
1:A:73:PHE:HB2	2:A:327:HOH:O	2.11	0.50
1:A:113:PHE:CZ	1:A:286:GLN:HB2	2.46	0.50
1:C:124:CYS:HB3	1:C:208:VAL:HG11	1.92	0.50
1:B:18:PRO:HD2	1:B:64:GLU:OE1	2.12	0.50
1:B:241:THR:O	1:B:245:GLU:HG3	2.12	0.50
1:B:14:ILE:HG22	1:B:39:LEU:CD1	2.42	0.50
1:A:288:LYS:HE2	1:A:296:ILE:CD1	2.41	0.50
1:C:39:LEU:O	1:C:62:ILE:HG23	2.12	0.50
1:B:85:ASN:N	1:B:85:ASN:HD22	2.08	0.50
1:A:162:ALA:HB2	1:A:172:VAL:HG11	1.93	0.50
1:A:191:VAL:HG21	1:A:236:HIS:NE2	2.26	0.50
1:A:148:ASP:HB2	1:A:178:TYR:HE1	1.76	0.50
1:A:220:TYR:N	1:A:220:TYR:CD1	2.80	0.50
1:C:41:VAL:CG2	2:C:343:HOH:O	2.59	0.50
1:A:289:LYS:NZ	1:A:295:ARG:CZ	2.74	0.50
1:C:45:GLN:O	1:C:49:VAL:HG12	2.12	0.49
1:A:137:LYS:HE3	2:A:420:HOH:O	2.11	0.49
1:B:99:LEU:HD11	1:B:299:VAL:HG23	1.95	0.49
1:A:289:LYS:HE3	1:A:295:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:THR:O	1:C:27:LYS:HG3	2.12	0.49
1:A:310:VAL:HG12	1:A:311:VAL:N	2.27	0.49
1:A:75:THR:HG22	1:A:78:GLU:CD	2.33	0.49
1:B:323:GLU:O	1:B:324:GLU:HB2	2.11	0.49
1:C:64:GLU:HA	1:C:67:ASP:OD1	2.12	0.49
1:C:200:LYS:HE3	2:C:577:HOH:O	2.12	0.49
1:B:100:LEU:O	1:B:101:ALA:HB3	2.12	0.49
1:A:158:ILE:HG23	2:A:518:HOH:O	2.12	0.49
1:B:13:THR:H	1:B:16:ASP:CG	2.16	0.49
1:B:169:ILE:HG12	2:B:460:HOH:O	2.13	0.49
1:A:298:ARG:HG3	1:A:308:GLY:C	2.33	0.49
1:C:187:GLN:HE21	1:C:236:HIS:HE1	1.60	0.49
1:A:249:ILE:HG22	1:A:250:ALA:N	2.28	0.49
1:A:156:GLU:HB2	2:A:444:HOH:O	2.13	0.48
1:C:33:TYR:HE2	1:C:42:ALA:HB1	1.78	0.48
1:B:104:ILE:CG2	1:B:252:ILE:HD11	2.43	0.48
1:B:187:GLN:HE21	1:B:236:HIS:CE1	2.31	0.48
1:A:207:ILE:HD11	1:A:249:ILE:HD13	1.94	0.48
1:B:323:GLU:O	1:B:324:GLU:CG	2.62	0.48
1:B:191:VAL:HG12	1:B:239:GLN:HG2	1.96	0.48
1:A:159:GLU:OE2	1:A:163:LYS:NZ	2.35	0.48
1:A:226:LEU:HA	1:A:229:ARG:HH21	1.78	0.48
1:A:298:ARG:HD2	1:A:309:GLU:HB3	1.96	0.48
1:B:49:VAL:HG13	1:B:50:ALA:N	2.28	0.48
1:A:87:LYS:HE3	2:A:373:HOH:O	2.13	0.48
1:A:88:LYS:HA	1:A:104:ILE:O	2.14	0.48
1:B:213:THR:HG22	1:B:233:LEU:HD21	1.95	0.47
1:A:74:LYS:CE	2:A:329:HOH:O	2.60	0.47
1:A:293:ASN:ND2	1:A:293:ASN:C	2.67	0.47
1:A:288:LYS:HG3	1:A:296:ILE:HB	1.95	0.47
1:A:195:GLN:O	1:A:199:SER:HB2	2.13	0.47
1:A:159:GLU:HG2	2:A:527:HOH:O	2.15	0.47
1:B:27:LYS:HD3	1:B:51:ALA:O	2.15	0.47
1:A:172:VAL:HG12	1:A:173:MET:N	2.30	0.47
1:B:165:LEU:HB2	1:B:167:LEU:HG	1.97	0.47
1:B:27:LYS:O	1:B:31:ALA:HB2	2.15	0.47
1:B:99:LEU:HD12	2:B:399:HOH:O	2.14	0.47
1:C:284:ARG:O	1:C:285:ILE:HD13	2.15	0.47
1:C:29:ILE:C	1:C:31:ALA:H	2.19	0.46
1:A:126:GLN:CB	1:A:319:ILE:HD12	2.45	0.46
1:A:171:ASN:O	1:A:174:ASN:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.29	0.46
1:A:184:THR:N	1:A:219:GLU:OE2	2.43	0.46
1:B:78:GLU:O	1:B:82:GLU:HG3	2.14	0.46
1:C:22:GLN:OE1	1:C:26:ASN:ND2	2.48	0.46
1:B:54:PRO:HG2	1:B:57:THR:OG1	2.15	0.46
1:A:310:VAL:HG12	1:A:311:VAL:H	1.79	0.46
1:C:220:TYR:HB2	1:C:229:ARG:HG3	1.96	0.46
1:C:17:LEU:HA	1:C:18:PRO:HD3	1.70	0.46
1:B:194:LEU:CD1	1:B:207:ILE:HD13	2.38	0.46
1:A:82:GLU:O	1:A:82:GLU:OE2	2.34	0.46
1:C:16:ASP:OD1	1:C:16:ASP:N	2.49	0.46
1:B:14:ILE:HG22	1:B:39:LEU:HD11	1.98	0.46
1:C:18:PRO:HG3	2:C:632:HOH:O	2.15	0.46
1:A:122:GLN:HB2	1:A:314:LEU:HD21	1.98	0.45
1:B:226:LEU:HD11	2:B:610:HOH:O	2.14	0.45
1:B:22:GLN:HG3	1:B:26:ASN:ND2	2.29	0.45
1:B:63:LYS:HE2	1:B:67:ASP:OD2	2.16	0.45
1:B:293:ASN:HD22	1:B:294:ARG:N	2.13	0.45
1:A:148:ASP:HB3	1:A:180:ARG:HA	1.99	0.45
1:C:12:LYS:HE2	1:C:12:LYS:HB3	1.76	0.45
1:A:288:LYS:HE2	1:A:296:ILE:HD13	1.98	0.45
1:C:249:ILE:HG22	1:C:250:ALA:N	2.32	0.45
1:B:20:ILE:HG12	1:B:21:SER:N	2.31	0.45
1:B:309:GLU:CD	1:C:298:ARG:HH22	2.21	0.44
1:B:30:GLU:O	1:B:30:GLU:HG3	2.17	0.44
1:C:38:THR:O	1:C:41:VAL:C	2.56	0.44
1:B:223:ARG:HG2	1:B:226:LEU:HD22	1.99	0.44
1:C:37:GLU:CD	1:C:37:GLU:N	2.68	0.44
1:B:191:VAL:CG1	1:B:239:GLN:HG2	2.48	0.44
1:A:204:ILE:HG21	2:A:424:HOH:O	2.16	0.44
1:A:170:ASP:O	1:A:174:ASN:HB2	2.16	0.44
1:B:133:LEU:O	1:B:139:GLY:HA3	2.18	0.44
1:A:158:ILE:HG21	2:A:607:HOH:O	2.16	0.44
1:A:79:VAL:CA	2:A:352:HOH:O	2.59	0.44
1:B:23:THR:CG2	1:B:24:VAL:N	2.81	0.44
1:C:180:ARG:C	1:C:180:ARG:HD3	2.38	0.44
1:C:223:ARG:HA	1:C:226:LEU:HB2	1.99	0.44
1:B:310:VAL:HG12	1:B:311:VAL:N	2.32	0.44
1:B:88:LYS:CE	1:B:105:GLU:HB2	2.48	0.44
1:C:223:ARG:CD	1:C:223:ARG:H	2.31	0.43
1:A:300:VAL:O	1:A:300:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG22	1:A:109:MET:N	2.33	0.43
1:C:224:GLU:HG3	2:C:592:HOH:O	2.19	0.43
1:A:156:GLU:O	1:A:156:GLU:OE2	2.37	0.43
1:C:104:ILE:CG2	1:C:252:ILE:HD11	2.48	0.43
1:B:235:LYS:HB2	1:B:235:LYS:HE2	1.80	0.43
1:B:28:LEU:O	1:B:31:ALA:N	2.51	0.43
1:A:181:ALA:HB2	1:A:190:ILE:HD12	2.00	0.43
1:A:83:ARG:NH1	1:A:83:ARG:CG	2.79	0.43
1:A:230:GLN:O	1:A:234:ASN:HB3	2.19	0.43
1:A:95:ALA:HB1	1:A:310:VAL:CG1	2.49	0.43
1:A:152:THR:CG2	2:A:407:HOH:O	2.57	0.43
1:A:284:ARG:HB2	1:A:301:ASP:HB3	2.01	0.43
1:A:243:LEU:HD12	1:A:247:TYR:CD1	2.54	0.43
1:A:301:ASP:OD1	1:A:301:ASP:O	2.36	0.43
1:A:224:GLU:CG	1:A:225:ASN:N	2.81	0.43
1:B:63:LYS:O	1:B:67:ASP:OD2	2.37	0.43
1:A:118:SER:O	1:A:295:ARG:HD3	2.18	0.42
1:C:169:ILE:HG12	2:C:466:HOH:O	2.19	0.42
1:B:309:GLU:CD	1:C:298:ARG:NH2	2.72	0.42
1:A:109:MET:CE	1:A:237:LEU:HD22	2.49	0.42
1:A:207:ILE:HD13	1:A:243:LEU:CD2	2.49	0.42
1:C:285:ILE:N	1:C:285:ILE:HD13	2.32	0.42
1:B:227:ALA:HB3	2:B:514:HOH:O	2.19	0.42
1:B:17:LEU:HA	1:B:18:PRO:HD3	1.80	0.42
1:A:148:ASP:OD2	1:A:153:PHE:HB3	2.19	0.42
1:B:281:PRO:CB	2:B:421:HOH:O	2.60	0.42
1:C:28:LEU:O	1:C:31:ALA:HB3	2.20	0.42
1:A:293:ASN:HD22	1:A:293:ASN:C	2.23	0.42
1:C:14:ILE:HG22	1:C:39:LEU:HD12	2.02	0.42
1:A:81:LYS:HE3	2:A:347:HOH:O	2.19	0.42
1:A:223:ARG:HA	1:A:226:LEU:HB2	2.01	0.42
1:A:289:LYS:CE	1:A:295:ARG:NH2	2.83	0.42
1:C:305:LEU:O	1:C:307:GLU:OE1	2.38	0.42
1:B:31:ALA:HB1	1:B:50:ALA:O	2.20	0.42
1:A:121:THR:O	1:A:122:GLN:C	2.57	0.42
1:C:60:LYS:HB2	2:C:651:HOH:O	2.20	0.41
1:A:123:LEU:CD2	1:A:127:LEU:CD1	2.97	0.41
1:A:289:LYS:HB3	1:A:295:ARG:HH21	1.86	0.41
1:C:293:ASN:ND2	1:C:293:ASN:C	2.74	0.41
1:B:13:THR:O	1:B:16:ASP:N	2.51	0.41
1:B:104:ILE:HG21	1:B:252:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:HA	1:A:202:PRO:HD2	1.90	0.41
1:A:123:LEU:HG	1:A:319:ILE:HD11	2.00	0.41
1:B:29:ILE:O	1:B:31:ALA:N	2.52	0.41
1:A:293:ASN:N	1:A:293:ASN:HD22	2.19	0.41
1:B:228:VAL:CG1	1:B:232:LYS:HE2	2.50	0.41
1:A:317:GLU:CD	1:A:317:GLU:N	2.74	0.40
1:A:149:THR:HB	1:A:210:ASP:O	2.21	0.40
1:A:75:THR:CG2	1:A:78:GLU:HG3	2.51	0.40
1:A:289:LYS:CE	1:A:295:ARG:HH21	2.34	0.40
1:C:217:ARG:HA	1:C:229:ARG:HD3	2.03	0.40
1:B:37:GLU:CD	1:B:37:GLU:N	2.75	0.40
1:A:160:ASN:ND2	2:A:446:HOH:O	2.54	0.40
1:B:281:PRO:N	2:B:412:HOH:O	2.55	0.40
1:A:136:GLU:N	1:A:136:GLU:CD	2.72	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	224/324 (69%)	216 (96%)	7 (3%)	1 (0%)	39	26
1	B	286/324 (88%)	271 (95%)	11 (4%)	4 (1%)	14	4
1	C	285/324 (88%)	270 (95%)	11 (4%)	4 (1%)	14	4
All	All	795/972 (82%)	757 (95%)	29 (4%)	9 (1%)	17	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	GLU
1	C	20	ILE
1	C	30	GLU

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Mol	Chain	Res	Type
1	B	19	GLY
1	B	28	LEU
1	A	302	ALA
1	B	282	GLY
1	C	19	GLY
1	C	282	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/275 (71%)	174 (89%)	21 (11%)	8	1
1	B	246/275 (90%)	239 (97%)	7 (3%)	51	38
1	C	245/275 (89%)	234 (96%)	11 (4%)	34	18
All	All	686/825 (83%)	647 (94%)	39 (6%)	25	10

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	A	83	ARG
1	A	123	LEU
1	A	136	GLU
1	A	146	TYR
1	A	154	ARG
1	A	156	GLU
1	A	159	GLU
1	A	172	VAL
1	A	180	ARG
1	A	182	ILE
1	A	198	VAL
1	A	205	LYS
1	A	220	TYR
1	A	223	ARG
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	293	ASN
1	A	295	ARG
1	A	301	ASP
1	A	320	ARG
1	B	16	ASP
1	B	23	THR
1	B	55	LEU
1	B	85	ASN
1	B	154	ARG
1	B	223	ARG
1	B	293	ASN
1	C	16	ASP
1	C	38	THR
1	C	154	ARG
1	C	180	ARG
1	C	199	SER
1	C	214	SER
1	C	223	ARG
1	C	239	GLN
1	C	293	ASN
1	C	303	PRO
1	C	323	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	236	HIS
1	A	256	GLN
1	A	293	ASN
1	B	22	GLN
1	B	26	ASN
1	B	85	ASN
1	B	160	ASN
1	B	195	GLN
1	B	231	GLN
1	B	236	HIS
1	B	293	ASN
1	C	85	ASN
1	C	160	ASN
1	C	236	HIS

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Mol	Chain	Res	Type
1	C	293	ASN

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 carbohydrates 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 ⓘ

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	228/324 (70%)	-0.14	2 (0%) 85 89	29, 46, 73, 88	0
1	B	290/324 (89%)	-0.15	12 (4%) 41 50	16, 32, 82, 87	0
1	C	289/324 (89%)	-0.18	11 (3%) 44 54	15, 31, 82, 85	0
All	All	807/972 (83%)	-0.16	25 (3%) 52 61	15, 37, 82, 88	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	VAL	6.8
1	B	42	ALA	4.6
1	C	41	VAL	4.3
1	B	35	SER	3.8
1	C	50	ALA	3.8
1	A	226	LEU	3.3
1	C	32	GLY	3.3
1	B	29	ILE	3.2
1	C	257	VAL	3.1
1	B	32	GLY	3.1
1	C	34	SER	3.0
1	B	38	THR	2.7
1	C	42	ALA	2.5
1	C	35	SER	2.4
1	C	14	ILE	2.4
1	C	19	GLY	2.4
1	B	31	ALA	2.4
1	B	33	TYR	2.4
1	C	33	TYR	2.4
1	B	45	GLN	2.4
1	B	257	VAL	2.2
1	A	302	ALA	2.2
1	B	28	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	30	GLU	2.1
1	B	49	VAL	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 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.