



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 AM UTC

PDB ID : 6JDE / pdb_00006jde
Title : crystal structure of a DNA repair protein
Authors : Yan, X.X.; Tang, Q.
Deposited on : 2019-02-01
Resolution : 2.80 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

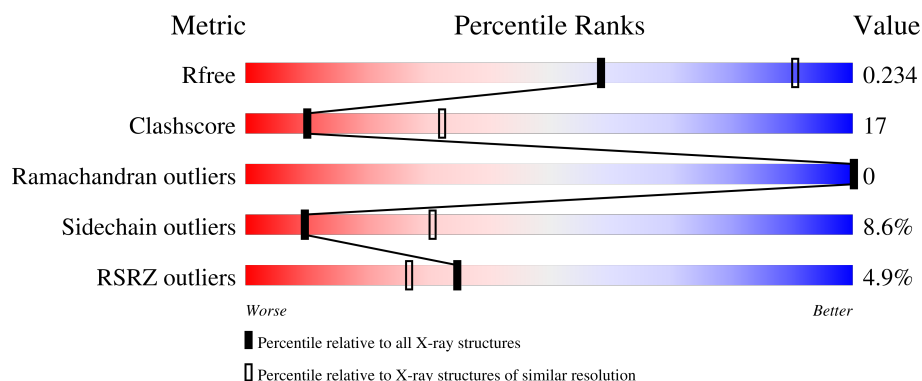
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	586	6% 63% 29% • •
1	B	586	3% 68% 25% • • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9030 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 Putative DNA repair helicase RadD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	567	Total	C	N	O	S	1	3	0
			4386	2798	786	784	18			
1	A	560	Total	C	N	O	S	1	2	0
			4266	2722	758	769	17			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

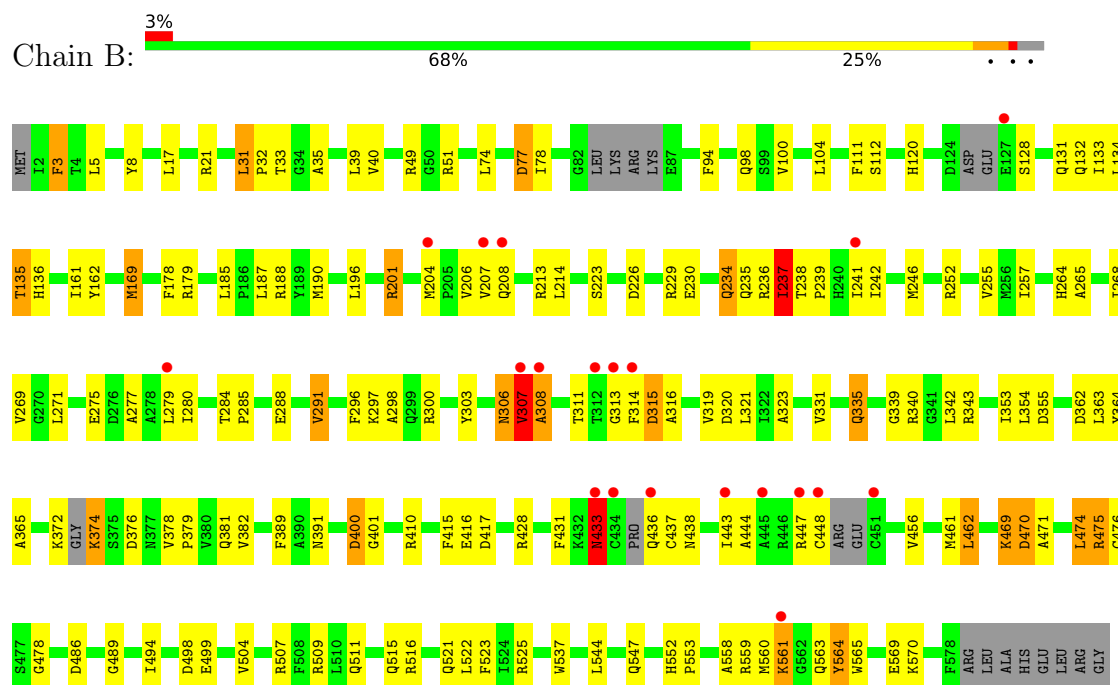
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	222	Total	O	0	0
			222	222		
3	A	154	Total	O	0	0
			154	154		

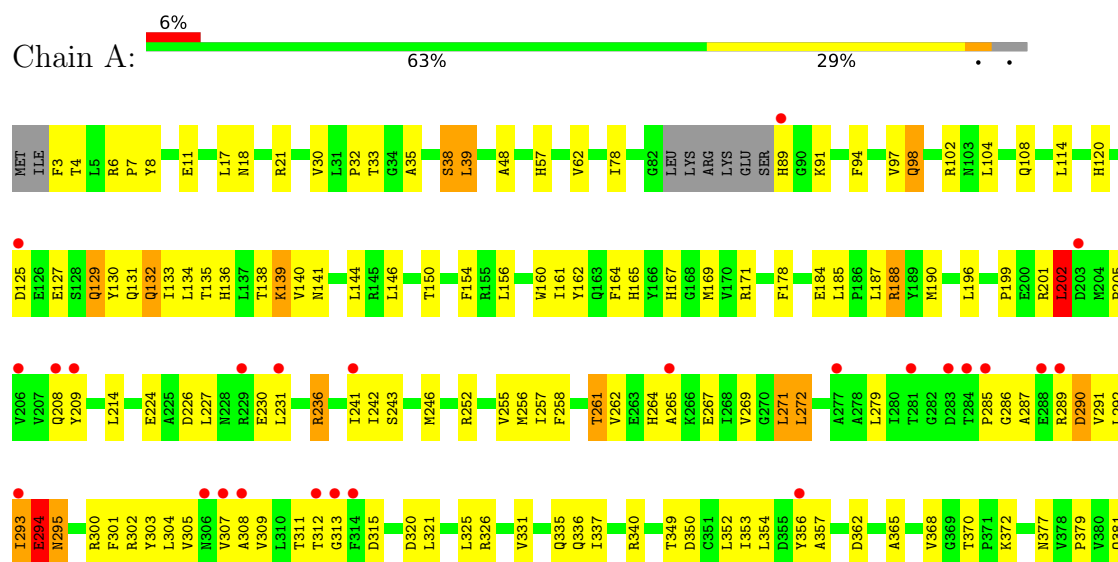
3 Residue-property plots

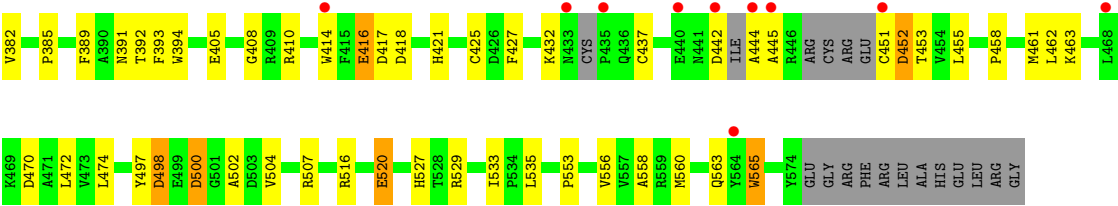
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Putative DNA repair helicase RadD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.52Å 78.45Å 110.59Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	19.95 – 2.80 19.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.95-2.80) 97.5 (19.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.228 , 0.240 0.231 , 0.234	Depositor DCC
R_{free} test set	1580 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3604e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.50	2/4367 (0.0%)	0.77	12/5940 (0.2%)
1	B	0.64	2/4490 (0.0%)	0.95	23/6099 (0.4%)
All	All	0.57	4/8857 (0.0%)	0.87	35/12039 (0.3%)

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	2
1	B	0	4
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	474	LEU	C-O	-5.47	1.17	1.23
1	A	38	SER	C-O	-5.16	1.18	1.24
1	A	188	ARG	C-O	-5.11	1.18	1.24
1	B	561	LYS	CA-C	-5.09	1.46	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	561	LYS	CA-C-N	22.77	166.03	121.41
1	B	561	LYS	C-N-CA	22.77	166.03	121.41
1	B	307	VAL	CB-CA-C	-13.11	89.80	111.29
1	B	315	ASP	N-CA-C	-12.41	84.36	110.80
1	B	307	VAL	N-CA-C	11.91	134.12	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	GLN	CB-CA-C	-11.75	90.48	110.81
1	B	561	LYS	N-CA-C	11.06	124.51	111.02
1	A	565	TRP	N-CA-C	10.93	134.09	110.80
1	A	294	GLU	CB-CA-C	-10.70	88.17	109.67
1	A	294	GLU	N-CA-C	10.68	126.89	112.90
1	B	204	MET	CB-CA-C	-10.55	99.57	110.33
1	A	293	ILE	CB-CA-C	-10.11	98.26	112.22
1	B	308	ALA	N-CA-C	-10.05	93.87	109.25
1	B	307	VAL	CA-C-N	9.86	136.01	121.72
1	B	307	VAL	C-N-CA	9.86	136.01	121.72
1	B	135	THR	N-CA-C	-8.74	102.75	113.41
1	B	237	ILE	CB-CA-C	-7.46	93.40	111.02
1	B	433	ASN	CA-C-N	7.38	134.99	121.70
1	B	433	ASN	C-N-CA	7.38	134.99	121.70
1	A	272	LEU	CB-CA-C	7.23	124.41	110.17
1	A	38	SER	N-CA-C	7.17	120.01	111.33
1	B	308	ALA	CB-CA-C	7.12	121.96	110.29
1	B	315	ASP	CB-CA-C	7.01	124.37	110.42
1	B	236	ARG	N-CA-C	-6.93	104.97	113.50
1	B	433	ASN	CB-CA-C	-6.92	97.69	112.78
1	A	140	VAL	CB-CA-C	-6.20	104.13	111.94
1	A	565	TRP	CB-CA-C	-6.07	98.35	110.42
1	B	474	LEU	CA-CB-CG	6.04	137.44	116.30
1	B	204	MET	N-CA-C	6.02	121.47	109.01
1	A	432	LYS	CB-CA-C	5.88	121.08	109.66
1	B	563	GLN	N-CA-C	5.37	122.23	110.80
1	A	133	ILE	N-CA-C	5.31	116.08	110.72
1	A	133	ILE	CB-CA-C	-5.13	105.15	112.22
1	B	40	VAL	N-CA-C	-5.09	105.75	110.53
1	A	202	LEU	N-CA-CB	-5.05	102.91	110.24

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	LEU	Peptide
1	A	309	VAL	Peptide
1	B	275	GLU	Peptide
1	B	307	VAL	Peptide
1	B	308	ALA	Peptide
1	B	561	LYS	Peptide

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	4266	0	4072	155	0
1	B	4386	0	4228	136	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	154	0	0	7	0
3	B	222	0	0	11	0
All	All	9030	0	8300	291	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 (291) 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:234:GLN:O	1:B:237:ILE:HG12	1.23	1.27
1:B:470:ASP:OD2	1:B:559:ARG:NH1	1.70	1.25
1:A:242:ILE:HD12	1:A:271:LEU:HD22	1.16	1.13
1:A:104:LEU:HB3	1:A:136:HIS:CD2	1.90	1.05
1:A:293:ILE:HD11	3:A:701:HOH:O	1.54	1.04
1:B:428:ARG:NE	1:B:438:ASN:OD1	1.99	0.95
1:B:433:ASN:ND2	1:B:448:CYS:O	1.97	0.95
1:A:132:GLN:O	1:A:135:THR:OG1	1.85	0.94
1:B:234:GLN:O	1:B:237:ILE:CG1	2.16	0.94
1:B:400:ASP:OD1	3:B:701:HOH:O	1.86	0.93
1:A:307:VAL:HG13	1:A:308:ALA:N	1.82	0.93
1:A:307:VAL:HG13	1:A:308:ALA:H	1.38	0.87
1:A:290:ASP:HA	1:A:293:ILE:CD1	2.05	0.86
1:A:290:ASP:HA	1:A:293:ILE:HD12	1.58	0.85
1:A:349:THR:HG23	1:A:350:ASP:OD2	1.77	0.83
1:A:257:ILE:HD11	1:A:325:LEU:HD11	1.60	0.83
1:B:187:LEU:HD21	1:B:363:LEU:HG	1.59	0.83
1:B:234:GLN:C	1:B:237:ILE:HG12	2.05	0.81
1:A:257:ILE:HD11	1:A:325:LEU:CD1	2.10	0.81
1:A:8:TYR:OH	1:A:35:ALA:O	1.98	0.81
1:B:433:ASN:HD22	1:B:448:CYS:C	1.89	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLY:HA2	1:A:289:ARG:HB3	1.64	0.80
1:B:8:TYR:OH	1:B:35:ALA:O	1.99	0.80
1:B:187:LEU:CD2	1:B:363:LEU:HG	2.12	0.79
1:A:246:MET:HE3	1:A:272:LEU:HD23	1.65	0.79
1:A:290:ASP:HA	1:A:293:ILE:CG1	2.13	0.78
1:B:32:PRO:HD2	1:B:185:LEU:HB3	1.65	0.78
1:A:242:ILE:CD1	1:A:271:LEU:HD22	2.07	0.78
1:A:242:ILE:HD12	1:A:271:LEU:CD2	2.08	0.77
1:B:311:THR:HG22	1:B:311:THR:O	1.85	0.75
1:A:290:ASP:CA	1:A:293:ILE:HG13	2.17	0.75
1:A:120:HIS:HA	1:A:161:ILE:HD13	1.69	0.74
1:B:206:VAL:HG12	1:B:207:VAL:H	1.54	0.73
1:B:433:ASN:O	1:B:436:GLN:HA	1.89	0.72
1:B:374:LYS:HG3	1:B:376:ASP:H	1.55	0.72
1:B:237:ILE:HD13	1:B:237:ILE:N	2.04	0.71
1:A:241:ILE:HG21	1:A:325:LEU:HD21	1.72	0.71
1:B:564:TYR:OH	3:B:702:HOH:O	2.08	0.71
1:A:290:ASP:HA	1:A:293:ILE:HG13	1.73	0.71
1:A:405:GLU:OE1	3:A:702:HOH:O	2.08	0.70
1:B:433:ASN:ND2	1:B:448:CYS:C	2.49	0.70
1:A:78:ILE:HA	1:A:94:PHE:O	1.92	0.69
1:A:417:ASP:OD1	1:A:418:ASP:N	2.22	0.69
1:B:475:ARG:HG2	1:B:475:ARG:HH11	1.58	0.69
1:B:437:CYS:SG	1:B:444:ALA:HA	2.33	0.69
1:B:314:PHE:O	1:B:316:ALA:N	2.26	0.69
1:A:169[A]:MET:HG2	1:A:389:PHE:HZ	1.58	0.69
1:A:372:LYS:O	1:A:377:ASN:ND2	2.26	0.68
1:B:255:VAL:HG22	1:B:321:LEU:HB3	1.76	0.68
1:A:307:VAL:CG1	1:A:308:ALA:H	2.07	0.68
1:B:315:ASP:OD2	1:B:343:ARG:NE	2.23	0.67
1:B:257:ILE:HG21	1:B:268:ILE:HG21	1.77	0.67
1:A:500:ASP:N	1:A:500:ASP:OD1	2.27	0.67
1:B:525[A]:ARG:NH1	3:B:705:HOH:O	2.27	0.67
1:B:100:VAL:HG12	1:B:133:ILE:HG12	1.77	0.67
1:A:307:VAL:CG1	1:A:308:ALA:N	2.55	0.66
1:A:311:THR:O	1:A:312:THR:HG23	1.95	0.66
1:A:451:CYS:O	1:A:453:THR:HG23	1.96	0.66
1:B:242:ILE:HG22	1:B:246:MET:HE2	1.79	0.65
1:A:289:ARG:O	1:A:293:ILE:HD11	1.95	0.65
1:B:321:LEU:HD11	1:B:354:LEU:HG	1.78	0.65
1:A:349:THR:HG23	1:A:350:ASP:CG	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:HD11	1:A:556:VAL:HB	1.77	0.65
1:B:316:ALA:HB3	1:B:319:VAL:HG23	1.79	0.65
1:B:230:GLU:HG3	1:B:234:GLN:HE21	1.60	0.65
1:B:280:ILE:HD11	1:B:306[A]:ASN:OD1	1.98	0.64
1:A:381:GLN:HA	1:A:391:ASN:O	1.97	0.64
1:A:62:VAL:HG12	1:A:78:ILE:HD11	1.78	0.64
1:A:97:VAL:HG12	1:A:129:GLN:HB2	1.80	0.64
1:A:18:ASN:ND2	3:A:706:HOH:O	2.31	0.64
1:A:269:VAL:HG21	1:A:279:LEU:HB2	1.79	0.63
1:B:476:CYS:HB3	1:B:553:PRO:O	1.99	0.63
1:B:31:LEU:HA	1:B:185:LEU:HB3	1.80	0.63
1:B:264:HIS:O	1:B:268:ILE:HG12	1.99	0.63
1:A:311:THR:O	1:A:312:THR:CG2	2.47	0.62
1:A:32:PRO:HG2	1:A:190:MET:HE2	1.82	0.62
1:B:49:ARG:NH2	3:B:709:HOH:O	2.33	0.61
1:B:77:ASP:OD1	1:B:77:ASP:N	2.33	0.61
1:A:104:LEU:CB	1:A:136:HIS:CD2	2.78	0.61
1:B:444:ALA:HB1	1:B:447:ARG:H	1.65	0.61
1:B:475:ARG:HH11	1:B:475:ARG:CG	2.14	0.61
1:A:313:GLY:C	1:A:315:ASP:OD1	2.44	0.61
1:A:3:PHE:N	3:A:707:HOH:O	2.33	0.61
1:A:114:LEU:HD23	1:A:146:LEU:HG	1.83	0.60
1:A:202:LEU:O	1:A:205:PRO:HD3	2.01	0.60
1:A:474:LEU:HD21	1:A:504:VAL:HG12	1.82	0.60
1:B:5:LEU:HD22	1:B:39:LEU:HB3	1.83	0.59
1:A:262:VAL:N	1:A:307:VAL:HG21	2.18	0.58
1:B:469:LYS:HD3	1:B:469:LYS:N	2.19	0.58
1:B:134:LEU:HG	1:B:134:LEU:O	2.04	0.58
1:A:445:ALA:HA	1:A:451:CYS:O	2.04	0.58
1:A:120:HIS:ND1	1:A:150:THR:OG1	2.37	0.58
1:A:202:LEU:HD22	1:A:354:LEU:CD2	2.33	0.58
1:B:169[B]:MET:HB3	1:B:389:PHE:HZ	1.69	0.58
1:B:471:ALA:HB2	1:B:559:ARG:HD3	1.84	0.57
1:B:504:VAL:HG21	1:B:558:ALA:HB2	1.86	0.57
1:B:339:GLY:HA2	1:B:342:LEU:HD12	1.87	0.57
1:A:291:VAL:HG23	1:A:292:LEU:N	2.19	0.57
1:A:246:MET:CE	1:A:272:LEU:HD23	2.35	0.57
1:B:489:GLY:HA3	1:B:511:GLN:HB2	1.87	0.56
1:A:520:GLU:OE2	3:A:703:HOH:O	2.17	0.56
1:B:223:SER:OG	1:B:226:ASP:HB2	2.05	0.56
1:A:202:LEU:HD22	1:A:354:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TYR:HA	1:B:178:PHE:O	2.07	0.54
1:A:290:ASP:N	1:A:293:ILE:HG13	2.22	0.54
1:B:242:ILE:HD11	1:B:268:ILE:HA	1.88	0.54
1:A:104:LEU:HD13	1:A:136:HIS:HB2	1.88	0.54
1:A:442:ASP:C	1:A:455:LEU:HB2	2.33	0.54
1:B:131:GLN:O	1:B:135:THR:HG23	2.08	0.54
1:B:169[B]:MET:HB3	1:B:389:PHE:CZ	2.43	0.54
1:B:32:PRO:HD3	1:B:185:LEU:O	2.08	0.54
1:B:206:VAL:HG12	1:B:207:VAL:N	2.21	0.54
1:B:331:VAL:O	1:B:335:GLN:HG2	2.07	0.54
1:B:78:ILE:HA	1:B:94:PHE:O	2.08	0.54
1:B:471:ALA:CB	1:B:559:ARG:HD3	2.37	0.54
1:A:33:THR:OG1	1:A:340:ARG:NH1	2.41	0.53
1:B:17:LEU:O	1:B:21:ARG:HG3	2.09	0.53
1:B:188:ARG:HG3	1:B:364:TYR:CE2	2.43	0.53
1:A:257:ILE:HD11	1:A:325:LEU:HD12	1.87	0.53
1:B:190:MET:HB3	1:B:196:LEU:HG	1.91	0.53
1:A:474:LEU:CD1	1:A:556:VAL:HB	2.37	0.53
1:B:307:VAL:O	1:B:307:VAL:CG1	2.44	0.53
1:A:17:LEU:O	1:A:21:ARG:HG3	2.09	0.53
1:B:478:GLY:HA2	1:B:552:HIS:CD2	2.43	0.53
1:A:125:ASP:C	1:A:127:GLU:H	2.17	0.53
1:B:516:ARG:HG3	1:B:537:TRP:CZ2	2.44	0.53
1:B:206:VAL:CG1	1:B:207:VAL:H	2.19	0.53
1:B:169[A]:MET:HB2	1:B:389:PHE:HZ	1.74	0.52
1:A:498:ASP:HB3	1:A:500:ASP:H	1.74	0.52
1:B:201:ARG:HB2	1:B:353:ILE:HB	1.91	0.52
1:B:560:MET:HG2	1:B:565:TRP:CZ3	2.45	0.52
1:B:381:GLN:HA	1:B:391:ASN:O	2.09	0.52
1:A:442:ASP:HA	1:A:455:LEU:HB2	1.91	0.52
1:B:410:ARG:NH1	3:B:712:HOH:O	2.36	0.52
1:A:162:TYR:HA	1:A:178:PHE:O	2.10	0.52
1:A:437:CYS:SG	1:A:444:ALA:HB3	2.50	0.52
1:B:461:MET:CE	1:B:462:LEU:HD13	2.40	0.52
1:A:98:GLN:O	1:A:102:ARG:HD3	2.10	0.52
1:A:190:MET:HE3	1:A:196:LEU:HG	1.92	0.52
1:B:311:THR:O	1:B:311:THR:CG2	2.56	0.51
1:B:315:ASP:OD2	1:B:343:ARG:NH2	2.43	0.51
1:A:214:LEU:HD22	1:A:226:ASP:HB3	1.92	0.51
1:A:311:THR:C	1:A:312:THR:HG23	2.36	0.51
1:B:428:ARG:HH21	1:B:438:ASN:HD21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HB	1:A:184:GLU:HG3	1.93	0.51
1:A:256:MET:HG2	1:A:304:LEU:HD23	1.92	0.51
1:B:208:GLN:NE2	1:B:355:ASP:O	2.43	0.51
1:B:169[A]:MET:HB2	1:B:389:PHE:CZ	2.45	0.51
1:B:187:LEU:HD23	1:B:363:LEU:HG	1.91	0.51
1:A:442:ASP:O	1:A:455:LEU:HB2	2.10	0.51
1:B:314:PHE:O	1:B:315:ASP:C	2.49	0.51
1:A:160:TRP:CE2	1:A:171:ARG:HD2	2.46	0.51
1:A:199:PRO:HB2	1:A:353:ILE:HD11	1.92	0.50
1:B:237:ILE:HG22	1:B:237:ILE:O	2.10	0.50
1:B:475:ARG:CG	1:B:475:ARG:NH1	2.72	0.50
1:A:372:LYS:HG2	1:A:377:ASN:HB2	1.94	0.50
1:B:185:LEU:HD21	1:B:190:MET:HE3	1.93	0.50
1:B:252:ARG:HH11	1:B:320:ASP:HB2	1.76	0.49
1:B:461:MET:HE3	1:B:462:LEU:HD13	1.93	0.49
1:B:382:VAL:O	1:B:391:ASN:HB2	2.13	0.49
1:A:35:ALA:HA	1:A:190:MET:HE1	1.95	0.48
1:B:288:GLU:O	1:B:291:VAL:HG12	2.13	0.48
1:B:313:GLY:C	1:B:315:ASP:H	2.20	0.48
1:B:207:VAL:HG12	1:B:208:GLN:N	2.28	0.48
1:A:265:ALA:HB1	1:A:279:LEU:HD11	1.96	0.48
1:B:362:ASP:CG	1:B:365:ALA:HB2	2.38	0.48
1:A:294:GLU:OE2	1:A:300:ARG:NH1	2.46	0.48
1:A:209:TYR:HB2	1:A:357:ALA:HA	1.96	0.48
1:A:362:ASP:HB2	1:A:365:ALA:HB2	1.95	0.48
1:B:315:ASP:HB3	1:B:340:ARG:HD2	1.95	0.48
1:A:125:ASP:C	1:A:127:GLU:N	2.72	0.48
1:B:300:ARG:NH2	3:B:718:HOH:O	2.46	0.47
1:A:285:PRO:HB2	1:A:287:ALA:H	1.78	0.47
1:A:414:TRP:HZ3	1:A:416:GLU:HG3	1.78	0.47
1:A:291:VAL:HG23	1:A:292:LEU:HG	1.96	0.47
1:B:185:LEU:HD11	1:B:190:MET:HE3	1.96	0.47
1:A:3:PHE:HB2	1:A:39:LEU:HD11	1.96	0.47
1:B:120:HIS:HA	1:B:161:ILE:HD13	1.96	0.47
1:B:32:PRO:HG2	1:B:190:MET:HG3	1.96	0.47
1:B:237:ILE:O	1:B:241:ILE:HD12	2.15	0.47
1:B:269:VAL:HG21	1:B:279:LEU:HB2	1.96	0.47
1:A:7:PRO:O	1:A:11:GLU:HG3	2.15	0.47
1:B:277:ALA:HA	1:B:303:TYR:O	2.15	0.47
1:A:129:GLN:H	1:A:129:GLN:HG2	1.43	0.47
1:A:504:VAL:HG21	1:A:558:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:356:TYR:HB2	1.97	0.46
1:A:527:HIS:HE1	1:A:553:PRO:HD3	1.81	0.46
1:A:169[A]:MET:HG2	1:A:389:PHE:CZ	2.44	0.46
1:A:368:VAL:HG22	1:A:392:THR:HG22	1.97	0.46
1:A:264:HIS:O	1:A:267:GLU:HB3	2.15	0.46
1:A:560:MET:HE3	1:A:560:MET:HB3	1.59	0.46
1:A:461:MET:HE3	1:A:461:MET:HB3	1.80	0.46
1:B:238:THR:HA	1:B:241:ILE:HD12	1.98	0.46
1:B:486:ASP:HB2	3:B:764:HOH:O	2.16	0.46
1:A:261:THR:C	1:A:307:VAL:HG21	2.40	0.46
1:A:8:TYR:CD1	1:A:185:LEU:HD22	2.51	0.45
1:A:57:HIS:CE1	1:A:97:VAL:HG21	2.52	0.45
1:A:104:LEU:HD22	1:A:136:HIS:HD2	1.81	0.45
1:A:405:GLU:HG3	1:A:529:ARG:HB3	1.98	0.45
1:B:320:ASP:OD1	1:B:320:ASP:N	2.49	0.45
1:A:154:PHE:HB2	1:A:160:TRP:CZ3	2.52	0.45
1:A:321:LEU:HD13	1:A:352:LEU:HB3	1.97	0.45
1:A:410:ARG:HH21	1:A:425:CYS:C	2.23	0.45
1:B:229:ARG:HE	1:B:229:ARG:HB2	1.45	0.45
1:B:51:ARG:HB2	1:B:111:PHE:CE1	2.51	0.45
1:B:161:ILE:HG13	1:B:178:PHE:HD2	1.82	0.45
1:B:3:PHE:CE2	1:B:74:LEU:HD11	2.52	0.44
1:A:331:VAL:HG12	1:A:335:GLN:NE2	2.32	0.44
1:B:553:PRO:HB3	1:B:570:LYS:HB3	1.98	0.44
1:B:559:ARG:NH2	3:B:721:HOH:O	2.50	0.44
1:A:4:THR:HA	3:A:718:HOH:O	2.17	0.44
1:A:417:ASP:HB3	1:A:421:HIS:H	1.82	0.44
1:A:255:VAL:HG13	1:A:321:LEU:HG	1.98	0.44
1:A:379:PRO:HD3	1:A:394:TRP:HZ3	1.82	0.44
1:A:458:PRO:O	1:A:462:LEU:HG	2.17	0.44
1:B:296:PHE:O	1:B:298:ALA:N	2.51	0.44
1:B:132:GLN:O	1:B:135:THR:OG1	2.32	0.44
1:B:456:VAL:O	1:B:456:VAL:HG13	2.17	0.44
1:A:257:ILE:HG23	1:A:305:VAL:HG22	2.00	0.44
1:B:214:LEU:HD11	1:B:230:GLU:HG2	2.00	0.44
1:B:428:ARG:HH21	1:B:438:ASN:ND2	2.15	0.44
1:B:470:ASP:CG	1:B:559:ARG:NH1	2.65	0.44
1:B:471:ALA:HB2	1:B:559:ARG:CD	2.48	0.44
1:B:521:GLN:HB3	1:B:522:LEU:HD23	1.99	0.44
1:A:208:GLN:HB2	1:A:356:TYR:O	2.18	0.44
1:A:295:ASN:HB2	1:A:301:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:HD2	1:A:414:TRP:CD1	2.36	0.44
1:B:475:ARG:NH1	3:B:722:HOH:O	2.51	0.43
1:B:431:PHE:N	1:B:431:PHE:CD1	2.86	0.43
1:A:162:TYR:CE2	1:A:165:HIS:HB2	2.52	0.43
1:A:289:ARG:HB3	1:A:289:ARG:HE	1.74	0.43
1:A:295:ASN:HA	1:A:300:ARG:HH11	1.83	0.43
1:A:382:VAL:HG13	1:A:533:ILE:HD11	1.99	0.43
1:B:296:PHE:O	1:B:297:LYS:HB2	2.17	0.43
1:A:372:LYS:HE3	1:A:377:ASN:O	2.18	0.43
1:A:410:ARG:NH2	1:A:425:CYS:O	2.45	0.43
1:A:527:HIS:CE1	1:A:553:PRO:HD3	2.54	0.43
1:B:187:LEU:HD21	1:B:363:LEU:CG	2.39	0.43
1:A:39:LEU:HD12	1:A:39:LEU:HA	1.92	0.43
1:B:207:VAL:CG1	1:B:208:GLN:N	2.82	0.43
1:A:336:GLN:O	1:A:340:ARG:HG2	2.18	0.43
1:A:227:LEU:O	1:A:230:GLU:O	2.37	0.43
1:A:444:ALA:HA	1:A:452:ASP:OD1	2.19	0.43
1:A:136:HIS:O	1:A:139:LYS:HB2	2.19	0.42
1:A:362:ASP:HB2	1:A:365:ALA:CB	2.49	0.42
1:A:393:PHE:CG	1:A:408:GLY:HA3	2.54	0.42
1:B:257:ILE:HA	1:B:323:ALA:HB3	2.01	0.42
1:B:400:ASP:OD1	1:B:401:GLY:N	2.52	0.42
1:A:560:MET:HG2	1:A:565:TRP:CE3	2.54	0.42
1:B:494:ILE:HG12	1:B:523:PHE:CE1	2.54	0.42
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.85	0.42
1:B:179:ARG:NE	3:B:713:HOH:O	2.39	0.42
1:A:291:VAL:CG2	1:A:292:LEU:N	2.82	0.42
1:A:313:GLY:C	1:A:315:ASP:H	2.26	0.42
1:A:340:ARG:HA	1:A:340:ARG:HD3	1.89	0.42
1:B:339:GLY:HA2	1:B:342:LEU:CD1	2.49	0.42
1:B:104:LEU:HB3	1:B:136:HIS:CE1	2.55	0.42
1:A:252:ARG:HB3	1:A:320:ASP:OD1	2.19	0.42
1:A:497:TYR:HA	1:A:502:ALA:O	2.20	0.42
1:A:560:MET:HE1	1:A:563:GLN:HA	2.02	0.42
1:B:433:ASN:O	1:B:436:GLN:CA	2.63	0.41
1:A:258:PHE:CE1	1:A:337:ILE:HG12	2.55	0.41
1:B:509:ARG:O	3:B:703:HOH:O	2.22	0.41
1:A:57:HIS:ND1	1:A:97:VAL:HG21	2.35	0.41
1:A:130:TYR:OH	1:A:146:LEU:HD11	2.20	0.41
1:B:242:ILE:HD11	1:B:268:ILE:HG23	2.01	0.41
1:B:242:ILE:CD1	1:B:271:LEU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HB2	1:A:144:LEU:HB2	2.03	0.41
1:B:315:ASP:OD2	1:B:343:ARG:CZ	2.69	0.41
1:B:443:ILE:HG22	1:B:444:ALA:O	2.21	0.41
1:A:160:TRP:CZ2	1:A:171:ARG:HD2	2.55	0.41
1:A:236:ARG:NE	3:A:714:HOH:O	2.54	0.41
1:A:165:HIS:CE1	1:A:167:HIS:HB2	2.56	0.41
1:B:265:ALA:HB1	1:B:279:LEU:HD11	2.03	0.41
1:A:472:LEU:HB2	1:A:565:TRP:CZ2	2.56	0.41
1:B:201:ARG:NH1	1:B:355:ASP:HB3	2.36	0.40
1:A:48:ALA:O	1:A:91:LYS:NZ	2.53	0.40
1:A:243:SER:O	1:A:246:MET:HB2	2.21	0.40
1:A:289:ARG:C	1:A:293:ILE:HG13	2.46	0.40
1:A:291:VAL:HG23	1:A:292:LEU:H	1.86	0.40
1:B:185:LEU:HD21	1:B:190:MET:CE	2.51	0.40
1:A:129:GLN:O	1:A:132:GLN:HB2	2.20	0.40
1:A:165:HIS:ND1	1:A:167:HIS:HB2	2.36	0.40
1:B:239:PRO:HB3	1:B:271:LEU:HD22	2.03	0.40
1:B:560:MET:HE2	1:B:565:TRP:CE2	2.56	0.40
1:A:370:THR:O	1:A:394:TRP:NE1	2.37	0.40
1:B:378:VAL:HG23	1:B:379:PRO:O	2.21	0.40
1:A:164:PHE:HB3	1:A:414:TRP:NE1	2.36	0.40
1:A:246:MET:HA	1:A:303:TYR:OH	2.21	0.40
1:A:385:PRO:HG2	1:A:427:PHE:CZ	2.57	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	552/586 (94%)	492 (89%)	60 (11%)	0	100	100
1	B	558/586 (95%)	511 (92%)	47 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1110/1172 (95%)	1003 (90%)	107 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	417/491 (85%)	381 (91%)	36 (9%)	10	31
1	B	436/491 (89%)	397 (91%)	39 (9%)	9	29
All	All	853/982 (87%)	778 (91%)	75 (9%)	10	29

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	PHE
1	B	31	LEU
1	B	33	THR
1	B	77	ASP
1	B	98	GLN
1	B	112	SER
1	B	128	SER
1	B	169[A]	MET
1	B	169[B]	MET
1	B	201	ARG
1	B	213	ARG
1	B	234	GLN
1	B	237	ILE
1	B	284	THR
1	B	285	PRO
1	B	291	VAL
1	B	306[A]	ASN
1	B	306[B]	ASN
1	B	335	GLN
1	B	372	LYS

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Mol	Chain	Res	Type
1	B	374	LYS
1	B	400	ASP
1	B	415	PHE
1	B	416	GLU
1	B	417	ASP
1	B	433	ASN
1	B	462	LEU
1	B	469	LYS
1	B	470	ASP
1	B	474	LEU
1	B	475	ARG
1	B	498	ASP
1	B	499	GLU
1	B	507	ARG
1	B	515	GLN
1	B	544	LEU
1	B	547	GLN
1	B	564	TYR
1	B	569	GLU
1	A	6	ARG
1	A	38	SER
1	A	39	LEU
1	A	89	HIS
1	A	98	GLN
1	A	108	GLN
1	A	129	GLN
1	A	131	GLN
1	A	132	GLN
1	A	134	LEU
1	A	138	THR
1	A	139	LYS
1	A	156	LEU
1	A	187	LEU
1	A	188	ARG
1	A	201	ARG
1	A	202	LEU
1	A	224	GLU
1	A	236	ARG
1	A	261	THR
1	A	271	LEU
1	A	290	ASP
1	A	294	GLU

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	302	ARG
1	A	326	ARG
1	A	416	GLU
1	A	452	ASP
1	A	463	LYS
1	A	470	ASP
1	A	498	ASP
1	A	500	ASP
1	A	507	ARG
1	A	516	ARG
1	A	520	GLU
1	A	535	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	64	GLN
1	B	70	GLN
1	B	98	GLN
1	B	208	GLN
1	B	235	GLN
1	B	240	HIS
1	B	433	ASN
1	B	483	HIS
1	B	547	GLN
1	B	552	HIS
1	A	23	HIS
1	A	98	GLN
1	A	129	GLN
1	A	131	GLN
1	A	132	GLN
1	A	235	GLN
1	A	336	GLN
1	A	482	GLN
1	A	566	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	560/586 (95%)	0.38	35 (6%)	26 19	7, 41, 76, 101	2 (0%)
1	B	567/586 (96%)	0.19	20 (3%)	47 38	9, 36, 65, 90	3 (0%)
All	All	1127/1172 (96%)	0.28	55 (4%)	35 27	7, 38, 72, 101	5 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	ASP	3.8
1	B	436	GLN	3.8
1	A	444	ALA	3.6
1	B	445	ALA	3.6
1	B	433	ASN	3.5
1	A	433	ASN	3.5
1	A	435	PRO	3.4
1	A	312	THR	3.4
1	B	307	VAL	3.3
1	B	204	MET	3.3
1	A	468	LEU	3.3
1	A	203	ASP	3.1
1	A	307	VAL	3.1
1	A	229	ARG	3.1
1	A	414	TRP	3.0
1	B	308	ALA	3.0
1	A	293	ILE	2.9
1	A	231	LEU	2.9
1	B	434	CYS	2.9
1	A	283	ASP	2.8
1	A	241	ILE	2.7
1	B	451	CYS	2.6
1	B	447	ARG	2.6
1	A	265	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	314	PHE	2.6
1	A	285	PRO	2.6
1	B	312	THR	2.6
1	A	356	TYR	2.5
1	A	451	CYS	2.5
1	A	89	HIS	2.5
1	B	127	GLU	2.5
1	B	561	LYS	2.4
1	B	241	ILE	2.4
1	A	288	GLU	2.4
1	B	314	PHE	2.4
1	B	279	LEU	2.3
1	A	308	ALA	2.3
1	A	209	TYR	2.3
1	A	208	GLN	2.3
1	A	313	GLY	2.3
1	B	443	ILE	2.2
1	B	448	CYS	2.2
1	A	440	GLU	2.2
1	B	207	VAL	2.2
1	B	208	GLN	2.2
1	A	281	THR	2.2
1	B	313	GLY	2.2
1	A	284	THR	2.1
1	A	289	ARG	2.1
1	A	277	ALA	2.1
1	A	564	TYR	2.1
1	A	206	VAL	2.0
1	A	445	ALA	2.0
1	A	306	ASN	2.0
1	A	125	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	601	1/1	0.97	0.08	38,38,38,38	0
2	ZN	B	601	1/1	0.99	0.06	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.