



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 12:48 AM EST

PDB ID : 1T5L
Title : Crystal structure of the DNA repair protein UvrB point mutant Y96A revealing a novel fold for domain 2
Authors : Truglio, J.J.; Croteau, D.L.; Skorvaga, M.; DellaVecchia, M.J.; Theis, K.; Mandavilli, B.S.; Van Houten, B.; Kisker, C.
Deposited on : 2004-05-04
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

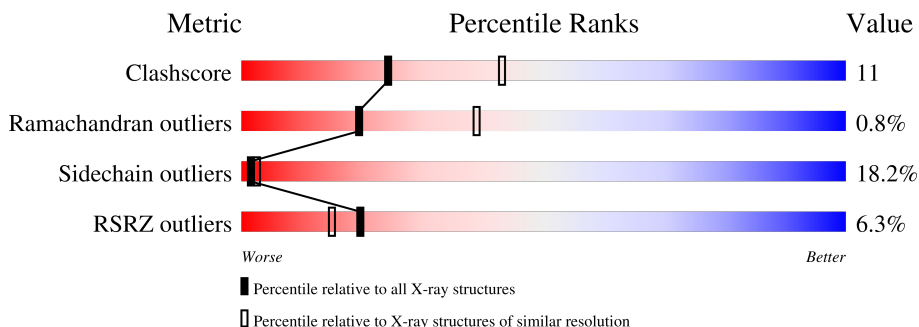
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	658	
1	B	658	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	660	-	-	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9812 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 UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4806	3027	858	909	12	0	0	0
1	B	595	4806	3027	858	909	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

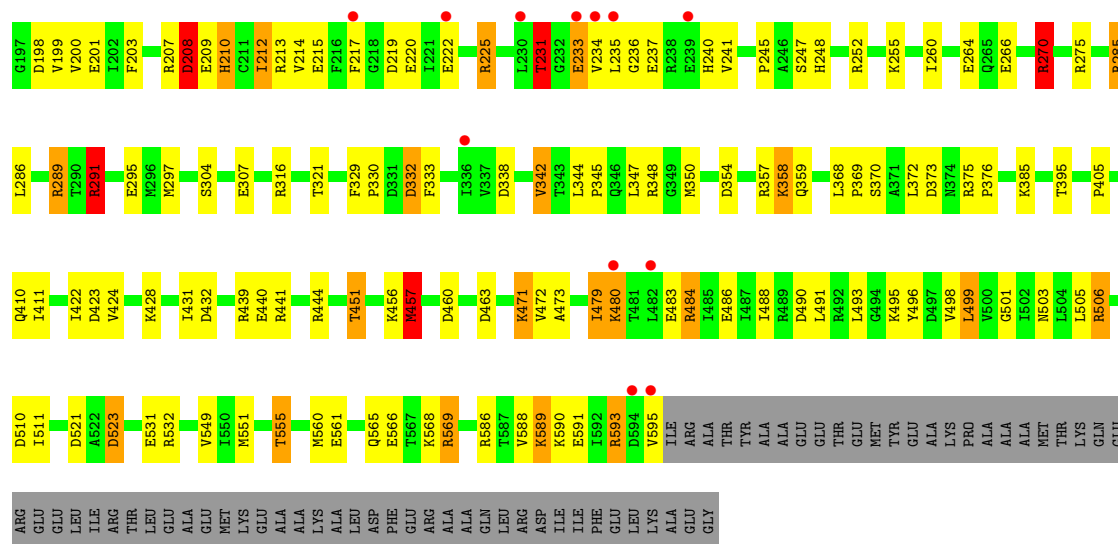
Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ARG	-	SEE REMARK 999	UNP P56981
A	233	GLU	LYS	SEE REMARK 999	UNP P56981
B	190	ARG	-	SEE REMARK 999	UNP P56981
B	233	GLU	LYS	SEE REMARK 999	UNP P56981

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		
3	B	116	Total	O	0	0
			116	116		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.81Å 150.81Å 159.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-2.60) 99.9 (24.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.60Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.230 , 0.287 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9812	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.43 % 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 8.2904e-06. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.81	1/4887 (0.0%)	1.00	20/6604 (0.3%)
1	B	0.95	1/4887 (0.0%)	1.08	28/6604 (0.4%)
All	All	0.88	2/9774 (0.0%)	1.04	48/13208 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	MET	SD-CE	5.12	2.06	1.77
1	A	457	MET	SD-CE	5.05	2.06	1.77

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	134	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	94	ASP	CB-CG-OD2	7.84	125.36	118.30
1	B	185	ASP	CB-CG-OD2	7.73	125.26	118.30
1	B	270	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	291	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	94	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	26	ASP	CB-CG-OD2	7.08	124.68	118.30
1	A	569	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	B	432	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	432	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	423	ASP	CB-CG-OD2	6.68	124.32	118.30
1	B	219	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	185	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	281	LEU	CA-CB-CG	6.27	129.72	115.30
1	B	350	MET	CG-SD-CE	6.25	110.21	100.20
1	B	208	ASP	CB-CG-OD2	6.21	123.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	LEU	CA-CB-CG	-6.17	101.11	115.30
1	B	182	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	289	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	510	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	228	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	106	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	198	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	463	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	354	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	570	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	332	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	523	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	423	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	332	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	460	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	208	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	270	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	569	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	B	112	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	373	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	338	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	111	LYS	N-CA-C	-5.24	96.84	111.00
1	B	289	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	134	ARG	CG-CD-NE	-5.16	100.96	111.80
1	B	285	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	270	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	176	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	521	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	219	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	570	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	106	ASP	CB-CG-OD2	5.02	122.82	118.30

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	4806	0	4843	105	0
1	B	4806	0	4843	108	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	80	0	0	12	0
3	B	116	0	0	11	0
All	All	9812	0	9686	213	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 11.

All (213) 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:457:MET:CE	1:A:457:MET:SD	2.06	1.44
1:B:457:MET:SD	1:B:457:MET:CE	2.06	1.42
1:B:291:ARG:O	1:B:295:GLU:HG3	1.65	0.95
1:A:60:THR:HG22	1:A:334:LEU:HB3	1.48	0.93
1:B:157:LEU:O	1:B:179:ILE:HD11	1.70	0.91
1:A:142:VAL:HG12	1:A:347:LEU:HD12	1.53	0.90
1:A:40:ALA:O	1:A:43:THR:HG22	1.74	0.87
1:A:133:ARG:HH11	1:A:133:ARG:HG3	1.41	0.83
1:A:202:ILE:O	1:A:204:PRO:HD3	1.81	0.80
1:B:67:LYS:HE2	1:B:94:ASP:OD1	1.81	0.80
1:A:395:THR:HB	1:A:532:ARG:HG2	1.63	0.80
1:A:155:ARG:O	1:A:158:VAL:HG12	1.82	0.79
1:B:589:LYS:HD2	1:B:590:LYS:H	1.48	0.78
1:A:130:LEU:O	3:A:729:HOH:O	2.02	0.77
1:A:162:ARG:HB3	3:A:733:HOH:O	1.84	0.76
1:B:115:ILE:H	1:B:115:ILE:HD13	1.51	0.75
1:B:43:THR:OG1	1:B:44:GLY:N	2.20	0.74
1:B:285:ARG:O	1:B:289:ARG:HG3	1.88	0.73
1:B:506:ARG:HG2	1:B:506:ARG:HH11	1.53	0.73
1:B:499:LEU:HD12	1:B:499:LEU:C	2.09	0.73
1:A:179:ILE:HG22	1:A:181:TYR:HD1	1.54	0.72
1:B:5:PHE:H	1:B:57:ASN:HD21	1.40	0.69
1:B:166:GLU:O	1:B:167:ILE:HG12	1.91	0.69
1:A:133:ARG:HG3	1:A:133:ARG:NH1	2.08	0.69
1:B:270:ARG:HD2	1:B:369:PRO:HD3	1.75	0.68
1:A:157:LEU:O	1:A:179:ILE:HD11	1.92	0.68
1:A:65:HIS:CD2	1:A:69:LEU:HD12	2.28	0.68
1:A:201:GLU:OE2	1:A:213:ARG:HD2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:O	1:B:192:THR:HB	1.94	0.67
1:B:162:ARG:HG3	3:B:737:HOH:O	1.93	0.67
1:A:162:ARG:HD3	3:A:733:HOH:O	1.94	0.66
1:B:395:THR:HB	1:B:532:ARG:HG2	1.76	0.66
1:A:33:LYS:HE3	1:A:34:HIS:HE2	1.59	0.66
1:B:159:VAL:HG23	1:B:179:ILE:HD12	1.78	0.65
1:B:83:HIS:HD2	3:B:767:HOH:O	1.78	0.65
1:A:224:ILE:HG21	1:A:241:VAL:HG11	1.78	0.64
1:A:509:LEU:HB2	1:A:540:ARG:HH21	1.62	0.64
1:A:484:ARG:CG	1:A:484:ARG:HH11	2.09	0.63
1:A:87:GLU:HB2	1:A:138:ILE:HG12	1.81	0.63
1:A:159:VAL:HG22	1:A:175:ARG:NH1	2.13	0.63
1:B:41:THR:HG22	3:B:760:HOH:O	1.97	0.63
1:B:97:GLN:OE1	1:B:109:ILE:HG21	1.98	0.63
1:B:566:GLU:CD	1:B:569:ARG:HH12	2.01	0.63
1:A:33:LYS:HE3	1:A:34:HIS:NE2	2.14	0.63
1:A:226:GLU:HB3	1:A:236:GLY:HA3	1.79	0.62
1:A:252:ARG:HD2	1:A:255:LYS:HD2	1.82	0.62
1:B:266:GLU:OE1	1:B:370:SER:HB3	2.00	0.61
1:B:200:VAL:HB	1:B:214:VAL:HG12	1.81	0.61
1:A:484:ARG:HH11	1:A:484:ARG:CB	2.14	0.61
1:A:289:ARG:NH1	1:A:366:PHE:O	2.33	0.60
1:B:33:LYS:HG2	1:B:34:HIS:CD2	2.37	0.60
1:B:225:ARG:HB3	1:B:236:GLY:O	2.02	0.60
1:A:49:ILE:CD1	1:A:392:VAL:HG21	2.32	0.60
1:A:12:GLU:OE2	1:A:13:PRO:HD2	2.01	0.59
1:A:316:ARG:NH2	1:A:321:THR:O	2.35	0.59
1:B:43:THR:HG21	1:B:410:GLN:HG2	1.84	0.59
1:B:179:ILE:HG23	1:B:245:PRO:HA	1.83	0.59
1:B:201:GLU:HG3	1:B:213:ARG:HG3	1.84	0.59
1:B:457:MET:CE	1:B:457:MET:HB3	2.32	0.59
1:A:521:ASP:HB3	1:A:524:LYS:HG2	1.85	0.58
1:B:270:ARG:HG2	1:B:286:LEU:CD2	2.33	0.58
1:A:507:GLU:H	1:A:507:GLU:CD	2.06	0.58
1:A:447:ARG:HD2	1:A:491:LEU:O	2.03	0.58
1:B:58:LYS:HD3	1:B:332:ASP:O	2.04	0.58
1:A:49:ILE:HD13	1:A:392:VAL:HG21	1.86	0.57
1:A:65:HIS:CD2	1:A:69:LEU:CD1	2.87	0.57
1:A:270:ARG:HD3	3:A:679:HOH:O	2.04	0.57
1:B:121:LYS:HE3	1:B:208:ASP:HB2	1.85	0.57
1:A:214:VAL:HG23	1:A:224:ILE:HG12	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:HA	1:A:194:ARG:HD3	1.85	0.57
1:A:287:GLU:OE2	1:A:291:ARG:NH1	2.38	0.57
1:B:589:LYS:HD2	1:B:590:LYS:N	2.17	0.57
1:A:39:GLY:O	1:A:45:LYS:HE3	2.05	0.57
1:A:30:ARG:HG3	3:A:723:HOH:O	2.04	0.57
1:B:260:ILE:HG12	1:B:297:MET:CE	2.34	0.57
1:A:7:LEU:HB3	3:A:671:HOH:O	2.04	0.56
1:B:551:MET:HE1	1:B:560:MET:HG2	1.88	0.56
1:B:199:VAL:HG23	1:B:215:GLU:HG2	1.89	0.55
1:B:266:GLU:HG2	1:B:368:LEU:HD22	1.88	0.55
1:B:506:ARG:HG2	1:B:506:ARG:NH1	2.20	0.55
1:A:566:GLU:OE1	1:A:569:ARG:NH1	2.40	0.55
1:B:166:GLU:C	1:B:167:ILE:HG12	2.27	0.55
1:A:12:GLU:CD	1:A:13:PRO:HD2	2.28	0.54
1:A:430:GLN:HG3	1:A:431:ILE:HD12	1.88	0.54
1:B:471:LYS:N	1:B:471:LYS:HD3	2.23	0.54
1:A:158:VAL:HG21	1:A:242:ALA:HB1	1.90	0.54
1:B:252:ARG:HD2	1:B:255:LYS:HE3	1.90	0.53
1:B:358:LYS:HB3	1:B:372:LEU:HD23	1.89	0.53
1:B:201:GLU:CG	1:B:213:ARG:HG3	2.39	0.53
1:B:498:VAL:HG12	1:B:499:LEU:N	2.23	0.53
1:B:14:GLN:O	1:B:17:GLN:HB2	2.09	0.53
1:B:67:LYS:CE	1:B:94:ASP:OD1	2.57	0.53
1:A:207:ARG:HD3	3:A:666:HOH:O	2.08	0.52
1:A:176:LEU:O	1:A:181:TYR:HB2	2.10	0.52
1:B:97:GLN:OE1	1:B:109:ILE:CG2	2.57	0.52
1:B:472:VAL:HG12	1:B:473:ALA:N	2.25	0.51
1:A:348:ARG:NH1	3:A:661:HOH:O	2.43	0.51
1:B:566:GLU:OE1	1:B:569:ARG:NH1	2.42	0.51
1:A:179:ILE:O	1:A:179:ILE:HG23	2.11	0.51
1:A:342:VAL:O	1:A:345:PRO:HD2	2.11	0.51
1:B:270:ARG:O	1:B:270:ARG:HG3	2.11	0.51
1:A:484:ARG:HH11	1:A:484:ARG:HG3	1.74	0.51
1:A:58:LYS:O	1:A:60:THR:HG23	2.11	0.50
1:A:145:ILE:O	1:A:376:PRO:HA	2.11	0.50
1:A:270:ARG:HD2	1:A:369:PRO:HD3	1.93	0.50
1:B:503:ASN:OD1	1:B:505:LEU:N	2.44	0.50
1:A:150:SER:HB3	3:A:697:HOH:O	2.11	0.50
1:B:212:ILE:HG12	1:B:241:VAL:HG21	1.94	0.50
1:B:115:ILE:HD13	1:B:115:ILE:N	2.23	0.50
1:B:40:ALA:O	1:B:43:THR:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ARG:HG2	1:B:286:LEU:HD21	1.94	0.49
1:A:484:ARG:HH11	1:A:484:ARG:HB3	1.78	0.49
1:B:479:ILE:CG2	1:B:484:ARG:HG2	2.41	0.49
1:A:395:THR:CB	1:A:532:ARG:HG2	2.37	0.49
1:B:491:LEU:HD12	1:B:496:TYR:O	2.11	0.49
1:A:17:GLN:HB2	1:A:18:PRO:HD3	1.94	0.49
1:A:185:ASP:OD2	1:A:185:ASP:N	2.46	0.49
1:B:348:ARG:NH1	3:B:666:HOH:O	2.45	0.49
1:B:160:SER:HB2	1:B:240:HIS:NE2	2.27	0.49
1:A:179:ILE:HG22	1:A:181:TYR:CD1	2.42	0.49
1:A:375:ARG:HB2	1:A:376:PRO:HD2	1.95	0.49
1:A:16:ASP:HB2	1:A:19:GLN:NE2	2.27	0.48
1:B:422:ILE:HG12	1:B:549:VAL:HB	1.95	0.48
1:A:34:HIS:O	1:A:405:PRO:HD3	2.13	0.48
1:A:141:SER:C	1:A:143:SER:H	2.16	0.48
1:B:342:VAL:O	1:B:345:PRO:HD2	2.14	0.48
1:B:270:ARG:HD2	1:B:369:PRO:CD	2.41	0.48
1:B:451:THR:HA	1:B:501:GLY:O	2.14	0.48
1:B:155:ARG:O	1:B:158:VAL:HG23	2.15	0.47
1:B:184:ASN:ND2	1:B:187:ASP:O	2.48	0.47
1:B:289:ARG:HB3	3:B:716:HOH:O	2.14	0.47
1:B:143:SER:HA	1:B:146:TYR:CE2	2.49	0.47
1:A:141:SER:C	1:A:143:SER:N	2.68	0.47
1:B:344:LEU:HB2	1:B:345:PRO:HD3	1.97	0.47
1:B:503:ASN:OD1	1:B:503:ASN:C	2.54	0.47
1:A:270:ARG:HG2	1:A:286:LEU:CD2	2.44	0.47
1:B:200:VAL:HB	1:B:214:VAL:CG1	2.44	0.47
1:A:484:ARG:NH2	1:A:506:ARG:HB2	2.31	0.46
1:A:566:GLU:CD	1:A:569:ARG:HH12	2.18	0.46
1:B:523:ASP:HB2	1:B:555:THR:HG22	1.97	0.46
1:A:229:ALA:O	1:A:230:LEU:HG	2.16	0.46
1:A:358:LYS:HB3	1:A:372:LEU:HD23	1.96	0.46
1:B:316:ARG:NH2	1:B:321:THR:O	2.48	0.46
1:B:4:ARG:NH1	1:B:57:ASN:HB2	2.31	0.46
1:B:83:HIS:CD2	3:B:767:HOH:O	2.61	0.46
1:B:94:ASP:OD2	1:B:95:TYR:N	2.49	0.46
1:B:162:ARG:CG	3:B:737:HOH:O	2.56	0.46
1:B:307:GLU:H	1:B:307:GLU:CD	2.18	0.46
1:A:201:GLU:OE2	1:A:213:ARG:CD	2.63	0.46
1:B:440:GLU:CG	3:B:770:HOH:O	2.64	0.46
1:B:275:ARG:HD2	3:B:721:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:PHE:HA	1:B:201:GLU:O	2.17	0.45
1:A:133:ARG:HH11	1:A:133:ARG:CG	2.20	0.45
1:B:210:HIS:H	1:B:210:HIS:CD2	2.34	0.45
1:A:40:ALA:O	1:A:43:THR:CG2	2.56	0.45
1:A:65:HIS:HA	3:A:688:HOH:O	2.16	0.45
1:A:342:VAL:C	1:A:345:PRO:HD2	2.37	0.45
1:A:507:GLU:N	1:A:507:GLU:OE1	2.48	0.45
1:A:32:VAL:O	1:A:388:GLN:HG2	2.17	0.45
1:B:511:ILE:HG21	1:B:511:ILE:HD13	1.66	0.45
1:A:270:ARG:O	1:A:270:ARG:HG3	2.15	0.44
1:A:49:ILE:HD11	1:A:392:VAL:CG2	2.47	0.44
1:B:142:VAL:HB	1:B:347:LEU:HD12	2.00	0.44
1:A:153:GLU:O	1:A:157:LEU:HB2	2.17	0.44
1:B:138:ILE:HD12	1:B:329:PHE:CZ	2.52	0.44
1:B:225:ARG:CB	1:B:236:GLY:O	2.65	0.44
1:B:593:ARG:H	1:B:593:ARG:HG2	1.65	0.44
1:B:499:LEU:C	1:B:499:LEU:CD1	2.83	0.44
1:B:375:ARG:HB2	1:B:376:PRO:HD2	1.99	0.43
1:A:148:LEU:HD23	1:A:328:TYR:CE1	2.54	0.43
1:B:480:LYS:HB2	1:B:483:GLU:H	1.83	0.43
1:A:171:ALA:O	1:A:175:ARG:HG2	2.19	0.43
1:B:161:LEU:HD21	1:B:172:LEU:HD13	2.01	0.43
1:A:192:THR:HG22	1:A:193:PHE:N	2.34	0.43
1:A:179:ILE:CG2	1:A:181:TYR:CD1	3.02	0.43
1:B:472:VAL:HG12	1:B:473:ALA:H	1.83	0.42
1:A:475:LEU:HD11	1:A:484:ARG:HD2	2.01	0.42
1:A:171:ALA:O	1:A:175:ARG:CG	2.67	0.42
1:A:498:VAL:HG12	1:A:499:LEU:N	2.34	0.42
1:B:17:GLN:O	1:B:21:ILE:HG13	2.19	0.42
1:B:196:ARG:O	1:B:199:VAL:HG12	2.19	0.42
1:A:189:ARG:O	1:A:192:THR:HB	2.19	0.42
1:B:207:ARG:NH1	1:B:210:HIS:O	2.53	0.42
1:A:134:ARG:HG2	3:A:732:HOH:O	2.19	0.42
1:B:87:GLU:HB3	3:B:683:HOH:O	2.18	0.42
1:B:270:ARG:HD3	3:B:671:HOH:O	2.19	0.42
1:A:65:HIS:NE2	1:A:69:LEU:HD11	2.35	0.42
1:A:92:TYR:O	1:A:96:ALA:HB3	2.20	0.42
1:A:333:PHE:H	1:A:333:PHE:HD2	1.68	0.42
1:A:524:LYS:HD3	1:A:524:LYS:HA	1.62	0.42
1:B:59:PRO:HG3	1:B:330:PRO:HG2	2.01	0.42
1:A:307:GLU:H	1:A:307:GLU:CD	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:OE1	1:A:367:ARG:NE	2.45	0.41
1:B:2:GLU:HB3	1:B:134:ARG:HG3	2.03	0.41
1:B:266:GLU:OE1	1:B:370:SER:CB	2.69	0.41
1:A:43:THR:OG1	1:A:44:GLY:N	2.53	0.41
1:B:252:ARG:CD	1:B:255:LYS:HE3	2.51	0.41
1:A:4:ARG:HB2	1:A:57:ASN:OD1	2.21	0.41
1:B:252:ARG:NE	1:B:255:LYS:HE3	2.36	0.41
1:A:224:ILE:HG21	1:A:241:VAL:CG1	2.46	0.41
1:A:406:GLY:N	3:A:722:HOH:O	2.52	0.41
1:B:87:GLU:OE1	1:B:125:SER:HB2	2.21	0.41
1:B:149:GLY:HA3	1:B:248:HIS:O	2.21	0.41
1:B:252:ARG:HE	1:B:255:LYS:HE3	1.85	0.41
1:B:405:PRO:HG2	1:B:405:PRO:O	2.21	0.41
1:A:188:PHE:HB2	1:A:194:ARG:NH1	2.35	0.41
1:A:346:GLN:O	1:A:350:MET:HG2	2.21	0.41
1:A:419:ASP:O	1:A:571:ARG:NH1	2.48	0.40
1:A:491:LEU:HD22	1:A:499:LEU:HD13	2.03	0.40
1:B:148:LEU:HA	1:B:148:LEU:HD12	1.72	0.40
1:A:183:ARG:NH1	1:A:195:VAL:HG11	2.37	0.40
1:B:231:THR:HB	1:B:233:GLU:H	1.86	0.40
1:B:488:ILE:HG23	1:B:511:ILE:HD11	2.04	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	593/658 (90%)	552 (93%)	37 (6%)	4 (1%)	22	43
1	B	593/658 (90%)	565 (95%)	23 (4%)	5 (1%)	19	39
All	All	1186/1316 (90%)	1117 (94%)	60 (5%)	9 (1%)	19	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASP
1	B	115	ILE
1	B	186	ILE
1	A	113	ALA
1	A	237	GLU
1	B	113	ALA
1	A	477	SER
1	B	114	LYS
1	B	231	THR

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	521/569 (92%)	419 (80%)	102 (20%)	1 2
1	B	521/569 (92%)	433 (83%)	88 (17%)	2 3
All	All	1042/1138 (92%)	852 (82%)	190 (18%)	1 2

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	4	ARG
1	A	12	GLU
1	A	19	GLN
1	A	23	LYS
1	A	43	THR
1	A	49	ILE
1	A	62	VAL
1	A	67	LYS
1	A	72	GLN
1	A	75	SER
1	A	92	TYR
1	A	93	TYR
1	A	94	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	GLN
1	A	105	THR
1	A	107	THR
1	A	110	GLU
1	A	114	LYS
1	A	115	ILE
1	A	118	GLU
1	A	120	ASP
1	A	128	SER
1	A	132	GLU
1	A	133	ARG
1	A	134	ARG
1	A	155	ARG
1	A	166	GLU
1	A	167	ILE
1	A	169	ARG
1	A	172	LEU
1	A	179	ILE
1	A	180	GLN
1	A	185	ASP
1	A	186	ILE
1	A	189	ARG
1	A	203	PHE
1	A	208	ASP
1	A	210	HIS
1	A	212	ILE
1	A	213	ARG
1	A	214	VAL
1	A	217	PHE
1	A	219	ASP
1	A	220	GLU
1	A	225	ARG
1	A	226	GLU
1	A	235	LEU
1	A	237	GLU
1	A	238	ARG
1	A	239	GLU
1	A	247	SER
1	A	281	LEU
1	A	288	GLN
1	A	300	MET
1	A	304	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	326	LEU
1	A	333	PHE
1	A	336	ILE
1	A	342	VAL
1	A	347	LEU
1	A	358	LYS
1	A	385	LYS
1	A	411	ILE
1	A	415	THR
1	A	424	VAL
1	A	428	LYS
1	A	441	ARG
1	A	444	ARG
1	A	451	THR
1	A	455	LYS
1	A	456	LYS
1	A	464	TYR
1	A	471	LYS
1	A	472	VAL
1	A	477	SER
1	A	478	GLU
1	A	479	ILE
1	A	480	LYS
1	A	481	THR
1	A	482	LEU
1	A	484	ARG
1	A	486	GLU
1	A	489	ARG
1	A	493	LEU
1	A	495	LYS
1	A	499	LEU
1	A	506	ARG
1	A	507	GLU
1	A	520	LEU
1	A	524	LYS
1	A	540	ARG
1	A	543	ARG
1	A	558	LYS
1	A	561	GLU
1	A	565	GLN
1	A	568	LYS
1	A	586	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	588	VAL
1	A	591	GLU
1	A	592	ILE
1	A	594	ASP
1	B	12	GLU
1	B	19	GLN
1	B	43	THR
1	B	45	LYS
1	B	57	ASN
1	B	62	VAL
1	B	72	GLN
1	B	75	SER
1	B	91	SER
1	B	92	TYR
1	B	93	TYR
1	B	94	ASP
1	B	97	GLN
1	B	104	GLN
1	B	110	GLU
1	B	111	LYS
1	B	114	LYS
1	B	115	ILE
1	B	120	ASP
1	B	125	SER
1	B	132	GLU
1	B	133	ARG
1	B	134	ARG
1	B	155	ARG
1	B	162	ARG
1	B	166	GLU
1	B	169	ARG
1	B	179	ILE
1	B	183	ARG
1	B	187	ASP
1	B	196	ARG
1	B	198	ASP
1	B	203	PHE
1	B	208	ASP
1	B	209	GLU
1	B	210	HIS
1	B	212	ILE
1	B	217	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	220	GLU
1	B	222	GLU
1	B	225	ARG
1	B	231	THR
1	B	233	GLU
1	B	234	VAL
1	B	235	LEU
1	B	237	GLU
1	B	247	SER
1	B	264	GLU
1	B	270	ARG
1	B	291	ARG
1	B	304	SER
1	B	333	PHE
1	B	342	VAL
1	B	357	ARG
1	B	358	LYS
1	B	359	GLN
1	B	385	LYS
1	B	411	ILE
1	B	424	VAL
1	B	428	LYS
1	B	431	ILE
1	B	439	ARG
1	B	441	ARG
1	B	444	ARG
1	B	451	THR
1	B	456	LYS
1	B	457	MET
1	B	471	LYS
1	B	479	ILE
1	B	480	LYS
1	B	484	ARG
1	B	486	GLU
1	B	490	ASP
1	B	493	LEU
1	B	495	LYS
1	B	499	LEU
1	B	506	ARG
1	B	531	GLU
1	B	555	THR
1	B	561	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	565	GLN
1	B	568	LYS
1	B	586	ARG
1	B	588	VAL
1	B	589	LYS
1	B	591	GLU
1	B	593	ARG
1	B	595	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	97	GLN
1	A	210	HIS
1	A	277	GLN
1	A	536	GLN
1	B	57	ASN
1	B	210	HIS
1	B	288	GLN
1	B	346	GLN
1	B	536	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](#)

Of 4 ligands modelled in this entry, 4 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	595/658 (90%)	0.20	46 (7%) 13 10	29, 59, 161, 211	0
1	B	595/658 (90%)	-0.09	29 (4%) 29 23	26, 45, 98, 113	0
All	All	1190/1316 (90%)	0.05	75 (6%) 20 15	26, 53, 131, 211	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	8.9
1	A	95	TYR	8.1
1	B	95	TYR	7.7
1	A	230	LEU	7.3
1	A	93	TYR	5.5
1	A	595	VAL	5.4
1	A	217	PHE	5.0
1	A	223	ARG	4.8
1	B	94	ASP	4.5
1	A	112	ASP	4.4
1	B	217	PHE	4.3
1	A	186	ILE	4.3
1	A	202	ILE	4.2
1	A	231	THR	4.2
1	A	214	VAL	4.0
1	B	114	LYS	3.9
1	A	229	ALA	3.7
1	B	234	VAL	3.7
1	B	235	LEU	3.7
1	A	2	GLU	3.7
1	A	183	ARG	3.5
1	A	237	GLU	3.5
1	A	9	ALA	3.2
1	A	208	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	3.1
1	A	189	ARG	3.1
1	B	595	VAL	3.0
1	A	10	PRO	2.9
1	A	94	ASP	2.9
1	A	235	LEU	2.8
1	A	593	ARG	2.8
1	A	480	LYS	2.8
1	B	482	LEU	2.8
1	A	187	ASP	2.7
1	B	594	ASP	2.7
1	A	83	HIS	2.7
1	A	209	GLU	2.7
1	A	238	ARG	2.7
1	B	104	GLN	2.6
1	B	222	GLU	2.6
1	A	114	LYS	2.6
1	B	163	VAL	2.6
1	A	170	ASN	2.6
1	A	197	GLY	2.6
1	B	187	ASP	2.6
1	A	225	ARG	2.5
1	A	477	SER	2.5
1	A	113	ALA	2.5
1	B	480	LYS	2.4
1	B	113	ALA	2.4
1	A	171	ALA	2.4
1	B	195	VAL	2.4
1	A	200	VAL	2.4
1	B	107	THR	2.4
1	B	102	VAL	2.4
1	A	337	VAL	2.3
1	A	116	ASN	2.3
1	A	115	ILE	2.3
1	B	239	GLU	2.2
1	B	117	ASP	2.2
1	B	115	ILE	2.2
1	B	1	VAL	2.2
1	A	204	PRO	2.2
1	A	594	ASP	2.2
1	B	164	GLY	2.2
1	A	336	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2	GLU	2.2
1	A	174	ARG	2.2
1	B	183	ARG	2.1
1	B	336	ILE	2.1
1	B	93	TYR	2.1
1	B	230	LEU	2.1
1	A	450	VAL	2.0
1	B	233	GLU	2.0
1	A	165	MET	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 [\(i\)](#)

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(Å ²)	Q<0.9
2	ZN	A	660	1/1	0.72	0.90	89,89,89,89	1
2	ZN	B	660	1/1	0.80	0.19	72,72,72,72	1
2	ZN	A	659	1/1	0.93	0.11	87,87,87,87	0
2	ZN	B	659	1/1	0.97	0.13	83,83,83,83	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.