



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:52 AM UTC

PDB ID : 9PI5 / pdb_00009pi5
Title : Poly dA bound form of Single stranded DNA-binding protein(ICP8) from Herpes simplex virus-1. Mutations: C254S, C455S
Authors : Erlandsen, H.; Wright, D.
Deposited on : 2025-07-10
Resolution : 3.00 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

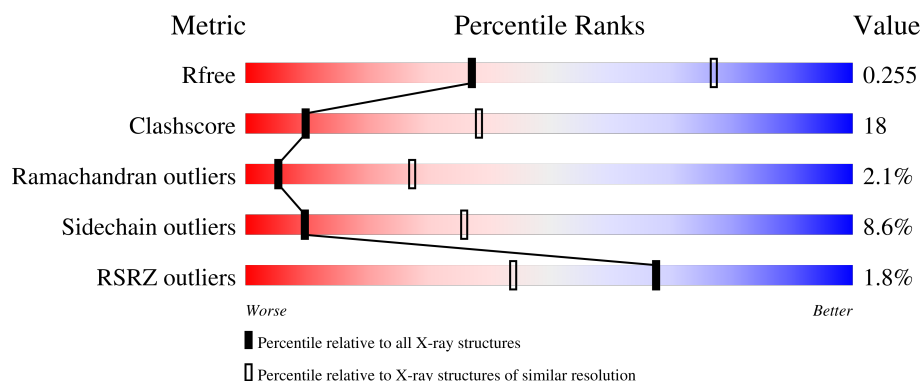
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1127	
2	G	8	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8231 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 Major DNA-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1057	Total	C	N	O	S	0	1	0
			8063	5094	1432	1490	47			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	SER	conflict	UNP P04296
A	224	ASN	LYS	conflict	UNP P04296
A	254	SER	CYS	engineered mutation	UNP P04296
A	306	PRO	ALA	conflict	UNP P04296
A	348	CYS	PHE	conflict	UNP P04296
A	455	SER	CYS	engineered mutation	UNP P04296
A	1039	ASN	SER	conflict	UNP P04296

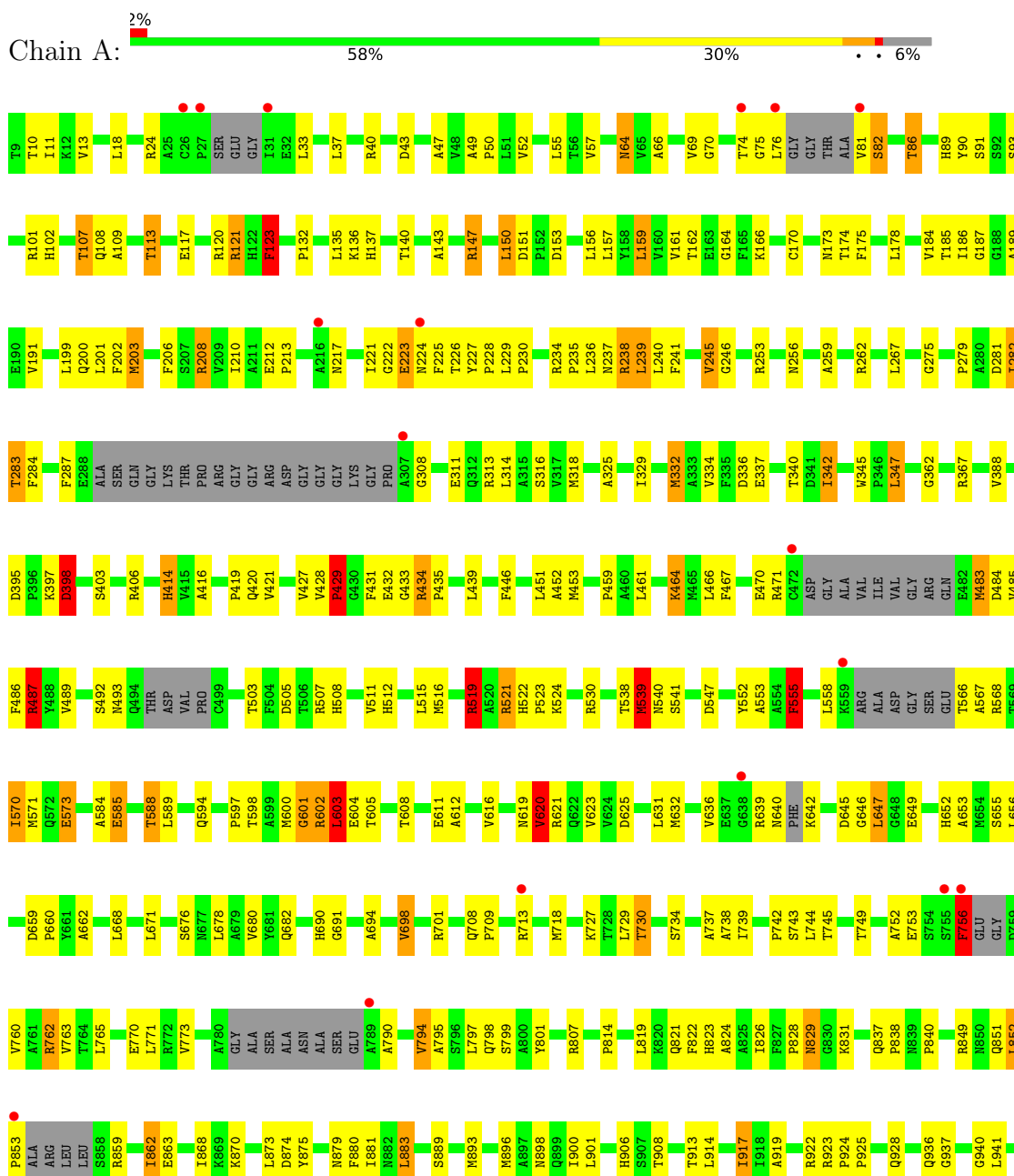
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*A)-3').

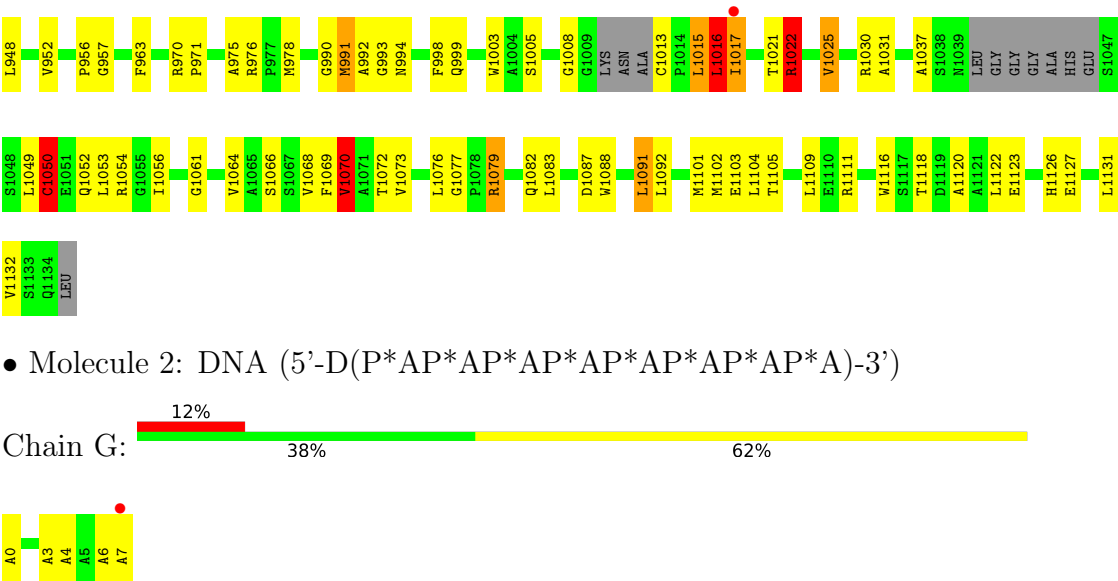
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			168	80	40	40	8			

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: Major DNA-binding protein





● Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.17Å 151.17Å 154.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	130.92 – 3.00 130.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (130.92-3.00) 100.0 (130.92-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.126), PDB-REDO 8.20	Depositor
R, R_{free}	0.200 , 0.238 0.205 , 0.255	Depositor DCC
R_{free} test set	2119 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 103.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8231	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.333 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	0.64	2/8230 (0.0%)	1.03	16/11168 (0.1%)
2	G	0.28	0/191	1.00	0/292
All	All	0.63	2/8421 (0.0%)	1.03	16/11460 (0.1%)

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	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CA-CB	5.82	1.56	1.52
1	A	453	MET	SD-CE	5.26	1.92	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	LEU	N-CA-C	-6.88	101.45	110.33
1	A	555	PHE	CA-CB-CG	6.75	120.56	113.80
1	A	1070	VAL	N-CA-CB	5.98	117.55	110.55
1	A	756	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	123	PHE	N-CA-C	-5.55	101.49	110.32
1	A	217	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	645	ASP	N-CA-C	-5.26	103.53	110.43
1	A	151	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	770	GLU	N-CA-C	5.10	116.59	108.79
1	A	647	LEU	N-CA-C	-5.10	105.36	112.45
1	A	620	VAL	N-CA-C	-5.09	105.58	110.72
1	A	653	ALA	N-CA-C	5.07	116.55	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	539	MET	CB-CA-C	5.06	120.12	111.68
1	A	398	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	659	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	1022	ARG	Sidechain
1	A	1030	ARG	Sidechain
1	A	1079	ARG	Sidechain
1	A	121	ARG	Sidechain
1	A	147	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	406	ARG	Sidechain
1	A	434	ARG	Sidechain
1	A	487	ARG	Sidechain
1	A	519	ARG	Sidechain
1	A	521	ARG	Sidechain
1	A	530	ARG	Sidechain
1	A	701	ARG	Sidechain
1	A	713[A]	ARG	Sidechain
1	A	762	ARG	Sidechain
1	A	807	ARG	Sidechain
1	A	859	ARG	Sidechain
1	A	922	ARG	Sidechain
1	A	923	ARG	Sidechain

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	8063	0	7964	281	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	168	0	89	4	0
All	All	8231	0	8053	284	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 18.

All (284) 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:652:HIS:CG	1:A:914:LEU:HD11	2.10	0.85
1:A:170:CYS:HA	1:A:237:ASN:OD1	1.79	0.81
1:A:519:ARG:HG3	1:A:519:ARG:HH11	1.47	0.77
1:A:1022:ARG:HG3	1:A:1022:ARG:HH11	1.50	0.76
1:A:485:VAL:O	1:A:489:VAL:HG23	1.87	0.75
1:A:1088:TRP:O	1:A:1092:LEU:HD12	1.88	0.74
1:A:555:PHE:CD1	1:A:570:ILE:HD11	2.23	0.73
1:A:140:THR:HG23	1:A:143:ALA:HB2	1.71	0.73
1:A:1050:CYS:O	1:A:1054:ARG:HG2	1.89	0.72
1:A:1069:PHE:O	1:A:1073:VAL:HG23	1.90	0.71
1:A:573:GLU:OE1	1:A:573:GLU:HA	1.91	0.70
1:A:117:GLU:O	1:A:121:ARG:HG3	1.92	0.70
1:A:519:ARG:HH11	1:A:519:ARG:CG	2.04	0.69
1:A:175:PHE:HD2	1:A:199:LEU:HD23	1.58	0.68
1:A:332:MET:HE2	1:A:332:MET:HA	1.74	0.68
1:A:519:ARG:HG3	1:A:519:ARG:NH1	2.09	0.67
1:A:801:TYR:CE1	1:A:1021:THR:HG22	2.30	0.67
1:A:862:ILE:HD12	1:A:863:GLU:N	2.09	0.67
1:A:200:GLN:OE1	1:A:210:ILE:HD12	1.94	0.67
1:A:483:MET:HE3	1:A:516:MET:HG2	1.76	0.67
1:A:1003:TRP:HZ2	1:A:1025:VAL:HG22	1.60	0.65
1:A:471:ARG:NH1	1:A:957:GLY:O	2.30	0.65
1:A:340:THR:HB	1:A:345:TRP:HE1	1.63	0.64
1:A:1122:LEU:O	1:A:1126:HIS:CD2	2.50	0.64
1:A:140:THR:HG23	1:A:143:ALA:CB	2.29	0.63
1:A:239:LEU:O	1:A:240:LEU:HB2	1.97	0.62
1:A:147:ARG:CZ	1:A:178:LEU:HD23	2.28	0.61
1:A:159:LEU:CD2	1:A:161:VAL:HG22	2.30	0.61
1:A:203:MET:HE2	1:A:206:PHE:CD2	2.35	0.61
1:A:831:LYS:HG2	1:A:838:PRO:N	2.14	0.61
1:A:948:LEU:C	1:A:948:LEU:HD23	2.24	0.61
1:A:55:LEU:HB2	1:A:342:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:CD2	1:A:698:VAL:HG23	2.30	0.61
1:A:159:LEU:HD22	1:A:161:VAL:HG22	1.82	0.61
1:A:824:ALA:O	1:A:828:PRO:HA	2.01	0.60
1:A:259:ALA:HB1	1:A:279:PRO:HG3	1.82	0.60
1:A:602:ARG:O	1:A:604:GLU:N	2.35	0.60
1:A:1073:VAL:HG13	1:A:1116:TRP:HZ2	1.66	0.60
1:A:90:TYR:HA	1:A:162:THR:HA	1.84	0.60
1:A:505:ASP:O	1:A:508:HIS:CE1	2.54	0.60
1:A:203:MET:HE2	1:A:206:PHE:CE2	2.38	0.59
1:A:397:LYS:O	1:A:398:ASP:C	2.46	0.59
1:A:434:ARG:HD3	1:A:435:PRO:HD2	1.84	0.58
1:A:512:HIS:CE1	1:A:516:MET:HE3	2.38	0.58
1:A:862:ILE:HD12	1:A:862:ILE:C	2.28	0.58
1:A:81:VAL:HG13	1:A:82:SER:H	1.68	0.58
1:A:914:LEU:CD2	1:A:1003:TRP:CH2	2.86	0.58
1:A:1111:ARG:HB3	1:A:1120:ALA:HB1	1.86	0.58
1:A:159:LEU:HD12	1:A:236:LEU:HD11	1.85	0.58
1:A:616:VAL:O	1:A:620:VAL:HG13	2.03	0.58
1:A:914:LEU:CD2	1:A:1003:TRP:CZ3	2.88	0.57
1:A:64:ASN:OD1	1:A:334:VAL:CG1	2.53	0.57
1:A:570:ILE:C	1:A:570:ILE:HD12	2.30	0.57
1:A:762:ARG:O	1:A:763:VAL:HG12	2.04	0.57
1:A:632:MET:O	1:A:636:VAL:HG23	2.04	0.57
1:A:647:LEU:HD21	1:A:901:LEU:HD23	1.85	0.57
1:A:428:VAL:HB	1:A:429:PRO:HD2	1.85	0.57
1:A:570:ILE:HD12	1:A:571:MET:N	2.19	0.57
1:A:221:ILE:HG22	1:A:222:GLY:O	2.04	0.56
1:A:282:ILE:HD13	1:A:283:THR:N	2.19	0.56
1:A:503:THR:O	1:A:507:ARG:HG3	2.04	0.56
1:A:147:ARG:NE	1:A:178:LEU:HD23	2.20	0.56
1:A:602:ARG:O	1:A:605:THR:N	2.35	0.56
1:A:318:MET:HA	1:A:708:GLN:HE22	1.71	0.56
2:G:6:DA:H2"	2:G:7:DA:OP1	2.04	0.56
1:A:829:ASN:HA	1:A:831:LYS:NZ	2.21	0.56
1:A:829:ASN:HA	1:A:831:LYS:HZ2	1.71	0.55
1:A:852:LEU:HD12	1:A:853:PRO:HD2	1.87	0.55
1:A:24:ARG:HB3	1:A:191:VAL:HG12	1.88	0.55
1:A:1015:LEU:O	1:A:1017:ILE:HD13	2.06	0.55
1:A:568:ARG:HA	1:A:568:ARG:NE	2.21	0.55
1:A:936:GLN:HE21	1:A:940:GLY:CA	2.20	0.55
1:A:1015:LEU:HD23	1:A:1016:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:ALA:HB1	2:G:0:DA:H4'	1.89	0.55
1:A:140:THR:CG2	1:A:143:ALA:HB2	2.36	0.55
1:A:875:TYR:HE2	1:A:879:ASN:HD22	1.54	0.55
1:A:107:THR:CG2	1:A:470:GLU:OE2	2.55	0.55
1:A:584:ALA:HA	1:A:594:GLN:NE2	2.22	0.54
1:A:849:ARG:O	1:A:851:GLN:HG3	2.08	0.54
1:A:64:ASN:OD1	1:A:334:VAL:HG13	2.07	0.54
1:A:282:ILE:HD13	1:A:283:THR:H	1.73	0.54
1:A:597:PRO:HG3	1:A:971:PRO:HG2	1.87	0.54
1:A:730:THR:HA	1:A:763:VAL:O	2.07	0.54
1:A:484:ASP:HA	1:A:928:GLN:HE22	1.72	0.54
1:A:175:PHE:CD2	1:A:199:LEU:HD23	2.42	0.54
1:A:446:PHE:HB3	1:A:522:HIS:CD2	2.43	0.54
1:A:313:ARG:O	1:A:316:SER:HB3	2.07	0.53
1:A:521:ARG:O	1:A:522:HIS:C	2.51	0.53
1:A:540:ASN:O	1:A:976:ARG:HD2	2.08	0.53
1:A:822:PHE:HB2	1:A:826:ILE:HD11	1.90	0.53
1:A:1073:VAL:CG1	1:A:1116:TRP:HZ2	2.21	0.53
2:G:3:DA:H2''	2:G:4:DA:OP2	2.07	0.53
1:A:150:LEU:HD12	1:A:150:LEU:N	2.24	0.53
1:A:367:ARG:O	1:A:919:ALA:HB1	2.08	0.53
1:A:880:PHE:CD2	1:A:906:HIS:HD2	2.26	0.53
1:A:464:LYS:O	1:A:467:PHE:HB3	2.08	0.53
1:A:538:THR:HG22	1:A:978:MET:HG2	1.91	0.53
1:A:1118:THR:O	1:A:1122:LEU:HD12	2.08	0.53
1:A:538:THR:HG21	1:A:662:ALA:O	2.09	0.52
1:A:164:GLY:HA3	1:A:332:MET:HE3	1.92	0.52
1:A:229:LEU:C	1:A:229:LEU:HD23	2.35	0.52
1:A:879:ASN:OD1	1:A:881:ILE:N	2.42	0.52
1:A:831:LYS:HG2	1:A:837:GLN:C	2.34	0.52
1:A:734:SER:O	1:A:737:ALA:HB2	2.10	0.51
1:A:1061:GLY:O	1:A:1064:VAL:HG23	2.10	0.51
1:A:539:MET:HE2	1:A:655:SER:H	1.75	0.51
1:A:49:ALA:O	1:A:93:SER:HB2	2.11	0.51
1:A:1022:ARG:HG3	1:A:1022:ARG:NH1	2.24	0.51
2:G:7:DA:H2'	2:G:7:DA:N3	2.26	0.51
1:A:708:GLN:N	1:A:709:PRO:CD	2.73	0.51
1:A:238:ARG:C	1:A:239:LEU:O	2.51	0.51
1:A:573:GLU:OE2	1:A:631:LEU:HA	2.10	0.51
1:A:936:GLN:HE21	1:A:940:GLY:HA3	1.75	0.50
1:A:64:ASN:N	1:A:64:ASN:HD22	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:O	1:A:225:PHE:N	2.44	0.50
1:A:970:ARG:HB3	1:A:971:PRO:HD3	1.94	0.50
1:A:1049:LEU:O	1:A:1050:CYS:C	2.55	0.50
1:A:821:GLN:HG2	1:A:822:PHE:CE2	2.46	0.50
1:A:917:ILE:HG22	1:A:963:PHE:CD1	2.47	0.50
1:A:1088:TRP:CE3	1:A:1101:MET:HG3	2.47	0.50
1:A:403:SER:HB2	1:A:690:HIS:ND1	2.27	0.50
1:A:1076:LEU:HB3	1:A:1079:ARG:HB2	1.94	0.50
1:A:234:ARG:HB2	1:A:235:PRO:HD3	1.94	0.50
1:A:539:MET:SD	1:A:539:MET:C	2.94	0.50
1:A:159:LEU:HD22	1:A:161:VAL:CG2	2.41	0.49
1:A:113:THR:HA	1:A:459:PRO:HG3	1.94	0.49
1:A:362:GLY:HA3	1:A:956:PRO:O	2.11	0.49
1:A:1076:LEU:O	1:A:1077:GLY:C	2.55	0.49
1:A:1053:LEU:HD12	1:A:1091:LEU:HD12	1.94	0.49
1:A:69:VAL:HG11	1:A:86:THR:HG22	1.94	0.49
1:A:466:LEU:O	1:A:470:GLU:HG3	2.13	0.49
1:A:879:ASN:HA	1:A:898:ASN:ND2	2.27	0.49
1:A:18:LEU:C	1:A:18:LEU:HD12	2.37	0.49
1:A:585:GLU:O	1:A:589:LEU:HD12	2.13	0.49
1:A:639:ARG:O	1:A:640:ASN:C	2.56	0.49
1:A:336:ASP:O	1:A:337:GLU:C	2.55	0.48
1:A:1053:LEU:HD22	1:A:1068:VAL:HG13	1.95	0.48
1:A:52:VAL:HG23	1:A:340:THR:OG1	2.13	0.48
1:A:975:ALA:HA	1:A:1031:ALA:HB3	1.95	0.48
1:A:185:THR:HA	1:A:189:ALA:O	2.13	0.48
1:A:585:GLU:O	1:A:588:THR:HB	2.14	0.48
1:A:555:PHE:CD1	1:A:555:PHE:C	2.90	0.48
1:A:870:LYS:HE2	1:A:874:ASP:OD2	2.13	0.48
1:A:489:VAL:HG21	1:A:941:LEU:CD2	2.44	0.48
1:A:484:ASP:CG	1:A:487:ARG:HB2	2.39	0.48
1:A:69:VAL:HG11	1:A:86:THR:CG2	2.44	0.48
1:A:267:LEU:HD13	1:A:325:ALA:HA	1.96	0.48
1:A:1082:GLN:O	1:A:1083:LEU:C	2.57	0.48
1:A:40:ARG:HG3	1:A:47:ALA:HB2	1.95	0.47
1:A:70:GLY:HA2	1:A:201:LEU:HA	1.95	0.47
1:A:157:LEU:N	1:A:157:LEU:HD12	2.29	0.47
1:A:240:LEU:O	1:A:245:VAL:HG23	2.13	0.47
1:A:420:GLN:HB2	1:A:431:PHE:CE2	2.49	0.47
1:A:896:MET:O	1:A:900:ILE:HG13	2.15	0.47
1:A:161:VAL:HG11	1:A:166:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:MET:CE	1:A:206:PHE:CE2	2.97	0.47
1:A:1079:ARG:HA	1:A:1082:GLN:OE1	2.15	0.47
1:A:223:GLU:OE1	1:A:223:GLU:N	2.48	0.47
1:A:523:PRO:O	1:A:524:LYS:HD3	2.14	0.47
1:A:284:PHE:CG	1:A:313:ARG:HD2	2.50	0.47
1:A:600:MET:O	1:A:601:GLY:C	2.57	0.47
1:A:10:THR:HA	1:A:730:THR:O	2.15	0.47
1:A:552:TYR:O	1:A:553:ALA:C	2.57	0.47
1:A:602:ARG:O	1:A:603:LEU:C	2.58	0.47
1:A:727:LYS:HE2	1:A:729:LEU:HD21	1.97	0.46
1:A:991:MET:SD	1:A:992:ALA:N	2.75	0.46
1:A:102:HIS:NE2	1:A:153:ASP:O	2.39	0.46
1:A:948:LEU:C	1:A:948:LEU:CD2	2.88	0.46
1:A:879:ASN:OD1	1:A:879:ASN:C	2.58	0.46
1:A:222:GLY:HA3	1:A:225:PHE:CE2	2.50	0.46
1:A:822:PHE:O	1:A:823:HIS:C	2.59	0.46
1:A:57:VAL:C	1:A:186:ILE:HD12	2.40	0.46
1:A:883:LEU:HD22	1:A:913:THR:HG21	1.98	0.46
1:A:1105:THR:O	1:A:1109:LEU:HD23	2.15	0.46
1:A:156:LEU:C	1:A:156:LEU:HD23	2.40	0.46
1:A:566:THR:O	1:A:567:ALA:HB3	2.15	0.46
1:A:814:PRO:HB3	1:A:875:TYR:CD2	2.51	0.46
1:A:998:PHE:C	1:A:999:GLN:HG3	2.41	0.46
1:A:226:THR:OG1	1:A:745:THR:O	2.32	0.46
1:A:991:MET:HE3	1:A:994:ASN:N	2.30	0.46
1:A:676:SER:O	1:A:680:VAL:HG23	2.16	0.45
1:A:1003:TRP:CZ2	1:A:1025:VAL:HG22	2.47	0.45
1:A:1016:LEU:H	1:A:1016:LEU:HD23	1.82	0.45
1:A:619:ASN:O	1:A:623:VAL:HG23	2.17	0.45
1:A:823:HIS:HB2	1:A:840:PRO:HB3	1.97	0.45
1:A:555:PHE:CD1	1:A:570:ILE:CD1	2.98	0.45
1:A:1073:VAL:HG13	1:A:1116:TRP:CZ2	2.50	0.45
1:A:210:ILE:HG21	1:A:213:PRO:HA	1.98	0.45
1:A:873:LEU:HD23	1:A:873:LEU:C	2.42	0.45
1:A:1111:ARG:HH11	1:A:1111:ARG:HG2	1.81	0.45
1:A:558:LEU:N	1:A:558:LEU:HD23	2.32	0.45
1:A:237:ASN:O	1:A:241:PHE:HB2	2.16	0.45
1:A:519:ARG:HA	1:A:522:HIS:CE1	2.52	0.45
1:A:132:PRO:HA	1:A:135:LEU:CD1	2.46	0.45
1:A:568:ARG:HA	1:A:568:ARG:CZ	2.47	0.45
1:A:646:GLY:HA2	1:A:649:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD13	1:A:161:VAL:CG2	2.47	0.44
1:A:466:LEU:HD11	1:A:511:VAL:HG22	1.98	0.44
1:A:428:VAL:O	1:A:429:PRO:C	2.60	0.44
1:A:52:VAL:HG12	1:A:55:LEU:HB3	2.00	0.44
1:A:652:HIS:CG	1:A:914:LEU:CD1	2.93	0.44
1:A:1068:VAL:HG11	1:A:1092:LEU:HD21	1.99	0.44
1:A:1118:THR:O	1:A:1122:LEU:CD1	2.65	0.44
1:A:1053:LEU:HA	1:A:1056:ILE:HD12	1.98	0.44
1:A:284:PHE:CD1	1:A:313:ARG:HD2	2.53	0.44
1:A:419:PRO:HA	1:A:431:PHE:CD1	2.53	0.44
1:A:120:ARG:O	1:A:123:PHE:O	2.35	0.44
1:A:225:PHE:CE1	1:A:744:LEU:HD23	2.53	0.44
1:A:227:TYR:HA	1:A:228:PRO:HD3	1.88	0.44
1:A:547:ASP:OD1	1:A:970:ARG:HD2	2.18	0.44
1:A:555:PHE:C	1:A:555:PHE:HD1	2.25	0.44
1:A:794:VAL:HG12	1:A:795:ALA:N	2.32	0.44
1:A:161:VAL:HG12	1:A:162:THR:N	2.33	0.43
1:A:573:GLU:OE1	1:A:573:GLU:CA	2.63	0.43
1:A:738:ALA:O	1:A:739:ILE:C	2.61	0.43
1:A:108:GLN:O	1:A:109:ALA:C	2.61	0.43
1:A:275:GLY:HA2	1:A:708:GLN:HB3	2.00	0.43
1:A:202:PHE:CE2	1:A:744:LEU:HA	2.53	0.43
1:A:13:VAL:HG23	1:A:66:ALA:HB2	2.00	0.43
1:A:164:GLY:HA3	1:A:332:MET:CE	2.48	0.43
1:A:414:HIS:ND1	1:A:414:HIS:N	2.66	0.43
1:A:69:VAL:CG1	1:A:86:THR:HG22	2.48	0.43
1:A:914:LEU:HD21	1:A:1003:TRP:CZ3	2.54	0.43
1:A:136:LYS:HG3	1:A:137:HIS:CD2	2.53	0.43
1:A:287:PHE:CD1	1:A:287:PHE:C	2.96	0.43
1:A:678:LEU:O	1:A:682:GLN:HG3	2.18	0.43
1:A:43:ASP:OD1	1:A:113:THR:OG1	2.37	0.43
1:A:691:GLY:O	1:A:694:ALA:HB2	2.18	0.43
1:A:1083:LEU:HD22	1:A:1087:ASP:HB3	2.01	0.43
1:A:1103:GLU:O	1:A:1104:LEU:C	2.61	0.43
1:A:1111:ARG:HH22	1:A:1127:GLU:CD	2.27	0.43
1:A:52:VAL:CG1	1:A:55:LEU:HB3	2.49	0.43
1:A:505:ASP:O	1:A:937:GLY:HA3	2.19	0.43
1:A:1015:LEU:CD2	1:A:1016:LEU:N	2.82	0.43
1:A:492:SER:O	1:A:493:ASN:C	2.62	0.43
1:A:539:MET:HE1	1:A:541:SER:HB3	2.00	0.43
1:A:601:GLY:O	1:A:602:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ASN:OD1	1:A:829:ASN:N	2.52	0.43
1:A:914:LEU:HD22	1:A:1003:TRP:CH2	2.54	0.42
1:A:924:PRO:HA	1:A:925:PRO:HD3	1.88	0.42
1:A:427:VAL:HG12	1:A:428:VAL:N	2.33	0.42
1:A:991:MET:CG	1:A:992:ALA:H	2.32	0.42
1:A:1066:SER:O	1:A:1070:VAL:HG13	2.19	0.42
1:A:893:MET:HE2	1:A:893:MET:HA	2.01	0.42
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.84	0.42
1:A:342:ILE:H	1:A:342:ILE:HD12	1.83	0.42
1:A:1123:GLU:O	1:A:1127:GLU:HG3	2.20	0.42
1:A:990:GLY:O	1:A:991:MET:C	2.62	0.42
1:A:515:LEU:O	1:A:522:HIS:HE1	2.02	0.42
1:A:37:LEU:HB3	1:A:50:PRO:HG3	2.02	0.42
1:A:540:ASN:O	1:A:976:ARG:CD	2.66	0.42
1:A:797:LEU:O	1:A:798:GLN:C	2.63	0.42
1:A:43:ASP:CG	1:A:113:THR:OG1	2.63	0.42
1:A:89:HIS:NE2	1:A:660:PRO:HG3	2.34	0.42
1:A:203:MET:CE	1:A:206:PHE:CD2	3.02	0.42
1:A:395:ASP:OD1	1:A:397:LYS:HG2	2.20	0.42
1:A:668:LEU:O	1:A:671:LEU:HB3	2.20	0.42
1:A:718:MET:HE2	1:A:999:GLN:NE2	2.35	0.42
1:A:229:LEU:HD23	1:A:230:PRO:N	2.34	0.42
1:A:287:PHE:CD1	1:A:439:LEU:HD13	2.55	0.41
1:A:819:LEU:HD21	1:A:868:ILE:HG12	2.02	0.41
1:A:245:VAL:O	1:A:246:GLY:C	2.63	0.41
1:A:256:ASN:ND2	1:A:259:ALA:HB2	2.35	0.41
1:A:123:PHE:CD2	1:A:416:ALA:HB3	2.55	0.41
1:A:756:PHE:N	1:A:756:PHE:CD1	2.89	0.41
1:A:64:ASN:OD1	1:A:334:VAL:HG12	2.20	0.41
1:A:75:GLY:O	1:A:76:LEU:C	2.64	0.41
1:A:186:ILE:O	1:A:187:GLY:C	2.63	0.41
1:A:267:LEU:CD1	1:A:325:ALA:HA	2.51	0.41
1:A:283:THR:OG1	1:A:420:GLN:HB3	2.20	0.41
1:A:621:ARG:HG2	1:A:625:ASP:OD2	2.21	0.41
1:A:486:PHE:CE2	1:A:928:GLN:HG2	2.55	0.41
1:A:1072:THR:HG21	1:A:1088:TRP:CZ3	2.55	0.41
1:A:253:ARG:O	1:A:282:ILE:HD11	2.20	0.41
1:A:1102:MET:HE3	1:A:1102:MET:HB3	1.92	0.41
1:A:184:VAL:HG12	1:A:185:THR:N	2.36	0.40
1:A:611:GLU:O	1:A:612:ALA:C	2.63	0.40
1:A:601:GLY:O	1:A:602:ARG:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LYS:HG2	1:A:838:PRO:CA	2.51	0.40
1:A:451:LEU:O	1:A:452:ALA:C	2.62	0.40
1:A:539:MET:CE	1:A:655:SER:H	2.34	0.40
1:A:236:LEU:O	1:A:240:LEU:HD12	2.22	0.40
1:A:461:LEU:HD13	1:A:671:LEU:HD22	2.04	0.40
1:A:762:ARG:HB3	1:A:765:LEU:CD2	2.52	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	1032/1127 (92%)	910 (88%)	100 (10%)	22 (2%)	5 27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	GLU
1	A	224	ASN
1	A	398	ASP
1	A	603	LEU
1	A	991	MET
1	A	1017	ILE
1	A	82	SER
1	A	347	LEU
1	A	433	GLY
1	A	601	GLY
1	A	602	ARG
1	A	742	PRO
1	A	1016	LEU
1	A	308	GLY
1	A	799	SER

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Mol	Chain	Res	Type
1	A	1008	GLY
1	A	429	PRO
1	A	1037	ALA
1	A	1050	CYS
1	A	752	ALA
1	A	993	GLY
1	A	1015	LEU

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	839/880 (95%)	767 (91%)	72 (9%)	10	36

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	33	LEU
1	A	64	ASN
1	A	74	THR
1	A	86	THR
1	A	91	SER
1	A	107	THR
1	A	113	THR
1	A	123	PHE
1	A	150	LEU
1	A	159	LEU
1	A	173	ASN
1	A	174	THR
1	A	203	MET
1	A	245	VAL
1	A	282	ILE
1	A	283	THR
1	A	311	GLU
1	A	329	ILE

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Mol	Chain	Res	Type
1	A	332	MET
1	A	342	ILE
1	A	347	LEU
1	A	388	VAL
1	A	414	HIS
1	A	421	VAL
1	A	429	PRO
1	A	432	GLU
1	A	464	LYS
1	A	483	MET
1	A	487	ARG
1	A	519	ARG
1	A	539	MET
1	A	555	PHE
1	A	570	ILE
1	A	573	GLU
1	A	585	GLU
1	A	588	THR
1	A	598	THR
1	A	603	LEU
1	A	608	THR
1	A	620	VAL
1	A	642	LYS
1	A	656	LEU
1	A	698	VAL
1	A	730	THR
1	A	743	SER
1	A	749	THR
1	A	753	GLU
1	A	756	PHE
1	A	760	VAL
1	A	771	LEU
1	A	773	VAL
1	A	794	VAL
1	A	829	ASN
1	A	852	LEU
1	A	862	ILE
1	A	883	LEU
1	A	889	SER
1	A	908	THR
1	A	917	ILE
1	A	952	VAL

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Mol	Chain	Res	Type
1	A	1005	SER
1	A	1013	CYS
1	A	1016	LEU
1	A	1022	ARG
1	A	1025	VAL
1	A	1050	CYS
1	A	1052	GLN
1	A	1070	VAL
1	A	1091	LEU
1	A	1131	LEU
1	A	1132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	200	GLN
1	A	233	ASN
1	A	420	GLN
1	A	493	ASN
1	A	512	HIS
1	A	522	HIS
1	A	594	GLN
1	A	614	HIS
1	A	688	GLN
1	A	705	ASN
1	A	708	GLN
1	A	821	GLN
1	A	836	ASN
1	A	848	GLN
1	A	898	ASN
1	A	906	HIS
1	A	928	GLN
1	A	936	GLN
1	A	999	GLN
1	A	1039	ASN
1	A	1052	GLN
1	A	1126	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1057/1127 (93%)	-0.06	18 (1%) 69 45	45, 90, 135, 173	1 (0%)
2	G	8/8 (100%)	0.91	1 (12%) 8 5	154, 168, 204, 224	0
All	All	1065/1135 (93%)	-0.06	19 (1%) 67 44	45, 90, 138, 224	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	713[A]	ARG	5.0
1	A	76	LEU	4.2
1	A	853	PRO	3.9
1	A	1017	ILE	3.5
1	A	31	ILE	3.4
1	A	27	PRO	3.3
1	A	81	VAL	3.3
1	A	789	ALA	3.2
1	A	756	PHE	3.1
1	A	638	GLY	2.9
1	A	74	THR	2.8
2	G	7	DA	2.7
1	A	224	ASN	2.7
1	A	216	ALA	2.6
1	A	559	LYS	2.3
1	A	755	SER	2.2
1	A	307	ALA	2.2
1	A	472	CYS	2.2
1	A	26	CYS	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.