



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:58 PM UTC

PDB ID : 5B2S / pdb_00005b2s
Title : Crystal structure of the Streptococcus pyogenes Cas9 EQR variant in complex with sgRNA and target DNA (TGAG PAM)
Authors : Hirano, S.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2016-02-02
Resolution : 2.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

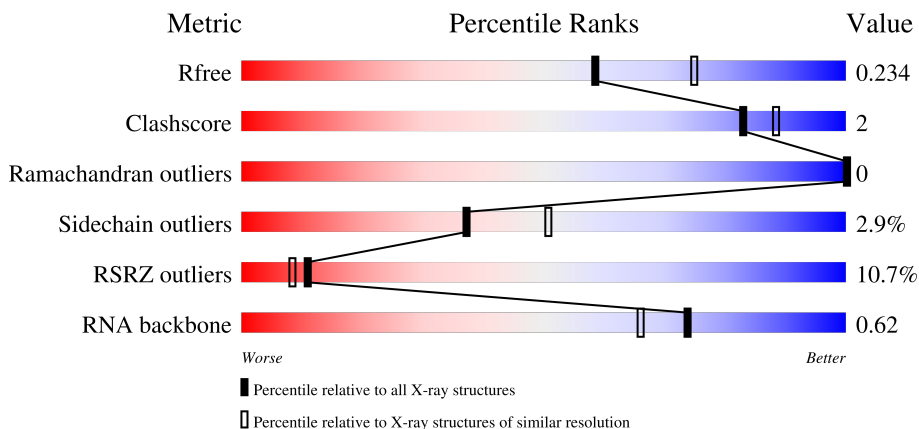
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

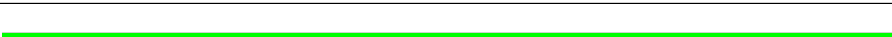
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	81	 79% 20%
2	B	1372	 11% 88% 8%
3	C	28	 79% 21%
4	D	8	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13535 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 RNA chain called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	P	0	0	0
			1739	778	319	561	81			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1319	Total	C	N	O	S	0	1	0
			10494	6695	1820	1959	20			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q99ZW2
B	-2	SER	-	expression tag	UNP Q99ZW2
B	-1	GLY	-	expression tag	UNP Q99ZW2
B	0	HIS	-	expression tag	UNP Q99ZW2
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	80	LEU	CYS	engineered mutation	UNP Q99ZW2
B	574	GLU	CYS	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1135	GLU	ASP	engineered mutation	UNP Q99ZW2
B	1335	GLN	ARG	engineered mutation	UNP Q99ZW2
B	1337	ARG	THR	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called Target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			560	269	100	164	27			

- Molecule 4 is a DNA chain called Non-target DNA, DNA (5'-D(*TP*GP*AP*GP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			165	80	31	47	7			

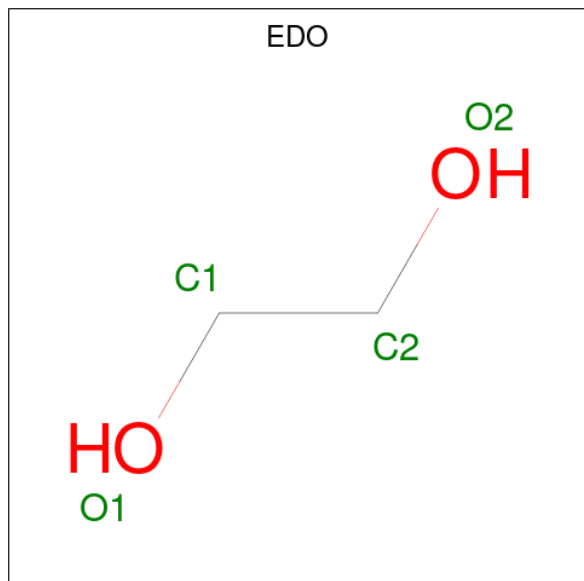
- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	K	0	0
			3	3		
5	B	8	Total	K	0	0
			8	8		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

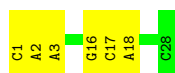


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	161	Total	O	0	0
			161	161		
9	B	343	Total	O	0	0
			343	343		
9	C	30	Total	O	0	0
			30	30		
9	D	9	Total	O	0	0
			9	9		

Chain C:  79% 21%



- Molecule 4: Non-target DNA, DNA (5'-D(*TP*GP*AP*GP*AP*TP*TP*G)-3')

Chain D:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.02Å 67.82Å 187.57Å 90.00° 111.12° 90.00°	Depositor
Resolution (Å)	48.01 – 2.20 48.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.01-2.20) 97.5 (48.01-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.207 , 0.231 0.210 , 0.234	Depositor DCC
R_{free} test set	5177 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13535	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACT, EDO, K

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	0.11	0/1949	0.26	0/3037
2	B	0.10	0/10682	0.28	0/14409
3	C	0.21	0/626	0.41	0/961
4	D	0.19	0/185	0.42	0/285
All	All	0.11	0/13442	0.29	0/18692

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1739	0	870	6	0
2	B	10494	0	10384	50	0
3	C	560	0	316	5	0
4	D	165	0	93	0	0
5	A	3	0	0	0	0
5	B	8	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	12	0	18	0	0
8	A	4	0	3	0	0
9	A	161	0	0	0	0
9	B	343	0	0	2	0
9	C	30	0	0	0	0
9	D	9	0	0	0	0
All	All	13535	0	11690	59	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 2.

All (59) 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:18:G:N7	2:B:71:ARG:NH2	2.29	0.81
2:B:240:ASN:ND2	2:B:255:ASN:OD1	2.31	0.62
2:B:251:ASN:HD21	2:B:262:ALA:H	1.48	0.62
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.83	0.60
3:C:2:DA:H2'	3:C:3:DA:C8	2.36	0.60
2:B:342:GLN:HB2	2:B:383:MET:HE3	1.83	0.59
1:A:44:U:O2'	2:B:402:GLN:NE2	2.36	0.58
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.36	0.56
2:B:251:ASN:ND2	2:B:262:ALA:H	2.04	0.55
2:B:1256:GLN:NE2	2:B:1260:GLU:OE2	2.37	0.55
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.89	0.54
2:B:279:LEU:HG	2:B:284:ASP:HA	1.90	0.53
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.90	0.53
2:B:193:ASN:ND2	2:B:201:ILE:O	2.34	0.51
2:B:870:VAL:HG22	2:B:871:PRO:HD2	1.93	0.51
2:B:784:ILE:HD12	2:B:806:LEU:HD13	1.92	0.51
2:B:349:GLU:HG3	2:B:356:LYS:HG3	1.93	0.51
2:B:841:ILE:HD12	2:B:854:ASN:HA	1.95	0.49
2:B:1114:ARG:HG3	2:B:1116:SER:H	1.76	0.48
2:B:1297:HIS:HD2	2:B:1300:LYS:HE3	1.77	0.48
1:A:73:G:H3'	1:A:74:A:C5'	2.43	0.48
2:B:826:GLN:NE2	2:B:859:ARG:HD2	2.28	0.48
2:B:869:ASN:OD1	2:B:870:VAL:N	2.34	0.47
2:B:839:ASP:OD2	2:B:864:ARG:NE	2.37	0.47
2:B:336:LYS:NZ	9:B:1507:HOH:O	2.40	0.47
2:B:1048:THR:HG22	2:B:1076:LYS:HD3	1.95	0.47
2:B:1044:ASN:HB3	2:B:1050:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.36	0.46
3:C:17:DC:H2'	3:C:18:DA:C8	2.50	0.46
2:B:1256:GLN:O	2:B:1260:GLU:HG2	2.16	0.46
2:B:312:ILE:HG23	2:B:313:THR:HG22	1.97	0.45
2:B:901:THR:O	2:B:904:GLU:HG2	2.16	0.45
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.97	0.44
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.99	0.44
2:B:1231:LYS:HE3	2:B:1232:TYR:CZ	2.52	0.44
3:C:1:DC:H2'	3:C:2:DA:C8	2.51	0.44
2:B:216:LEU:HD22	2:B:220:ARG:HG2	2.00	0.44
2:B:846:PHE:O	2:B:920:GLN:NE2	2.46	0.44
2:B:822:MET:HG3	2:B:856:VAL:HB	1.99	0.44
2:B:301:LEU:HG	2:B:302:LEU:HD13	2.00	0.44
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.83	0.43
2:B:985:HIS:CG	2:B:1087:LEU:HD22	2.53	0.43
2:B:1060:ARG:HB2	2:B:1076:LYS:NZ	2.33	0.43
2:B:1339:THR:O	2:B:1342:VAL:HG22	2.19	0.43
1:A:71:U:H2'	1:A:72:U:C6	2.54	0.43
2:B:196:PHE:CZ	2:B:286:TYR:HE1	2.36	0.43
3:C:16:DG:H2'	3:C:17:DC:C6	2.54	0.42
2:B:882:TYR:CZ	2:B:886:LEU:HD11	2.54	0.42
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.51	0.42
2:B:338:LEU:C	2:B:383:MET:HE1	2.44	0.42
2:B:192:TYR:HB2	2:B:289:LEU:HD11	2.01	0.42
1:A:3:A:H2'	1:A:4:A:C8	2.55	0.42
2:B:468:LYS:HE3	2:B:483:ASP:HA	2.02	0.42
2:B:218:LYS:HG3	2:B:221:ARG:NH1	2.35	0.41
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.82	0.41
1:A:38:A:H2'	1:A:39:G:C8	2.55	0.41
3:C:17:DC:H2'	3:C:18:DA:H8	1.86	0.41
2:B:1211:LYS:NZ	9:B:1535:HOH:O	2.54	0.41
2:B:821:ASP:HB3	2:B:824:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
2	B	1308/1372 (95%)	1264 (97%)	44 (3%)	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	
2	B	1106/1227 (90%)	1074 (97%)	32 (3%)	37	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	67	THR
2	B	112	LYS
2	B	123	VAL
2	B	216	LEU
2	B	219	SER
2	B	249	THR
2	B	261	ASP
2	B	289	LEU
2	B	301	LEU
2	B	309	ASN
2	B	310	THR
2	B	321	MET
2	B	334	LEU
2	B	390	LEU
2	B	419	LEU
2	B	524	LEU
2	B	638	THR
2	B	642	LEU
2	B	644	ASP

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Mol	Chain	Res	Type
2	B	847	LEU
2	B	853	ASP
2	B	870	VAL
2	B	900	LEU
2	B	911	LEU
2	B	971	GLN
2	B	998	ILE
2	B	1052	LEU
2	B	1072	ILE
2	B	1122	ARG
2	B	1192	LYS
2	B	1257	LEU
2	B	1302	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	265	GLN
2	B	402	GLN
2	B	412	HIS
2	B	511	HIS
2	B	726	ASN
2	B	739	GLN
2	B	926	GLN
2	B	980	ASN
2	B	1044	ASN
2	B	1115	ASN
2	B	1261	GLN
2	B	1262	HIS
2	B	1297	HIS
2	B	1317	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/81 (98%)	8 (10%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	28	A
1	A	40	C
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	74	A
1	A	75	A

There are no RNA pucker outliers to report.

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 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	A	106	-	3,3,3	0.43	0	2,2,2	0.42	0
8	ACT	A	107	-	3,3,3	0.79	0	3,3,3	1.31	0
7	EDO	B	1411	-	3,3,3	0.44	0	2,2,2	0.37	0
7	EDO	B	1410	-	3,3,3	0.44	0	2,2,2	0.35	0
7	EDO	B	1412	-	3,3,3	0.41	0	2,2,2	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	1411	-	-	0/1/1/1	-
7	EDO	A	106	-	-	0/1/1/1	-
7	EDO	B	1412	-	-	0/1/1/1	-
7	EDO	B	1410	-	-	0/1/1/1	-

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	81/81 (100%)	-0.52	0 100 100	28, 42, 127, 182	0
2	B	1319/1372 (96%)	0.62	153 (11%) 9 7	25, 53, 106, 140	1 (0%)
3	C	28/28 (100%)	-0.31	0 100 100	35, 47, 72, 86	0
4	D	8/8 (100%)	-0.12	0 100 100	37, 51, 97, 114	0
All	All	1436/1489 (96%)	0.54	153 (10%) 11 8	25, 53, 107, 182	1 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	299	ALA	7.9
2	B	244	LEU	7.3
2	B	247	GLY	6.5
2	B	264	LEU	6.3
2	B	189	VAL	6.3
2	B	296	LEU	6.1
2	B	248	LEU	5.9
2	B	246	LEU	5.9
2	B	184	LEU	5.8
2	B	1250	GLU	5.8
2	B	292	ALA	5.7
2	B	269	ASP	5.3
2	B	271	TYR	5.3
2	B	275	LEU	5.1
2	B	195	LEU	5.1
2	B	188	LEU	5.0
2	B	287	ALA	4.9
2	B	293	ALA	4.9
2	B	186	ILE	4.8
2	B	300	ILE	4.8
2	B	266	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	286	TYR	4.7
2	B	273	ASP	4.6
2	B	778	ARG	4.5
2	B	301	LEU	4.5
2	B	279	LEU	4.4
2	B	1243	GLU	4.4
2	B	1302	ILE	4.3
2	B	265	GLN	4.3
2	B	245	SER	4.3
2	B	291	LEU	4.3
2	B	270	THR	4.3
2	B	259	ALA	4.2
2	B	250	PRO	4.2
2	B	1366	GLY	4.2
2	B	249	THR	4.2
2	B	215	ARG	4.2
2	B	290	PHE	4.1
2	B	185	PHE	4.0
2	B	1251	ASP	4.0
2	B	243	ALA	3.8
2	B	178	ASN	3.7
2	B	297	SER	3.7
2	B	262	ALA	3.7
2	B	194	GLN	3.7
2	B	387	GLU	3.7
2	B	192	TYR	3.7
2	B	278	LEU	3.6
2	B	765	ARG	3.6
2	B	1249	PRO	3.6
2	B	911	LEU	3.5
2	B	309	ASN	3.5
2	B	187	GLN	3.5
2	B	1062	LEU	3.5
2	B	1077	GLY	3.5
2	B	302	LEU	3.4
2	B	191	THR	3.3
2	B	263	LYS	3.3
2	B	274	ASP	3.3
2	B	1242	TYR	3.3
2	B	295	ASN	3.3
2	B	218	LYS	3.2
2	B	1050	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	847	LEU	3.2
2	B	214	ALA	3.2
2	B	193	ASN	3.2
2	B	395	ARG	3.1
2	B	267	SER	3.1
2	B	730	SER	3.1
2	B	776	ASN	3.1
2	B	868	ASP	3.1
2	B	1241	HIS	3.0
2	B	210	ALA	3.0
2	B	1261	GLN	3.0
2	B	219	SER	3.0
2	B	294	LYS	3.0
2	B	174	LEU	3.0
2	B	298	ASP	3.0
2	B	1258	PHE	3.0
2	B	190	GLN	3.0
2	B	1031	LYS	2.9
2	B	285	GLN	2.9
2	B	728	ALA	2.9
2	B	1259	VAL	2.9
2	B	1051	THR	2.9
2	B	176	PRO	2.9
2	B	871	PRO	2.9
2	B	283	GLY	2.9
2	B	1260	GLU	2.9
2	B	1299	ASP	2.9
2	B	890	LYS	2.8
2	B	1055	GLY	2.8
2	B	200	PRO	2.8
2	B	280	ALA	2.8
2	B	289	LEU	2.8
2	B	783	ARG	2.8
2	B	795	ILE	2.8
2	B	308	VAL	2.8
2	B	804	THR	2.7
2	B	277	ASN	2.7
2	B	341	GLN	2.7
2	B	1253	GLU	2.7
2	B	779	GLU	2.7
2	B	803	ASN	2.7
2	B	1054	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	731	PRO	2.7
2	B	177	ASP	2.6
2	B	251	ASN	2.6
2	B	268	LYS	2.6
2	B	1034	ALA	2.5
2	B	1053	ALA	2.5
2	B	1070	GLY	2.5
2	B	216	LEU	2.5
2	B	791	LEU	2.5
2	B	917	ILE	2.4
2	B	1072	ILE	2.4
2	B	310	THR	2.4
2	B	1033	THR	2.4
2	B	866	LYS	2.4
2	B	260	GLU	2.4
2	B	729	GLY	2.3
2	B	789	LYS	2.3
2	B	867	SER	2.3
2	B	1264	HIS	2.3
2	B	869	ASN	2.3
2	B	253	LYS	2.3
2	B	261	ASP	2.3
2	B	213	SER	2.3
2	B	258	LEU	2.3
2	B	272	ASP	2.3
2	B	1057	ILE	2.2
2	B	888	ASN	2.2
2	B	1048	THR	2.2
2	B	852	ILE	2.2
2	B	276	ASP	2.2
2	B	916	PHE	2.2
2	B	1037	PHE	2.2
2	B	812	TYR	2.1
2	B	312	ILE	2.1
2	B	870	VAL	2.1
2	B	919	ARG	2.1
2	B	382	LYS	2.1
2	B	891	LEU	2.1
2	B	39	ASP	2.1
2	B	777	SER	2.1
2	B	1032	ALA	2.1
2	B	786	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1039	TYR	2.1
2	B	796	LEU	2.0
2	B	970	PHE	2.0
2	B	394	ASN	2.0
2	B	282	ILE	2.0
2	B	209	LYS	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
5	K	B	1408	1/1	0.40	0.26	160,160,160,160	0
5	K	B	1406	1/1	0.77	0.18	93,93,93,93	0
5	K	B	1403	1/1	0.87	0.10	74,74,74,74	0
7	EDO	B	1411	4/4	0.87	0.20	50,50,51,51	0
6	MG	A	105	1/1	0.91	0.15	49,49,49,49	0
8	ACT	A	107	4/4	0.91	0.13	50,50,50,51	0
7	EDO	A	106	4/4	0.92	0.10	30,32,34,35	0
5	K	B	1405	1/1	0.93	0.12	81,81,81,81	0
5	K	B	1407	1/1	0.95	0.06	60,60,60,60	0
7	EDO	B	1412	4/4	0.96	0.12	39,42,45,47	0
6	MG	B	1409	1/1	0.96	0.08	41,41,41,41	0
5	K	B	1404	1/1	0.97	0.09	52,52,52,52	0
5	K	A	103	1/1	0.98	0.06	38,38,38,38	0
5	K	A	102	1/1	0.98	0.07	38,38,38,38	0
7	EDO	B	1410	4/4	0.98	0.07	31,33,34,36	0
6	MG	A	104	1/1	0.99	0.03	43,43,43,43	0
5	K	A	101	1/1	0.99	0.05	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	B	1401	1/1	0.99	0.09	43,43,43,43	0
5	K	B	1402	1/1	0.99	0.02	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.