



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:29 PM UTC

PDB ID : 7OS0 / pdb_00007os0
Title : Structure of the Rhodobacter capsulatus Cas13a-crRNA binary complex
Authors : Kick, L.M.; Schneider, S.
Deposited on : 2021-06-07
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

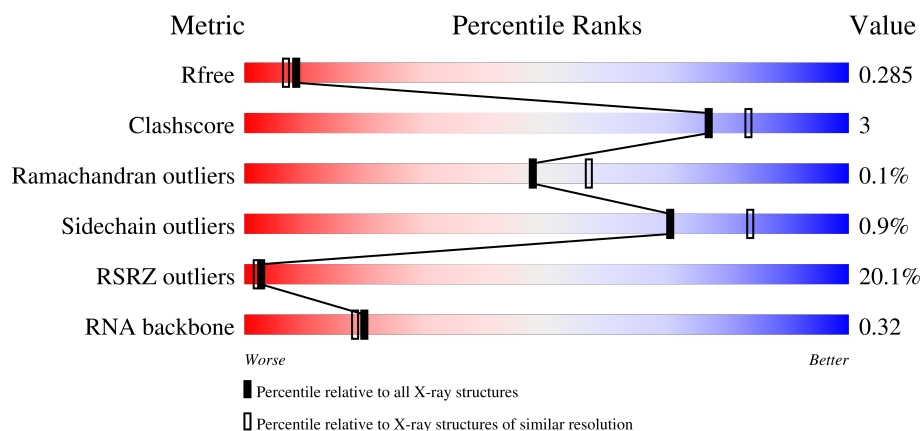
1 Overall quality at a glance

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	1304	
1	C	1304	
2	D	54	
2	F	54	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20467 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 Cas13a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1130	Total	C	N	O	S	0	8	0
			8945	5629	1653	1633	30			
1	C	1123	Total	C	N	O	S	0	1	0
			8850	5575	1634	1611	30			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	GLU	-	expression tag	UNP D5AUW0
A	1287	ASN	-	expression tag	UNP D5AUW0
A	1288	LEU	-	expression tag	UNP D5AUW0
A	1289	TYR	-	expression tag	UNP D5AUW0
A	1290	PHE	-	expression tag	UNP D5AUW0
A	1291	GLN	-	expression tag	UNP D5AUW0
A	1292	LYS	-	expression tag	UNP D5AUW0
A	1293	LEU	-	expression tag	UNP D5AUW0
A	1294	ALA	-	expression tag	UNP D5AUW0
A	1295	ALA	-	expression tag	UNP D5AUW0
A	1296	ALA	-	expression tag	UNP D5AUW0
A	1297	LEU	-	expression tag	UNP D5AUW0
A	1298	GLU	-	expression tag	UNP D5AUW0
A	1299	HIS	-	expression tag	UNP D5AUW0
A	1300	HIS	-	expression tag	UNP D5AUW0
A	1301	HIS	-	expression tag	UNP D5AUW0
A	1302	HIS	-	expression tag	UNP D5AUW0
A	1303	HIS	-	expression tag	UNP D5AUW0
A	1304	HIS	-	expression tag	UNP D5AUW0
C	1286	GLU	-	expression tag	UNP D5AUW0
C	1287	ASN	-	expression tag	UNP D5AUW0
C	1288	LEU	-	expression tag	UNP D5AUW0
C	1289	TYR	-	expression tag	UNP D5AUW0
C	1290	PHE	-	expression tag	UNP D5AUW0
C	1291	GLN	-	expression tag	UNP D5AUW0

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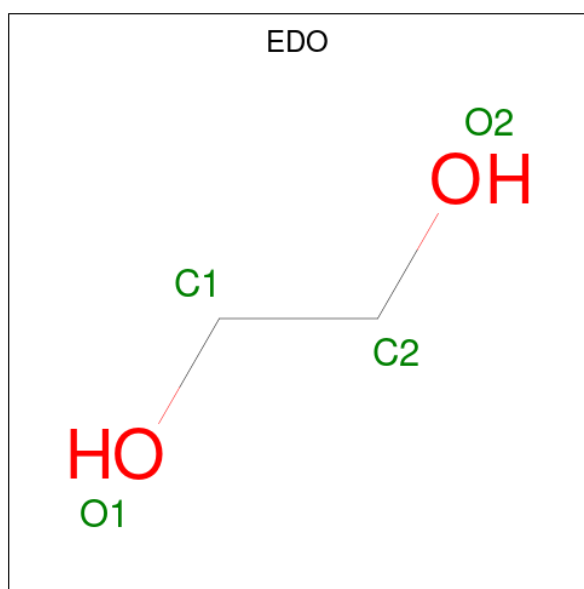
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1292	LYS	-	expression tag	UNP D5AUW0
C	1293	LEU	-	expression tag	UNP D5AUW0
C	1294	ALA	-	expression tag	UNP D5AUW0
C	1295	ALA	-	expression tag	UNP D5AUW0
C	1296	ALA	-	expression tag	UNP D5AUW0
C	1297	LEU	-	expression tag	UNP D5AUW0
C	1298	GLU	-	expression tag	UNP D5AUW0
C	1299	HIS	-	expression tag	UNP D5AUW0
C	1300	HIS	-	expression tag	UNP D5AUW0
C	1301	HIS	-	expression tag	UNP D5AUW0
C	1302	HIS	-	expression tag	UNP D5AUW0
C	1303	HIS	-	expression tag	UNP D5AUW0
C	1304	HIS	-	expression tag	UNP D5AUW0

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	48	Total	C	N	O	P	0	0	1
			993	444	172	330	47			
2	F	48	Total	C	N	O	P	0	0	1
			993	444	172	330	47			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



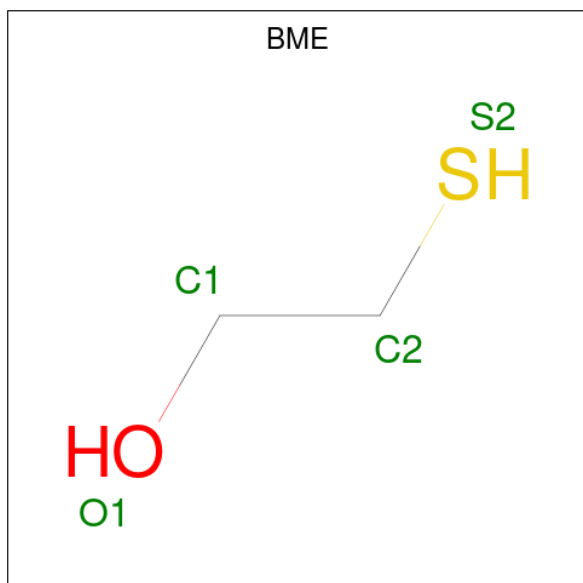
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

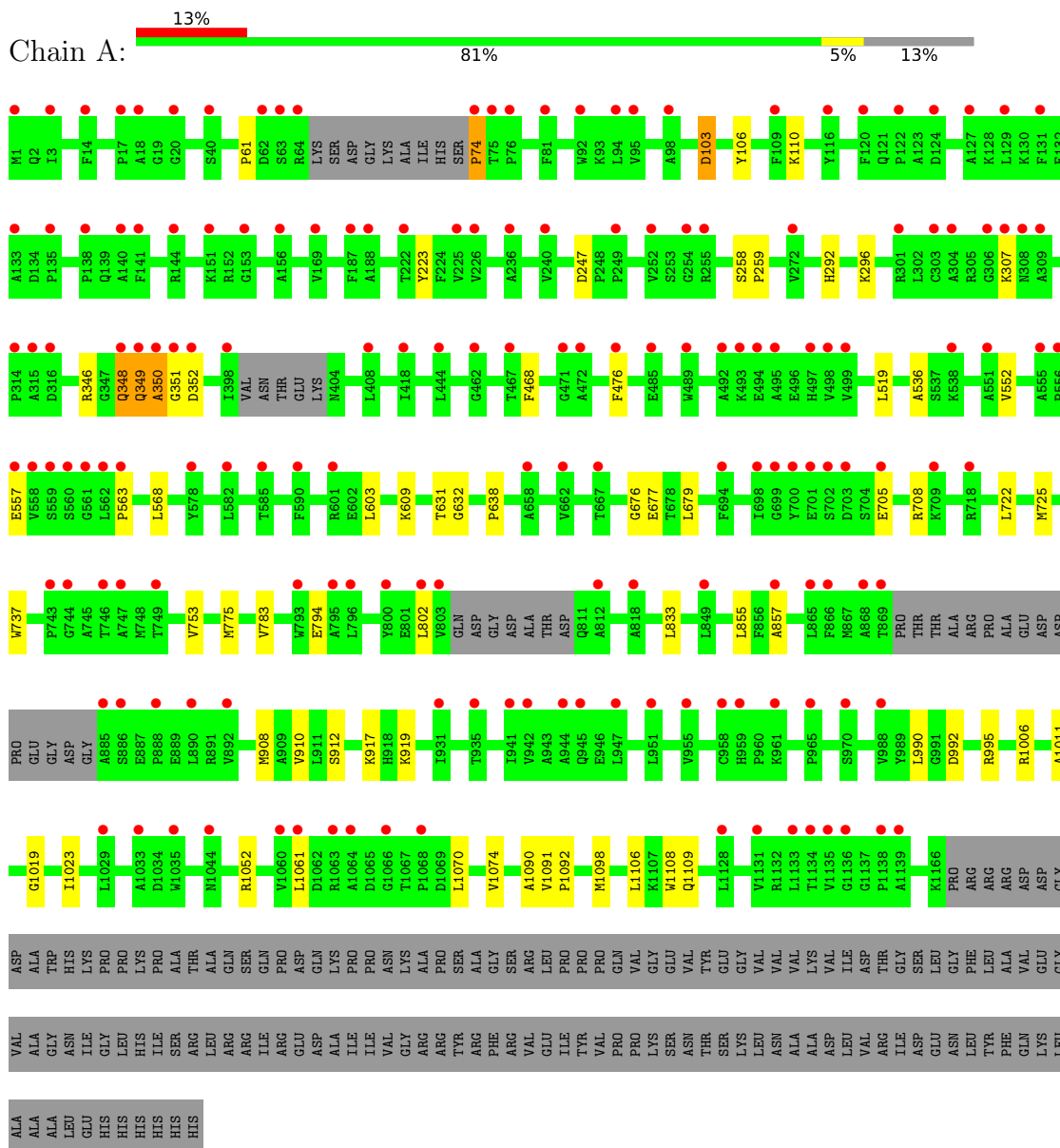
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	331	Total	O	0	0
			331	331		
5	C	177	Total	O	0	0
			177	177		
5	D	48	Total	O	0	0
			48	48		
5	F	74	Total	O	0	0
			74	74		

3 Residue-property plots [i](#)

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: Cas13a



• Molecule 1: Cas13a





● Molecule 2: crRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.39Å 91.08Å 136.51Å 89.99° 103.69° 97.65°	Depositor
Resolution (Å)	47.12 – 2.20 47.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.12-2.20) 97.7 (47.12-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.256 0.258 , 0.285	Depositor DCC
R_{free} test set	7063 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+1	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20467	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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

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

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	0.59	0/9130	1.03	0/12313
1	C	0.62	2/9028 (0.0%)	1.05	11/12174 (0.1%)
2	D	0.37	0/1107	0.77	2/1722 (0.1%)
2	F	0.36	0/1107	0.76	2/1722 (0.1%)
All	All	0.58	2/20372 (0.0%)	1.01	15/27931 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	718[A]	ARG	C-O	9.79	1.35	1.24
1	C	718[B]	ARG	C-O	9.79	1.35	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	718[A]	ARG	CA-C-O	11.19	132.41	120.55
1	C	718[B]	ARG	CA-C-O	11.19	132.41	120.55
2	D	20	A	C4'-C3'-O3'	7.08	120.03	109.40
1	C	718[A]	ARG	O-C-N	-7.07	114.63	122.12
1	C	718[B]	ARG	O-C-N	-7.07	114.63	122.12
2	F	20	A	C4'-C3'-O3'	7.05	119.97	109.40
1	C	560	SER	N-CA-C	-5.98	105.75	113.16
2	D	44	A	C2'-C3'-O3'	5.46	117.69	109.50
1	C	472	ALA	CA-C-N	5.30	127.91	120.28
1	C	472	ALA	C-N-CA	5.30	127.91	120.28
2	F	44	A	C2'-C3'-O3'	5.19	117.28	109.50
1	C	153	GLY	N-CA-C	5.16	117.29	112.08
1	C	151	LYS	N-CA-C	-5.13	102.27	109.96
1	C	128	LYS	CA-C-N	-5.10	115.91	123.05
1	C	128	LYS	C-N-CA	-5.10	115.91	123.05

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	8945	0	8995	45	0
1	C	8850	0	8909	61	0
2	D	993	0	507	6	0
2	F	993	0	507	6	0
3	A	16	0	24	0	0
3	C	16	0	24	0	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	331	0	0	1	0
5	C	177	0	0	0	0
5	D	48	0	0	0	0
5	F	74	0	0	0	0
All	All	20467	0	19002	112	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 3.

All (112) 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:C:1014:TYR:HB2	1:C:1081:MET:HE1	1.36	1.08
1:C:1060:VAL:HG11	1:C:1073:LEU:HD21	1.49	0.93
1:A:775:MET:HE3	1:A:783:VAL:HG22	1.53	0.87
1:C:332:VAL:HG12	1:C:336:MET:HE2	1.69	0.73
1:C:626:TYR:CE2	1:C:630:ILE:HD11	2.23	0.72
1:C:348:GLN:O	1:C:348:GLN:HG2	1.89	0.71
1:C:1080:MET:HE3	1:C:1081:MET:HE3	1.73	0.69
1:C:386:ARG:HE	1:C:907:HIS:HE2	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351[A]:GLY:O	1:A:352[A]:ASP:HB2	1.92	0.68
1:C:49:GLN:HE21	1:C:195:ARG:HH21	1.42	0.67
1:C:1131:VAL:O	1:C:1138:PRO:O	2.12	0.66
1:C:959:HIS:HB2	1:C:962:THR:HG22	1.77	0.65
1:C:1127:HIS:HB2	1:C:1141:VAL:HG22	1.80	0.63
1:A:292:HIS:CE1	1:A:296:LYS:HD2	2.35	0.62
1:A:348[A]:GLN:C	1:A:350[A]:ALA:H	2.08	0.61
2:F:40:C:O2	2:F:40:C:O4'	2.19	0.60
1:C:330:ASN:HD21	1:C:1085:ARG:H	1.50	0.60
1:A:563:PRO:HD3	1:A:722:LEU:HD13	1.85	0.59
1:C:336:MET:HE1	1:C:1040:ALA:HB2	1.84	0.59
1:C:336:MET:CE	1:C:1040:ALA:HB2	2.33	0.58
2:D:40:C:O4'	2:D:40:C:O2	2.20	0.58
1:C:1080:MET:HG2	1:C:1081:MET:CE	2.34	0.57
1:A:348[A]:GLN:O	1:A:350[A]:ALA:N	2.29	0.57
1:C:765:GLU:H	1:C:768:GLN:HE21	1.51	0.56
1:C:768:GLN:HE22	1:C:824:ARG:HH11	1.54	0.56
1:A:223:TYR:OH	1:A:292:HIS:HD2	1.90	0.55
1:C:519:LEU:HD21	1:C:552:VAL:HG11	1.87	0.55
1:C:398:ILE:CD1	1:C:423:MET:HE1	2.37	0.55
1:A:536:ALA:HB2	1:A:737:TRP:CZ3	2.43	0.54
1:C:1015:GLU:HB2	1:C:1052:ARG:HD2	1.90	0.53
1:C:536:ALA:HB2	1:C:737:TRP:CZ3	2.44	0.53
1:C:1055:LEU:HD21	1:C:1073:LEU:HD22	1.91	0.53
1:C:643:LYS:HG2	1:C:667:THR:HG22	1.91	0.52
1:C:910:VAL:HG13	1:C:911:LEU:HG	1.91	0.52
1:A:631:THR:HG22	1:A:632:GLY:H	1.74	0.52
1:A:855:LEU:HD23	1:A:990:LEU:HD22	1.91	0.52
1:A:631:THR:HG22	1:A:632:GLY:N	2.25	0.51
1:C:855:LEU:HD23	1:C:990:LEU:HD22	1.92	0.51
2:D:39:U:O2	2:D:39:U:O4'	2.27	0.51
1:C:211:LEU:O	1:C:328:HIS:HE1	1.94	0.50
1:A:61:PRO:HB2	1:A:74:PRO:HB3	1.93	0.50
1:A:1019:GLY:O	1:A:1023:ILE:HD12	2.12	0.49
1:C:627:ALA:HA	1:C:630:ILE:HD12	1.94	0.49
1:A:557:GLU:HG2	1:A:794:GLU:HG3	1.94	0.49
1:A:910:VAL:HG11	1:A:1061:LEU:HD22	1.94	0.49
1:C:626:TYR:CD2	1:C:630:ILE:HD11	2.47	0.49
1:A:468:PHE:CD2	1:A:476:PHE:CD1	3.01	0.49
1:C:468:PHE:CD2	1:C:476:PHE:CD1	3.01	0.49
1:A:631:THR:HG21	1:A:676:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1080:MET:C	1:C:1081:MET:HE2	2.39	0.48
1:A:908:MET:O	1:A:912:SER:HB3	2.14	0.48
1:A:603:LEU:O	1:A:609:LYS:HE2	2.13	0.48
1:C:49:GLN:HE21	1:C:195:ARG:NH2	2.09	0.47
1:C:695:ARG:NH2	2:D:33:G:N7	2.57	0.47
1:A:1091:VAL:HB	1:A:1092:PRO:HD3	1.97	0.46
1:A:349[B]:GLN:O	1:A:350[B]:ALA:HB2	2.16	0.46
1:C:568:LEU:C	1:C:568:LEU:HD23	2.41	0.46
1:C:683:LEU:HD12	1:C:683:LEU:HA	1.78	0.46
1:A:568:LEU:C	1:A:568:LEU:HD23	2.41	0.45
1:C:1006:ARG:HB2	1:C:1098:MET:HE1	1.96	0.45
1:C:1080:MET:CE	1:C:1081:MET:HE3	2.43	0.45
1:A:1011:ALA:HB1	1:A:1052[A]:ARG:HG2	1.97	0.45
2:D:20:A:H4'	2:D:21:C:OP1	2.16	0.45
1:C:1080:MET:HG2	1:C:1081:MET:HE3	1.99	0.45
1:A:705:GLU:OE1	1:A:708:ARG:NH1	2.50	0.45
1:A:348[B]:GLN:N	1:A:348[B]:GLN:CD	2.74	0.45
2:F:20:A:H4'	2:F:21:C:OP1	2.17	0.45
1:C:1091:VAL:HB	1:C:1092:PRO:HD3	1.98	0.45
1:C:1070:LEU:O	1:C:1074:VAL:HG23	2.17	0.45
1:A:258:SER:OG	2:F:25:G:OP2	2.34	0.45
1:A:348[A]:GLN:C	1:A:350[A]:ALA:N	2.73	0.45
1:A:1052[B]:ARG:HG2	1:A:1052[B]:ARG:HH21	1.83	0.44
1:A:631:THR:HG23	1:A:677:GLU:O	2.18	0.44
1:C:1138:PRO:O	1:C:1139:ALA:HB3	2.16	0.44
1:A:1109:GLN:NE2	5:A:1510:HOH:O	2.50	0.44
1:C:768:GLN:NE2	1:C:824:ARG:HH11	2.16	0.44
1:C:992:ASP:OD1	1:C:995:ARG:NH2	2.51	0.44
1:A:638:PRO:HG2	1:A:725:MET:HG2	2.00	0.43
1:C:258:SER:OG	2:D:25:G:OP2	2.34	0.43
1:A:679:LEU:HD22	1:A:725:MET:HE1	2.00	0.43
1:C:560:SER:HB2	1:C:788:HIS:ND1	2.33	0.43
1:A:1090:ALA:HB1	2:F:34:A:H4'	2.01	0.43
1:A:106:TYR:OH	1:A:110:LYS:HD2	2.19	0.43
1:A:857:ALA:HA	1:A:919:LYS:HD2	2.01	0.42
1:C:1014:TYR:HB2	1:C:1081:MET:CE	2.26	0.42
1:A:1070:LEU:O	1:A:1074:VAL:HG23	2.18	0.42
1:C:1081:MET:HE2	1:C:1081:MET:HA	2.02	0.42
1:C:348:GLN:O	1:C:348:GLN:CG	2.63	0.42
1:C:638:PRO:HG2	1:C:725:MET:HG2	2.01	0.42
1:A:1006:ARG:HB2	1:A:1098:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:N	1:A:103:ASP:OD1	2.53	0.42
1:A:346:ARG:NH2	1:A:351[B]:GLY:O	2.38	0.41
1:C:195:ARG:HD3	2:D:26:G:O2'	2.20	0.41
1:C:398:ILE:N	1:C:398:ILE:HD12	2.36	0.41
1:A:519:LEU:HD21	1:A:552:VAL:HG11	2.03	0.41
1:A:992:ASP:OD1	1:A:995:ARG:NH2	2.53	0.41
1:C:49:GLN:NE2	1:C:195:ARG:HH21	2.13	0.41
1:C:558:VAL:HG11	1:C:625:ALA:HA	2.03	0.41
1:C:802:LEU:HD22	1:C:802:LEU:N	2.36	0.41
1:C:293:ASP:OD2	1:C:297:LYS:HE2	2.20	0.41
1:C:679:LEU:HD22	1:C:725:MET:HE1	2.02	0.41
1:C:888:PRO:O	1:C:892:VAL:HG12	2.21	0.41
1:A:258:SER:N	1:A:259:PRO:HD2	2.35	0.41
1:A:1106:LEU:HD21	1:A:1108:TRP:CZ2	2.57	0.40
1:C:293:ASP:O	1:C:297:LYS:HG3	2.22	0.40
2:F:12:C:H2'	2:F:13:C:C6	2.56	0.40
1:A:833:LEU:HD22	2:F:39:U:C6	2.57	0.40
1:C:258:SER:N	1:C:259:PRO:HD2	2.36	0.40
1:C:1075:ASN:HD21	1:C:1115:LEU:H	1.68	0.40
1:C:1106:LEU:HD21	1:C:1108:TRP:CZ2	2.56	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	1128/1304 (86%)	1106 (98%)	18 (2%)	4 (0%)	30	34
1	C	1112/1304 (85%)	1092 (98%)	20 (2%)	0	100	100
All	All	2240/2608 (86%)	2198 (98%)	38 (2%)	4 (0%)	48	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350[A]	ALA
1	A	350[B]	ALA
1	A	349[A]	GLN
1	A	349[B]	GLN

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	910/1049 (87%)	901 (99%)	9 (1%)	68	81
1	C	901/1049 (86%)	892 (99%)	9 (1%)	68	81
All	All	1811/2098 (86%)	1793 (99%)	18 (1%)	70	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	PRO
1	A	103	ASP
1	A	247	ASP
1	A	307	LYS
1	A	348[A]	GLN
1	A	348[B]	GLN
1	A	753	VAL
1	A	802	LEU
1	A	917	LYS
1	C	104	SER
1	C	124	ASP
1	C	183	LYS
1	C	683	LEU
1	C	801	GLU
1	C	802	LEU
1	C	892	VAL
1	C	917	LYS
1	C	1141	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	292	HIS
1	A	355	GLN
1	A	357	HIS
1	A	449	ASN
1	A	540	HIS
1	A	674	ASN
1	A	918	HIS
1	A	945	GLN
1	A	1044	ASN
1	A	1059	ASN
1	A	1148	GLN
1	A	1164	ASN
1	C	38	HIS
1	C	49	GLN
1	C	268	HIS
1	C	328	HIS
1	C	330	ASN
1	C	540	HIS
1	C	768	GLN
1	C	918	HIS
1	C	997	HIS
1	C	1075	ASN
1	C	1113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	46/54 (85%)	16 (34%)	7 (15%)
2	F	46/54 (85%)	18 (39%)	8 (17%)
All	All	92/108 (85%)	34 (36%)	15 (16%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	10	C
2	D	11	A
2	D	17	A
2	D	18	A
2	D	21	C
2	D	22	G
2	D	30	A

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Mol	Chain	Res	Type
2	D	32	U
2	D	40	C
2	D	41	A
2	D	42	U
2	D	43	U
2	D	44	A
2	D	45	C
2	D	50	G
2	D	51	U
2	F	10	C
2	F	11	A
2	F	17	A
2	F	18	A
2	F	21	C
2	F	22	G
2	F	30	A
2	F	32	U
2	F	38	U
2	F	39	U
2	F	40	C
2	F	41	A
2	F	42	U
2	F	43	U
2	F	44	A
2	F	45	C
2	F	50	G
2	F	51	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	17	A
2	D	18	A
2	D	20	A
2	D	21	C
2	D	41	A
2	D	44	A
2	D	50	G
2	F	17	A
2	F	18	A
2	F	20	A
2	F	21	C

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Mol	Chain	Res	Type
2	F	38	U
2	F	41	A
2	F	44	A
2	F	50	G

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](#)

14 ligands are modelled in this entry.

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	$\# Z > 2$
3	EDO	A	1402	-	3,3,3	0.05	0	2,2,2	0.07	0
3	EDO	A	1401	-	3,3,3	0.07	0	2,2,2	0.12	0
3	EDO	D	101	-	3,3,3	0.05	0	2,2,2	0.11	0
3	EDO	F	101	-	3,3,3	0.05	0	2,2,2	0.16	0
4	BME	D	103	-	3,3,3	0.18	0	2,2,2	0.22	0
3	EDO	A	1403	-	3,3,3	0.06	0	2,2,2	0.12	0
3	EDO	C	1403	-	3,3,3	0.06	0	2,2,2	0.11	0
4	BME	A	1405	-	3,3,3	0.18	0	2,2,2	0.16	0
3	EDO	C	1401	-	3,3,3	0.07	0	2,2,2	0.20	0
3	EDO	C	1404	-	3,3,3	0.06	0	2,2,2	0.12	0
4	BME	C	1405	-	3,3,3	0.18	0	2,2,2	0.23	0
3	EDO	C	1402	-	3,3,3	0.07	0	2,2,2	0.11	0
3	EDO	D	102	-	3,3,3	0.06	0	2,2,2	0.10	0
3	EDO	A	1404	-	3,3,3	0.07	0	2,2,2	0.12	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
3	EDO	A	1402	-	-	0/1/1/1	-
3	EDO	A	1401	-	-	0/1/1/1	-
3	EDO	D	101	-	-	1/1/1/1	-
3	EDO	F	101	-	-	1/1/1/1	-
4	BME	D	103	-	-	1/1/1/1	-
3	EDO	A	1403	-	-	1/1/1/1	-
3	EDO	C	1403	-	-	1/1/1/1	-
4	BME	A	1405	-	-	0/1/1/1	-
3	EDO	C	1401	-	-	1/1/1/1	-
3	EDO	C	1404	-	-	0/1/1/1	-
4	BME	C	1405	-	-	0/1/1/1	-
3	EDO	C	1402	-	-	1/1/1/1	-
3	EDO	D	102	-	-	0/1/1/1	-
3	EDO	A	1404	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	101	EDO	O1-C1-C2-O2
3	A	1404	EDO	O1-C1-C2-O2
3	C	1403	EDO	O1-C1-C2-O2
4	D	103	BME	O1-C1-C2-S2
3	A	1403	EDO	O1-C1-C2-O2
3	C	1401	EDO	O1-C1-C2-O2
3	C	1402	EDO	O1-C1-C2-O2
3	D	101	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1130/1304 (86%)	1.24	167 (14%) 5 4	41, 81, 132, 211	8 (0%)
1	C	1123/1304 (86%)	1.61	294 (26%) 1 1	42, 95, 149, 206	1 (0%)
2	D	48/54 (88%)	0.66	4 (8%) 17 15	54, 83, 178, 252	0
2	F	48/54 (88%)	1.11	8 (16%) 4 3	33, 48, 125, 164	0
All	All	2349/2716 (86%)	1.40	473 (20%) 3 2	33, 88, 146, 252	9 (0%)

All (473) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350[A]	ALA	8.4
1	A	349[A]	GLN	6.5
1	A	561	GLY	6.4
1	C	561	GLY	6.1
1	A	560	SER	6.0
1	A	351[A]	GLY	6.0
1	C	916	ALA	4.8
1	C	926	ALA	4.7
1	C	920	VAL	4.7
1	C	955	VAL	4.7
1	A	556	PRO	4.7
1	C	399	VAL	4.6
1	C	951	LEU	4.3
1	A	1135	VAL	4.3
1	C	915	PHE	4.3
1	C	856	PHE	4.2
1	C	1135	VAL	4.2
1	C	560	SER	4.2
1	C	866	PHE	4.2
1	C	802	LEU	4.2
1	A	558	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	812	ALA	4.1
1	C	868	ALA	4.1
1	C	865	LEU	4.1
1	A	1131	VAL	4.0
1	C	556	PRO	4.0
1	C	911	LEU	4.0
1	C	914	LEU	4.0
1	A	1134	THR	4.0
1	A	1133	LEU	3.9
1	C	963	ILE	3.9
1	A	494	GLU	3.9
1	C	984	LEU	3.9
1	C	1133	LEU	3.9
1	A	885	ALA	3.9
1	C	977	THR	3.9
1	A	252	VAL	3.7
1	C	76	PRO	3.7
1	C	890	LEU	3.7
1	C	188	ALA	3.6
1	C	896	LEU	3.5
1	C	947	LEU	3.5
1	C	1134	THR	3.5
1	A	699	GLY	3.5
1	C	555	ALA	3.5
1	C	925	VAL	3.4
1	C	747	ALA	3.4
1	A	408	LEU	3.4
1	C	922	ASP	3.4
1	A	694	PHE	3.4
1	C	694	PHE	3.4
1	A	802	LEU	3.4
1	C	855	LEU	3.4
1	C	857	ALA	3.4
1	C	931	ILE	3.4
1	C	1	MET	3.3
1	A	562	LEU	3.3
1	C	990	LEU	3.3
1	A	398	ILE	3.3
1	C	667	THR	3.3
1	C	962	THR	3.3
1	A	803	VAL	3.3
1	C	971	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	3.3
2	F	39	U	3.3
1	A	17	PRO	3.3
1	C	941	ILE	3.3
1	C	557	GLU	3.3
1	A	951	LEU	3.2
1	C	418	ILE	3.2
1	C	800	TYR	3.2
1	C	1035	TRP	3.2
1	A	1136	GLY	3.2
1	A	702	SER	3.2
1	C	908	MET	3.2
1	C	187	PHE	3.2
1	A	1066	GLY	3.2
1	C	533	ALA	3.2
1	C	923	GLU	3.2
1	C	1139	ALA	3.2
1	C	315	ALA	3.1
1	C	1136	GLY	3.1
1	A	1060	VAL	3.1
1	C	74	PRO	3.1
1	C	466	GLN	3.1
1	C	473	ARG	3.1
1	C	986	GLY	3.1
1	C	985	VAL	3.1
1	C	700	TYR	3.1
1	A	793	TRP	3.1
1	C	75	THR	3.1
1	C	912	SER	3.1
1	C	944	ALA	3.1
1	A	1064	ALA	3.1
1	C	974	ALA	3.1
1	C	252	VAL	3.1
1	C	942	VAL	3.1
1	A	129	LEU	3.1
1	C	129	LEU	3.1
1	A	698	ILE	3.0
1	C	1160	GLY	3.0
2	F	40	C	3.0
1	A	955	VAL	3.0
1	A	352[A]	ASP	3.0
1	C	983	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	495	ALA	3.0
1	C	156	ALA	3.0
1	C	854	ALA	3.0
1	C	1068	PRO	3.0
1	A	947	LEU	3.0
1	A	348[A]	GLN	3.0
1	A	718	ARG	3.0
1	C	898	GLY	3.0
1	C	131	PHE	3.0
1	A	74	PRO	3.0
1	A	944	ALA	3.0
1	C	1144	ALA	3.0
1	C	741	ILE	3.0
1	C	902	ILE	3.0
1	C	1128	LEU	2.9
1	C	169	VAL	2.9
1	C	753	VAL	2.9
1	C	989	TYR	2.9
1	C	965	PRO	2.9
1	C	860	ALA	2.9
1	A	498	VAL	2.9
1	C	949	THR	2.9
1	A	493	LYS	2.9
1	C	310	ALA	2.9
1	A	557	GLU	2.9
1	C	562	LEU	2.8
1	C	994	LEU	2.8
1	C	95	VAL	2.8
1	C	793	TRP	2.8
1	C	744	GLY	2.8
1	A	18	ALA	2.8
1	C	127	ALA	2.8
1	C	893	ALA	2.8
1	C	910	VAL	2.8
1	A	667	THR	2.8
1	C	895	THR	2.8
1	C	978	ILE	2.8
1	C	899	LEU	2.8
1	C	133	ALA	2.8
1	C	362	ALA	2.8
1	C	929	ALA	2.8
1	C	892	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	75	THR	2.8
1	A	306	GLY	2.8
1	C	1148	GLN	2.8
1	C	626	TYR	2.8
1	C	1031	ALA	2.8
1	C	81	PHE	2.8
1	A	153	GLY	2.7
1	A	489	TRP	2.7
1	C	859	PRO	2.7
1	A	315	ALA	2.7
1	A	868	ALA	2.7
1	A	1063	ARG	2.7
1	C	345	TYR	2.7
1	C	973	ALA	2.7
1	A	590	PHE	2.7
2	F	43	U	2.7
2	F	7	C	2.7
2	D	54	G	2.7
1	A	138	PRO	2.7
1	C	928	LEU	2.7
1	C	1118	ALA	2.7
1	A	81	PHE	2.7
1	C	584	ASP	2.7
1	C	3	ILE	2.7
1	A	555	ALA	2.7
1	C	1156	ALA	2.7
1	C	120	PHE	2.7
1	A	705	GLU	2.7
1	A	127	ALA	2.6
1	A	309	ALA	2.6
1	C	658	ALA	2.6
1	C	943	ALA	2.6
1	A	578	TYR	2.6
1	C	192	VAL	2.6
1	C	699	GLY	2.6
1	A	64	ARG	2.6
1	C	606	PRO	2.6
1	C	151	LYS	2.6
1	A	472	ALA	2.6
1	C	230	ALA	2.6
1	A	131	PHE	2.6
1	C	975	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	45	C	2.6
1	C	21	LEU	2.6
1	C	100	LEU	2.6
2	F	42	U	2.6
1	C	140	ALA	2.6
1	C	737	TRP	2.6
1	C	972	ALA	2.6
1	A	255	ARG	2.6
1	C	91	PHE	2.6
1	C	358	TYR	2.6
1	C	938	LYS	2.6
1	C	1153	MET	2.6
1	A	462	GLY	2.6
1	C	61	PRO	2.6
1	C	749	THR	2.6
1	C	662	VAL	2.6
1	C	54	ILE	2.6
1	C	698	ILE	2.6
1	C	905	TYR	2.6
1	C	1151	LEU	2.5
1	A	958	CYS	2.5
1	C	1030	GLY	2.5
1	A	240	VAL	2.5
1	C	368	LYS	2.5
1	C	552	VAL	2.5
1	C	398	ILE	2.5
1	C	918	HIS	2.5
1	A	700	TYR	2.5
1	C	94	LEU	2.5
1	C	1029	LEU	2.5
1	A	1	MET	2.5
1	C	189	PRO	2.5
1	C	306	GLY	2.5
1	C	327	THR	2.5
1	C	467	THR	2.5
1	C	1038	THR	2.5
1	A	476	PHE	2.5
1	C	558	VAL	2.5
1	C	164	TYR	2.5
1	A	582	LEU	2.5
1	A	890	LEU	2.5
1	C	159	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	444	LEU	2.5
1	C	565	LEU	2.5
2	F	44	A	2.5
1	A	551	ALA	2.5
1	A	857	ALA	2.5
1	C	554	ASP	2.5
1	C	711	ALA	2.5
1	C	462	GLY	2.5
1	C	676	GLY	2.5
1	C	184	THR	2.5
1	A	497	HIS	2.5
1	A	1139	ALA	2.5
1	C	495	ALA	2.5
1	A	254	GLY	2.5
1	C	249	PRO	2.5
2	F	50	G	2.5
1	A	701	GLU	2.4
1	A	935	THR	2.4
1	A	169	VAL	2.4
1	A	226	VAL	2.4
1	A	892	VAL	2.4
1	A	1128	LEU	2.4
1	C	535	TYR	2.4
1	A	307	LYS	2.4
1	A	961	LYS	2.4
1	A	959	HIS	2.4
1	C	29	GLY	2.4
1	C	861	THR	2.4
1	C	1067	THR	2.4
1	A	63	SER	2.4
1	A	141	PHE	2.4
1	A	988	VAL	2.4
1	C	25	ILE	2.4
1	C	1131	VAL	2.4
1	C	50	TRP	2.4
1	A	1044	ASN	2.4
1	C	242	ALA	2.4
1	C	743	PRO	2.4
1	C	1025	ALA	2.4
1	A	970	SER	2.4
1	C	546	SER	2.4
1	C	579	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1162	VAL	2.4
2	D	39	U	2.4
1	C	739	LEU	2.4
1	C	993	HIS	2.4
1	A	236	ALA	2.4
1	C	123	ALA	2.4
1	C	939	SER	2.4
1	A	187	PHE	2.4
1	C	339	MET	2.4
1	C	1102	LEU	2.4
1	C	927	ARG	2.4
1	C	924	GLU	2.4
1	A	122	PRO	2.3
1	A	888	PRO	2.3
1	C	153	GLY	2.3
1	A	98	ALA	2.3
1	A	1033	ALA	2.3
1	C	304	ALA	2.3
1	A	222	THR	2.3
1	C	222	THR	2.3
1	C	631	THR	2.3
1	A	95	VAL	2.3
1	C	109	PHE	2.3
1	C	288	VAL	2.3
1	C	852	PHE	2.3
1	C	988	VAL	2.3
1	A	301	ARG	2.3
1	C	649	LEU	2.3
1	C	701	GLU	2.3
1	A	316	ASP	2.3
1	A	92	TRP	2.3
1	C	145	TRP	2.3
1	C	1150	TYR	2.3
1	A	471	GLY	2.3
1	C	347	GLY	2.3
1	A	869	THR	2.3
1	C	746	THR	2.3
1	A	485[A]	GLU	2.3
1	C	225	VAL	2.3
1	C	226	VAL	2.3
1	C	1152	GLN	2.3
1	C	659	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	90	ALA	2.3
1	C	732	ALA	2.3
1	C	797	GLN	2.3
1	C	1163	GLN	2.3
1	A	109	PHE	2.3
1	A	499	VAL	2.3
1	A	866	PHE	2.3
1	A	94	LEU	2.3
1	C	858	ASN	2.3
1	C	148	ALA	2.3
1	C	589	ALA	2.3
1	C	921	ARG	2.3
1	C	542	SER	2.3
1	A	120	PHE	2.2
1	A	225	VAL	2.3
1	A	272	VAL	2.3
1	A	303	CYS	2.2
1	A	308	ASN	2.2
1	C	675	ASP	2.2
1	C	285	GLY	2.2
1	C	816	ARG	2.2
1	C	1101	ARG	2.2
1	C	83	ALA	2.2
1	C	146	TYR	2.2
1	C	610	ALA	2.2
1	C	903	ALA	2.2
1	C	981	HIS	2.2
1	A	942	VAL	2.2
1	C	1115	LEU	2.2
1	C	531	PHE	2.2
1	A	314	PRO	2.2
1	C	1000	MET	2.2
1	C	932	GLU	2.2
1	A	709	LYS	2.2
1	C	239	ALA	2.2
1	C	191	LEU	2.2
1	C	240	VAL	2.2
1	C	1154	VAL	2.2
1	A	144	ARG	2.2
1	C	308	ASN	2.2
1	C	755	PRO	2.2
1	C	166	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	46	C	2.2
1	A	492	ALA	2.2
1	A	795	ALA	2.2
1	C	354	ALA	2.2
1	C	472	ALA	2.2
1	C	646	ALA	2.2
1	C	647	THR	2.2
1	C	909	ALA	2.2
1	A	800	TYR	2.2
1	C	58	TYR	2.2
1	A	931	ILE	2.2
1	C	1073	LEU	2.2
1	A	62	ASP	2.2
1	A	124	ASP	2.2
1	C	395	MET	2.2
1	A	744	GLY	2.2
1	A	188	ALA	2.2
1	C	1121	THR	2.2
1	A	116	TYR	2.1
1	A	601	ARG	2.1
1	C	1010	TYR	2.1
1	A	3	ILE	2.1
1	C	748	MET	2.1
1	A	151	LYS	2.1
1	A	1068	PRO	2.1
1	A	1138	PRO	2.1
1	C	246	PHE	2.1
1	C	314	PRO	2.1
1	C	1057	HIS	2.1
1	C	207	GLY	2.1
1	C	798	GLY	2.1
1	A	133	ALA	2.1
1	A	304	ALA	2.1
1	A	658	ALA	2.1
1	A	747	ALA	2.1
1	C	492	ALA	2.1
1	C	745	ALA	2.1
1	C	970	SER	2.1
1	C	717	TYR	2.1
1	A	849	LEU	2.1
1	A	941	ILE	2.1
1	C	167	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	709	LYS	2.1
1	C	1004	ILE	2.1
1	C	913	ASP	2.1
1	A	743	PRO	2.1
1	A	1035	TRP	2.1
1	C	272	VAL	2.1
1	C	412	VAL	2.1
1	C	417	VAL	2.1
1	C	532	VAL	2.1
1	C	575	VAL	2.1
1	C	1141	VAL	2.1
1	C	313	PHE	2.1
1	C	710	GLN	2.1
1	C	862	PHE	2.1
1	A	20	GLY	2.1
1	A	585	THR	2.1
1	A	749	THR	2.1
1	C	543	THR	2.1
1	C	964	SER	2.1
1	A	538	LYS	2.1
1	A	865	LEU	2.1
1	C	946	GLU	2.1
1	C	1061	LEU	2.1
1	A	703	ASP	2.1
1	C	1127	HIS	2.1
1	A	249	PRO	2.1
1	A	662	VAL	2.1
1	C	193	VAL	2.1
1	A	14	PHE	2.1
1	C	718[A]	ARG	2.1
1	A	559	SER	2.1
1	C	27	THR	2.1
1	C	63	SER	2.1
1	C	1147	SER	2.1
1	A	140	ALA	2.1
1	A	818	ALA	2.1
1	C	814	ALA	2.1
1	C	775	MET	2.1
1	C	494	GLU	2.1
1	A	418	ILE	2.1
1	A	945	GLN	2.1
1	A	1061	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	57	ILE	2.1
1	C	1164	ASN	2.1
1	A	76	PRO	2.1
1	A	563	PRO	2.1
1	C	135	PRO	2.1
1	C	363	GLY	2.1
1	C	695	ARG	2.1
1	C	919	LYS	2.0
1	A	467	THR	2.0
1	A	746	THR	2.0
1	A	886	SER	2.0
1	C	536	ALA	2.0
1	C	1036	ALA	2.0
2	F	41	A	2.0
1	A	444	LEU	2.0
1	A	796	LEU	2.0
1	C	582	LEU	2.0
1	C	758	ILE	2.0
1	C	1138	PRO	2.0
1	C	578	TYR	2.0
1	C	301	ARG	2.0
1	C	917	LYS	2.0
1	C	954	LYS	2.0
1	C	663	MET	2.0
1	A	40	SER	2.0
1	C	350	ALA	2.0
1	C	357	HIS	2.0
1	C	940	GLN	2.0
1	A	1029	LEU	2.0
1	A	135	PRO	2.0
1	A	965	PRO	2.0
1	C	372	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
3	EDO	C	1403	4/4	0.56	0.25	78,78,80,82	0
3	EDO	A	1404	4/4	0.72	0.17	85,85,89,92	0
3	EDO	D	102	4/4	0.72	0.27	67,74,77,80	0
4	BME	C	1405	4/4	0.77	0.18	95,96,96,96	0
3	EDO	A	1402	4/4	0.81	0.18	63,64,69,70	0
3	EDO	A	1403	4/4	0.82	0.17	64,70,71,75	0
3	EDO	C	1402	4/4	0.86	0.17	61,66,68,69	0
3	EDO	A	1401	4/4	0.88	0.22	52,52,53,55	0
3	EDO	D	101	4/4	0.88	0.20	49,50,52,52	0
3	EDO	F	101	4/4	0.89	0.19	43,45,45,46	0
3	EDO	C	1401	4/4	0.90	0.22	51,52,56,59	0
4	BME	A	1405	4/4	0.91	0.12	74,76,76,81	0
4	BME	D	103	4/4	0.91	0.18	68,68,73,74	0
3	EDO	C	1404	4/4	0.94	0.17	68,68,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.