

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 13, 2022 - 09:16 am GMT

PDB ID	:	7OS0
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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.



Motria	Whole archive	Similar resolution				
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$				
R <sub>free</sub>	130704	4898 (2.20-2.20)				
Clashscore	141614	5594(2.20-2.20)				
Ramachandran outliers	138981	5503 (2.20-2.20)				
Sidechain outliers	138945	5504 (2.20-2.20)				
RSRZ outliers	127900	4800 (2.20-2.20)				
RNA backbone	3102	1032 (2.60-1.80)				

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 o	of chain		
			29%			
1	A	1304	81%		5%	13%
			37%			
1	С	1304	80%		6%	14%
			26%			
2	D	54	52%	31%	6%	11%
			22%			
2	F	54	48%	33%	7%	11%



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
3	EDO	А	1404	-	-	-	Х
3	EDO	D	102	-	-	-	Х



## 2 Entry composition (i)

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.

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

• Molecule 1 is a protein called Cas13a.

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

There are 38 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
С	1292	LYS	-	expression tag	UNP D5AUW0
С	1293	LEU	-	expression tag	UNP D5AUW0
С	1294	ALA	-	expression tag	UNP D5AUW0
С	1295	ALA	-	expression tag	UNP D5AUW0
С	1296	ALA	-	expression tag	UNP D5AUW0
С	1297	LEU	-	expression tag	UNP D5AUW0
С	1298	GLU	-	expression tag	UNP D5AUW0
С	1299	HIS	-	expression tag	UNP D5AUW0
С	1300	HIS	-	expression tag	UNP D5AUW0
С	1301	HIS	-	expression tag	UNP D5AUW0
С	1302	HIS	-	expression tag	UNP D5AUW0
С	1303	HIS	-	expression tag	UNP D5AUW0
С	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 993	C 444	N 172	O 330	Р 47	0	0	1
2	F	48	Total 993	C 444	N 172	O 330	Р 47	0	0	1

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 4	С 2	O 2	0	0

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 4	С 2	0 1	S 1	0	0



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
4	C	1	Total	С	0	S	0	0
4	U	1	4	2	1	1	0	0
4	Л	1	Total	С	0	S	0	0
4	D		4	2	1	1	0	

• Molecule 5 is water.

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



## 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









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	61.39Å $91.08$ Å $136.51$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$89.99^{\circ}$ $103.69^{\circ}$ $97.65^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.12 - 2.20	Depositor
Resolution (A)	47.08 - 2.20	EDS
% Data completeness	97.8 (47.12-2.20)	Depositor
(in resolution range)	97.8 (47.08-2.20)	EDS
$R_{merge}$	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.49 (at 2.20 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.218 , $0.256$	Depositor
$\Pi, \Pi_{free}$	0.258 , $0.285$	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 $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+l	Xtriage
$F_o, F_c$ correlation	0.94	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.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: BME, EDO

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).

Mal	Chain	Bo	nd lengths	Bond angles		
NIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.39	0/9130	0.57	0/12313	
1	С	0.40	2/9028~(0.0%)	0.58	4/12174~(0.0%)	
2	D	0.34	0/1107	0.77	0/1722	
2	F	0.33	0/1107	0.76	0/1722	
All	All	0.39	2/20372~(0.0%)	0.60	4/27931~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	718[A]	ARG	C-O	6.43	1.35	1.23
1	С	718[B]	ARG	C-O	6.43	1.35	1.23

 $\mathbf{Z}$ Mol Chain Res Observed(<sup>o</sup>) Ideal(°) Type Atoms  $\overline{\mathbf{C}}$ ARG 5.99132.67 718[A] CA-C-O 120.10 1 1 С ARG CA-C-O 5.99132.67 120.10 718|B| С 1 ARG O-C-N -5.04114.63 122.70 718 A  $\overline{\mathrm{C}}$ O-C-N 1 718[B] ARG -5.04114.63 122.70

All (4) bond angle outliers are listed below:

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.



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	8945	0	8995	44	0
1	С	8850	0	8909	54	0
2	D	993	0	507	5	0
2	F	993	0	507	5	0
3	А	16	0	24	0	0
3	С	16	0	24	0	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
4	А	4	0	6	0	0
4	С	4	0	6	0	0
4	D	4	0	6	0	0
5	А	331	0	0	1	0
5	С	177	0	0	0	0
5	D	48	0	0	0	0
5	F	74	0	0	0	0
All	All	20467	0	19002	104	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 (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:1060:VAL:HG11	1:C:1073:LEU:HD21	1.49	0.93
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:A:351[A]:GLY:O	1:A:352[A]:ASP:HB2	1.92	0.68
1:C:1014:TYR:HB2	1:C:1081:MET:HE1	1.77	0.67
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:1014:TYR:HB2	1:C:1081:MET:CE	2.26	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
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:907:HIS:HD1	1:C:997:HIS:HE1	1.49	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:348[A]:GLN:C	1:A:350[A]:ALA:H	2.08	0.56
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: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:A:775:MET:CE	1:A:783:VAL:HG22	2.41	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:C:332:VAL:HG12	1:C:336:MET:HE2	1.94	0.49
1:C:336:MET:HE3	1:C:1040:ALA:HB2	1.94	0.49
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
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:C:1080:MET:HG2	1:C:1081:MET:HE3	1.97	0.46
1:A:775:MET:HE3	1:A:783:VAL:HG22	1.95	0.46
1:A:349[B]:GLN:O	1:A:350[B]:ALA:HB2	2.16	0.46
1:C:683:LEU:HD12	1:C:683:LEU:HA	1.78	0.46
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:A:705:GLU:OE1	1:A:708:ARG:NH1	2.50	0.45



	• pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:1138:PRO:O	1:C:1139:ALA:HB3	2.16	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: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: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:560:SER:HB2	1:C:788:HIS:ND1	2.33	0.43
1:C:1014:TYR:HB2	1:C:1081:MET:HE2	1.99	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:A:79:MET:HE3	1:A:141:PHE:HE2	1.84	0.42
1:A:1070:LEU:O	1:A:1074:VAL:HG23	2.18	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: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:568:LEU:HD23	1:C:568:LEU:C	2.41	0.41
1:C:802:LEU:HD22	1:C:802:LEU:N	2.36	0.41
1:A:348[A]:GLN:C	1:A:350[A]:ALA:N	2.73	0.41
1:C:293:ASP:OD2	1:C:297:LYS:HE2	2.20	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:568:LEU:C	1:A:568:LEU:HD23	2.41	0.41
1:A:1106:LEU:HD21	1:A:1108:TRP:CZ2	2.57	0.40
1:A:348[B]:GLN:CD	1:A:348[B]:GLN:N	2.74	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



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Perce	entiles
1	А	1128/1304 (86%)	1106 (98%)	18 (2%)	4 (0%)	34	37
1	С	1112/1304 (85%)	1092 (98%)	20 (2%)	0	100	100
All	All	2240/2608~(86%)	2198 (98%)	38 (2%)	4 (0%)	51	55

All (4) Ramachandran outliers are listed below:

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

#### 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	А	910/1049~(87%)	897~(99%)	13~(1%)	67 80



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntile	$\mathbf{s}$
1	С	901/1049 (86%)	888 (99%)	13 (1%)	67	80	
All	All	1811/2098~(86%)	1785 (99%)	26 (1%)	69	80	

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	74	PRO
1	А	103	ASP
1	А	142	HIS
1	А	247	ASP
1	А	307	LYS
1	А	348[A]	GLN
1	А	348[B]	GLN
1	А	464[A]	ARG
1	A	464[B]	ARG
1	А	626	TYR
1	А	753	VAL
1	А	802	LEU
1	А	917	LYS
1	С	104	SER
1	С	124	ASP
1	С	142	HIS
1	С	183	LYS
1	С	187	PHE
1	С	244	GLN
1	С	406	ARG
1	С	683	LEU
1	С	801	GLU
1	С	892	VAL
1	С	946	GLU
1	С	1141	VAL
1	С	1166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	292	HIS
1	А	449	ASN
1	А	674	ASN
1	А	1044	ASN
1	А	1127	HIS



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Mol	Chain	Res	Type
1	С	49	GLN
1	С	328	HIS
1	С	330	ASN
1	С	768	GLN
1	С	918	HIS
1	С	997	HIS
1	С	1075	ASN
1	С	1127	HIS

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	46/54~(85%)	14 (30%)	7(15%)
2	F	46/54~(85%)	17 (36%)	8 (17%)
All	All	92/108~(85%)	31 (33%)	15~(16%)

All (31) RNA backbone outliers are listed below:

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



Mol	Chain	$\mathbf{Res}$	Type
2	F	39	U
2	F	40	С
2	F	41	А
2	F	42	U
2	F	43	U
2	F	44	А
2	F	45	С
2	F	50	G
2	F	51	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	17	А
2	D	18	А
2	D	20	А
2	D	21	С
2	D	41	А
2	D	44	А
2	D	50	G
2	F	17	А
2	F	18	А
2	F	20	А
2	F	21	С
2	F	38	U
2	F	41	А
2	F	44	А
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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

14 ligands are modelled in this entry.



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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).

Mal	Type	Chain	Dog	Link	B	ond leng	gths	E	Bond ang	gles
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	EDO	С	1403	-	3,3,3	0.06	0	2,2,2	0.18	0
3	EDO	A	1403	-	3,3,3	0.05	0	2,2,2	0.19	0
3	EDO	С	1404	-	3,3,3	0.06	0	2,2,2	0.19	0
3	EDO	F	101	-	3,3,3	0.05	0	2,2,2	0.24	0
4	BME	D	103	-	3,3,3	0.15	0	1,2,2	0.08	0
3	EDO	D	102	-	3,3,3	0.06	0	2,2,2	0.18	0
4	BME	С	1405	-	3,3,3	0.14	0	1,2,2	0.12	0
3	EDO	D	101	-	3,3,3	0.05	0	2,2,2	0.18	0
4	BME	А	1405	-	3,3,3	0.14	0	1,2,2	0.00	0
3	EDO	А	1404	-	3,3,3	0.06	0	2,2,2	0.19	0
3	EDO	С	1402	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	А	1401	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	С	1401	-	3,3,3	0.07	0	2,2,2	0.28	0
3	EDO	А	1402	-	3,3,3	0.05	0	2,2,2	0.14	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	С	1403	-	-	1/1/1/1	-
3	EDO	А	1403	-	-	1/1/1/1	-
3	EDO	С	1404	-	-	0/1/1/1	-
3	EDO	F	101	-	-	1/1/1/1	-
4	BME	D	103	-	-	1/1/1/1	-
3	EDO	D	102	-	-	0/1/1/1	-
4	BME	С	1405	-	-	0/1/1/1	-
3	EDO	D	101	-	-	1/1/1/1	-
4	BME	А	1405	-	-	0/1/1/1	-
3	EDO	А	1404	-	-	1/1/1/1	-
3	EDO	С	1402	-	-	1/1/1/1	-
3	EDO	А	1401	-	-	0/1/1/1	-
3	EDO	С	1401	-	-	1/1/1/1	-
3	EDO	А	1402	-	-	0/1/1/1	-



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
4	D	103	BME	O1-C1-C2-S2
3	F	101	EDO	O1-C1-C2-O2
3	А	1404	EDO	O1-C1-C2-O2
3	С	1403	EDO	O1-C1-C2-O2
3	С	1401	EDO	O1-C1-C2-O2
3	А	1403	EDO	O1-C1-C2-O2
3	С	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 (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,  $95^{th}$  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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	1130/1304~(86%)	1.88	379 (33%) 0	0	54, 81, 132, 211	0
1	С	1123/1304 (86%)	2.18	487 (43%) 0	0	64, 95, 149, 206	0
2	D	48/54~(88%)	1.89	14 (29%) 0	0	54, 83, 178, 252	0
2	F	48/54~(88%)	1.48	12 (25%) 0	0	33, 48, 125, 164	0
All	All	2349/2716 (86%)	2.01	892 (37%) 0	0	33, 88, 146, 252	0

All (892) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	399	VAL	15.6
1	А	74	PRO	14.2
1	А	243	ALA	11.8
1	А	802	LEU	10.8
1	А	125	SER	10.8
1	С	247	ASP	10.7
1	С	249	PRO	10.7
1	С	252	VAL	10.0
1	С	802	LEU	9.7
1	А	17	PRO	9.6
1	С	98	ALA	9.1
1	А	1064	ALA	9.1
1	С	251	GLN	9.1
1	А	561	GLY	9.0
1	А	887	GLU	8.8
1	С	350	ALA	8.6
1	С	243	ALA	8.4
1	А	124	ASP	8.3
1	С	128	LYS	8.3
1	С	129	LEU	8.3
1	А	247	ASP	8.1



Mol	Chain	Res	Type	RSRZ
1	С	74	PRO	8.0
1	А	472	ALA	7.9
1	А	246	PHE	7.9
1	А	121	GLN	7.8
1	С	1067	THR	7.8
1	С	136	PRO	7.7
2	F	41	A	7.6
1	А	136	PRO	7.4
1	С	248	PRO	7.4
1	С	246	PHE	7.4
1	А	494	GLU	7.3
1	С	955	VAL	7.3
1	С	242	ALA	7.2
1	C	245	ALA	7.2
1	С	123	ALA	7.2
1	С	121	GLN	7.0
1	С	244	GLN	6.9
1	А	554	ASP	6.9
1	С	973	ALA	6.8
1	А	1063	ARG	6.8
1	С	472	ALA	6.6
1	А	245	ALA	6.5
1	С	656	THR	6.5
1	С	125	SER	6.5
1	С	1165	PRO	6.5
1	А	252	VAL	6.5
1	А	249	PRO	6.4
2	F	42	U	6.4
1	С	187	PHE	6.4
1	А	128	LYS	6.3
1	С	942	VAL	6.3
2	F	54	G	6.2
1	С	556	PRO	6.2
1	C	984	LEU	6.1
1	А	935	THR	6.1
1	С	99	GLY	6.1
1	С	554	ASP	6.1
1	А	1065	ASP	6.0
1	C	1065	ASP	5.9
1	С	116	TYR	5.9
1	C	124	ASP	5.9
1	С	133	ALA	5.9



Mol	Chain	Res	Type	RSRZ
1	С	396	GLY	5.9
1	С	943	ALA	5.9
2	D	40	С	5.9
1	А	242	ALA	5.9
1	А	886	SER	5.9
1	А	16	ASP	5.9
1	С	941	ILE	5.8
1	А	351[A]	GLY	5.8
1	С	239	ALA	5.8
1	С	127	ALA	5.7
1	С	812	ALA	5.7
1	А	885	ALA	5.6
1	С	585	THR	5.6
1	С	417	VAL	5.6
1	А	127	ALA	5.6
1	С	16	ASP	5.5
1	С	714	ILE	5.5
2	D	54	G	5.5
1	С	95	VAL	5.5
1	А	751	ALA	5.5
1	С	691	ALA	5.4
1	А	248	PRO	5.4
1	С	132	GLU	5.4
1	С	351	GLY	5.4
1	А	18	ALA	5.4
1	А	129	LEU	5.3
1	А	350[A]	ALA	5.3
1	А	123	ALA	5.3
1	А	1031	ALA	5.3
1	А	869	THR	5.3
2	D	41	A	5.2
1	С	241	SER	5.2
1	С	372	ILE	5.1
1	А	251	GLN	5.1
1	А	812	ALA	5.1
1	А	347	GLY	5.1
1	А	417	VAL	5.1
1	А	63	SER	5.0
1	А	555	ALA	5.0
1	С	184	THR	5.0
1	С	120	PHE	5.0
1	С	349	GLN	5.0



Mol	Chain	Res	Type	RSRZ
1	С	250	ARG	4.9
1	С	1029	LEU	4.9
1	С	558	VAL	4.9
1	А	352[A]	ASP	4.9
1	А	90	ALA	4.9
1	С	868	ALA	4.9
1	А	418	ILE	4.9
1	С	561	GLY	4.9
1	С	139	GLN	4.9
1	С	1064	ALA	4.8
1	С	466	GLN	4.7
1	С	126	GLY	4.7
1	А	419	SER	4.7
2	F	40	С	4.7
1	С	908	MET	4.7
1	С	718[A]	ARG	4.7
1	А	239	ALA	4.7
1	С	45	ALA	4.7
1	А	77	SER	4.7
1	А	138	PRO	4.7
1	С	404	ASN	4.6
2	F	39	U	4.6
2	D	39	U	4.6
1	А	694	PHE	4.6
1	С	1112	ASP	4.6
1	С	916	ALA	4.6
1	А	15	GLY	4.6
1	А	1061	LEU	4.6
1	С	695	ARG	4.6
1	С	240	VAL	4.6
1	С	867	MET	4.6
1	А	813	ASP	4.6
1	A	698	ILE	4.5
1	С	842	GLY	4.5
1	А	92	TRP	4.5
1	A	811	GLN	4.5
1	С	863	ASP	4.5
1	C	983	PHE	4.5
1	А	888	PRO	4.5
1	С	448	GLY	4.5
1	С	889	GLU	4.5
1	С	683	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	С	18	ALA	4.5
1	C	155	ASP	4.5
1	C	887	GLU	4.5
1	C	1140	ALA	4.4
1	A	139	GLN	4.4
1	А	560	SER	4.4
1	C	698	ILE	4.4
1	C	711	ALA	4.4
1	C	443	ARG	4.4
1	C	542	SER	4.3
1	A	670	LEU	4.3
1	A	601	ARG	4.3
1	С	555	ALA	4.3
1	C	562	LEU	4.3
1	Ā	464[A]	ARG	4.3
1	A	937	GLU	4.3
1	C	1	MET	4.3
1	C	1138	PRO	4.3
1	C	209	ALA	4.3
1	A	126	GLY	4.3
1	С	17	PRO	4.2
1	C	888	PRO	4.2
1	A	98	ALA	4.2
1	С	744	GLY	4.2
1	С	352	ASP	4.2
1	А	253	SER	4.2
1	А	349[A]	GLN	4.2
1	С	347	GLY	4.2
1	С	966	GLU	4.2
1	С	77	SER	4.2
1	А	281	ASP	4.2
1	А	64	ARG	4.2
1	С	655	VAL	4.2
1	С	94	LEU	4.1
1	С	866	PHE	4.1
1	С	920	VAL	4.1
1	С	690	THR	4.1
1	С	161	ALA	4.1
1	С	662	VAL	4.1
1	С	923	GLU	4.1
1	А	99	GLY	4.1
1	А	705	GLU	4.1

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Mol	Chain	Res	Type	RSRZ		
1	А	348[A]	GLN	4.1		
1	С	951	LEU	4.1		
1	А	691	ALA	4.1		
1	С	365	THR	4.1		
1	А	20	GLY	4.1		
1	С	670	LEU	4.1		
1	С	914	LEU	4.1		
2	D	42	U	4.1		
1	А	556	PRO	4.0		
1	А	106	TYR	4.0		
1	С	787	LEU	4.0		
1	С	1118	ALA	4.0		
1	А	19	GLY	4.0		
1	А	116	TYR	4.0		
1	A	132	GLU	4.0		
1	С	367	ILE	4.0		
1	А	257	LEU	4.0		
1	С	694	PHE	4.0		
2	F	43	U	4.0		
1	С	978	ILE	4.0		
1	С	188	ALA	4.0		
1	С	986	GLY	4.0		
1	С	418	ILE	4.0		
1	А	135	PRO	4.0		
1	С	705	GLU	3.9		
1	А	372	ILE	3.9		
1	С	1066	GLY	3.9		
2	D	44	A	3.9		
1	А	563	PRO	3.9		
2	D	43	U	3.9		
1	С	204	LEU	3.9		
1	А	272	VAL	3.9		
1	С	106	TYR	3.8		
1	А	81	PHE	3.8		
1	С	339	MET	3.8		
1	С	829	LEU	3.8		
1	A	816	ARG	3.8		
1	А	499	VAL	3.8		
1	C	739	LEU	3.8		
1	С	934	GLU	3.8		
1	A	446	ALA	3.8		
1	A	585	THR	3.8		



Mol	Chain	Res	Type	RSRZ
1	С	792	LYS	3.8
1	С	626	TYR	3.8
1	С	931	ILE	3.8
1	С	423	MET	3.8
1	А	131	PHE	3.7
1	А	1	MET	3.7
1	А	889	GLU	3.7
1	А	303	CYS	3.7
1	С	530	ALA	3.7
1	А	714	ILE	3.7
1	С	783	VAL	3.7
1	С	376	LEU	3.7
1	С	788	HIS	3.7
1	С	1073	LEU	3.7
1	С	1032	GLY	3.7
1	С	373	PHE	3.7
1	С	1166	LYS	3.7
1	С	838	ALA	3.7
1	С	661	ASP	3.7
1	А	679	LEU	3.7
1	А	688	GLY	3.7
1	А	1166	LYS	3.7
2	F	44	А	3.7
1	С	140	ALA	3.7
1	С	63	SER	3.7
1	С	915	PHE	3.7
1	С	918	HIS	3.7
1	А	1037	VAL	3.7
1	С	62	ASP	3.7
1	А	690	THR	3.7
1	С	977	THR	3.7
1	С	1160	GLY	3.7
1	С	278	CYS	3.6
1	С	858	ASN	3.6
1	А	803	VAL	3.6
1	А	1067	THR	3.6
1	С	975	ILE	3.6
1	С	912	SER	3.6
1	А	485[A]	GLU	3.6
1	A	700	TYR	3.6
1	А	240	VAL	3.6
1	А	62	ASP	3.6



Mol	Chain	Res	Type	RSRZ
1	С	795	ALA	3.5
1	С	79	MET	3.5
1	С	1063	ARG	3.5
1	С	122	PRO	3.5
1	А	378	VAL	3.5
1	А	1029	LEU	3.5
1	С	199	ILE	3.5
1	А	75	THR	3.5
1	С	167	LEU	3.5
1	А	103	ASP	3.5
1	А	970	SER	3.5
1	С	419	SER	3.5
1	А	955	VAL	3.5
1	А	133	ALA	3.5
1	С	940	GLN	3.4
1	С	1046	ASP	3.4
1	С	471	GLY	3.4
1	С	378	VAL	3.4
1	С	19	GLY	3.4
1	С	688	GLY	3.4
1	С	860	ALA	3.4
1	С	20	GLY	3.4
1	А	711	ALA	3.4
1	А	745	ALA	3.4
1	С	686	LEU	3.4
1	С	750	ARG	3.4
1	С	857	ALA	3.4
1	С	130	LYS	3.4
1	А	562	LEU	3.4
1	A	814	ALA	3.4
1	A	255	ARG	3.3
1	С	1109	GLN	3.3
1	A	405	ASP	3.3
1	C	272	VAL	3.3
1	A	584	ASP	3.3
1	C	854	ALA	3.3
1	С	21	LEU	3.3
1	С	856	PHE	3.3
1	C	707	ALA	3.3
1	A	396	GLY	3.3
1	С	15	GLY	3.3
1	С	166	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	А	466	GLN	3.3
1	А	741	ILE	3.3
1	А	95	VAL	3.3
1	А	943	ALA	3.3
1	С	303	CYS	3.3
1	С	560	SER	3.3
1	А	134	ASP	3.3
1	С	844	ALA	3.2
1	С	186	LYS	3.2
1	С	790	LEU	3.2
1	А	309	ALA	3.2
1	А	591	ALA	3.2
1	А	265	LEU	3.2
1	А	376	LEU	3.2
1	С	567	LEU	3.2
1	С	1128	LEU	3.2
1	А	109	PHE	3.2
1	А	1036	ALA	3.2
1	С	1036	ALA	3.2
1	С	363	GLY	3.2
1	С	793	TRP	3.2
1	С	115	PRO	3.2
1	С	972	ALA	3.2
1	С	974	ALA	3.2
1	С	470	LEU	3.2
1	С	565	LEU	3.2
1	С	1134	THR	3.2
1	С	781	SER	3.2
1	С	76	PRO	3.2
1	С	238	ALA	3.2
1	A	254	GLY	3.2
1	А	721	MET	3.2
1	А	868	ALA	3.1
1	C	283	ALA	3.1
1	C	606	PRO	3.1
1	А	787	LEU	3.1
1	С	786	LEU	3.1
1	С	281	ASP	3.1
1	С	35	LEU	3.1
1	С	544	LEU	3.1
1	С	584	ASP	3.1
1	С	847	PHE	3.1



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Mol	Chain	Res	Type	RSRZ
1	С	732	ALA	3.1
1	С	1072	ALA	3.1
1	А	278	CYS	3.1
1	А	833	LEU	3.1
1	А	1115	LEU	3.1
1	С	163	LEU	3.1
1	С	861	THR	3.1
1	А	54	ILE	3.1
1	С	910	VAL	3.1
1	С	50	TRP	3.1
1	С	41	SER	3.1
1	С	191	LEU	3.1
1	С	896	LEU	3.1
1	А	667	THR	3.1
1	А	1165	PRO	3.1
1	А	471	GLY	3.1
1	С	134	ASP	3.1
1	А	635	LEU	3.1
1	А	627	ALA	3.1
1	А	944	ALA	3.1
1	С	944	ALA	3.1
1	А	702	SER	3.0
1	А	477	LEU	3.0
1	С	796	LEU	3.0
1	С	1153	MET	3.0
1	С	475	GLY	3.0
1	А	707	ALA	3.0
1	С	91	PHE	3.0
1	С	1158	PHE	3.0
2	D	11	А	3.0
1	С	1091	VAL	3.0
1	С	559	SER	3.0
1	С	700	TYR	3.0
1	А	94	LEU	3.0
1	А	250	ARG	3.0
1	С	699	GLY	3.0
1	А	404	ASN	3.0
1	С	581	GLY	3.0
1	С	603	LEU	3.0
1	С	1050	GLN	3.0
1	С	1127	HIS	3.0
2	D	37	С	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	104	SER	3.0
1	С	532	VAL	3.0
1	С	852	PHE	3.0
1	С	947	LEU	3.0
1	А	916	ALA	3.0
1	С	374	VAL	3.0
1	А	308	ASN	3.0
1	А	656	THR	3.0
1	С	791	ARG	3.0
1	А	569	LEU	2.9
1	С	236	ALA	2.9
1	С	348	GLN	2.9
1	С	953	ASP	2.9
1	С	398	ILE	2.9
1	А	669	ARG	2.9
1	С	397	LYS	2.9
1	С	706	ASN	2.9
1	С	46	LEU	2.9
1	С	150	SER	2.9
1	А	1090	ALA	2.9
1	С	463	CYS	2.9
1	С	898	GLY	2.9
1	С	501	THR	2.9
1	С	1051	THR	2.9
1	С	1117	ASP	2.9
1	А	1055	LEU	2.9
1	С	1115	LEU	2.9
1	С	965	PRO	2.9
1	С	778	VAL	2.9
1	А	119	LYS	2.9
1	А	695	ARG	2.9
1	С	849	LEU	2.9
1	А	973	ALA	2.9
1	А	1077	ALA	2.9
1	А	1138	PRO	2.9
1	С	689	GLU	2.9
1	С	131	PHE	2.9
1	А	783	VAL	2.9
1	А	699	GLY	2.9
1	С	117	GLY	2.9
1	А	204	LEU	2.9
1	С	309	ALA	2.9



Mol	Chain	Res	Type	RSRZ
1	А	847	PHE	2.9
1	С	713	PHE	2.9
1	С	102	GLN	2.9
1	С	771	LEU	2.9
1	С	1070	LEU	2.9
1	С	1139	ALA	2.9
1	А	244	GLN	2.8
1	А	228	VAL	2.8
1	А	532	VAL	2.8
1	А	942	VAL	2.8
1	А	1104	LEU	2.8
1	С	162	ALA	2.8
1	С	510	ALA	2.8
1	С	851	PRO	2.8
1	С	92	TRP	2.8
1	С	692	THR	2.8
1	С	81	PHE	2.8
1	А	79	MET	2.8
1	А	159	LEU	2.8
1	С	1090	ALA	2.8
1	С	789	GLN	2.8
1	А	1032	GLY	2.8
1	С	785	ASN	2.8
1	А	199	ILE	2.8
1	С	3	ILE	2.8
1	С	989	TYR	2.8
1	С	354	ALA	2.8
1	А	890	LEU	2.8
1	С	75	THR	2.8
1	А	717	TYR	2.8
1	С	59	ARG	2.8
1	А	558	VAL	2.8
1	А	1091	VAL	2.8
1	А	236	ALA	2.8
1	А	1139	ALA	2.8
1	А	154	ASN	2.8
1	А	191	LEU	2.8
1	А	500	LEU	2.8
1	А	739	LEU	2.8
1	С	684	SER	2.8
1	С	922	ASP	2.8
1	А	497	HIS	2.8



Mol	Chain	<b>Bos</b>	Type	<b>BSB7</b>
1	Cliain	205		
1	C	295	VAL	2.8
1		957		2.8
1	A	414	ILE	2.8
1	C	981	HIS	2.8
1	C	225	VAL	2.7
1	C	455	ALA	2.7
1	С	495	ALA	2.7
1	С	967	GLU	2.8
1	A	964	SER	2.7
1	А	1030	GLY	2.7
1	С	473	ARG	2.7
1	А	1025	ALA	2.7
1	С	696	VAL	2.7
1	С	1141	VAL	2.7
1	С	211	LEU	2.7
1	С	924	GLU	2.7
1	А	785	ASN	2.7
1	С	528	SER	2.7
1	С	717	TYR	2.7
1	А	307	LYS	2.7
1	С	753	VAL	2.7
1	А	820	ASP	2.7
1	А	51	ILE	2.7
1	А	969	GLN	2.7
1	А	628	SER	2.7
1	A	929	ALA	2.7
1	С	745	ALA	2.7
1	A	332	VAL	2.7
1	С	9	ARG	2.7
1	C	407	ASP	2.7
1	C	1045	THR	2.7
1	Ā	801	GLU	2.7
- 1	C	919	LYS	2.7
1	Ă	1008	ILE	2.7
1	C	392	ILE	2.7
1	C	601	ARG	2.7
1		800	TVR	2.7
1	Δ	832	PHE	2.1 2.7
1	Δ	052	LEU	2.1
1		551	VAT	2.1
1		1/0	VAL MET	2.1
1	A	149		2.1
T	A	104	$\mid 1 \Pi K$	2.1



Mol	Chain	Res	Type	RSRZ
1	С	667	THR	2.7
1	С	538	LYS	2.7
1	С	583	ARG	2.7
1	А	770	ALA	2.7
2	F	50	G	2.7
1	А	289	LEU	2.7
1	А	498	VAL	2.7
1	С	631	THR	2.7
1	С	687	THR	2.7
1	С	1164	ASN	2.6
1	А	448	GLY	2.6
1	А	683	LEU	2.6
1	А	708	ARG	2.6
1	А	1087	ARG	2.6
1	С	109	PHE	2.6
1	С	594	LEU	2.6
1	А	781	SER	2.6
1	А	130	LYS	2.6
1	С	135	PRO	2.6
1	С	563	PRO	2.6
1	А	789	GLN	2.6
1	С	364	GLN	2.6
1	С	90	ALA	2.6
1	С	474	ALA	2.6
1	С	650	ALA	2.6
1	А	46	LEU	2.6
1	С	345	TYR	2.6
1	С	1159	ASN	2.6
1	А	88	GLY	2.6
1	А	1098	MET	2.6
1	A	443	ARG	2.6
1	С	311	ARG	2.6
1	С	815	ARG	2.6
1	А	57	ILE	2.6
1	А	367	ILE	2.6
1	С	1008	ILE	2.6
1	A	241	SER	2.6
1	A	120	PHE	2.6
1	С	381	PHE	2.6
1	С	649	LEU	2.6
1	С	800	TYR	2.6
1	С	1060	VAL	2.6



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Mol	Chain	Res	Type	RSRZ
1	А	59	ARG	2.6
1	С	648	ALA	2.6
1	А	407	ASP	2.6
1	С	964	SER	2.6
1	А	416	GLN	2.6
1	А	3	ILE	2.6
1	А	542	SER	2.5
1	А	793	TRP	2.5
1	С	321	LEU	2.5
1	С	928	LEU	2.5
1	А	261	VAL	2.5
1	А	295	VAL	2.5
1	А	374	VAL	2.5
1	А	744	GLY	2.5
1	С	557	GLU	2.5
1	А	284	ALA	2.5
1	А	1164	ASN	2.5
2	D	50	G	2.5
1	С	406	ARG	2.5
1	А	1004	ILE	2.5
1	А	269	LEU	2.5
1	А	565	LEU	2.5
1	С	185	ASP	2.5
1	А	959	HIS	2.5
1	А	777	PHE	2.5
1	С	263	PHE	2.5
1	С	337	VAL	2.5
1	A	380	ALA	2.5
1	А	455	ALA	2.5
1	А	692	THR	2.5
1	A	738	ILE	2.5
1	С	902	ILE	2.5
1	A	445	GLY	2.5
1	А	484	LEU	2.5
1	A	527	LEU	2.5
1	A	829	LEU	2.5
1	С	152	ARG	2.5
1	С	831	LEU	2.5
1	С	192	VAL	2.5
1	С	332	VAL	2.5
1	С	1081	MET	2.5
1	А	844	ALA	2.5



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Mol	Chain	Res	Type	RSRZ
1	С	1010	TYR	2.5
1	С	447	447 GLU	
1	А	792	LYS	2.5
1	А	564	564 ARG	
1	С	855	855 LEU	
1	А	452	452 PHE	
1	С	226	VAL	2.5
1	А	238	ALA	2.5
1	С	202	SER	2.5
1	С	380	ALA	2.5
1	А	592	THR	2.5
1	С	360	THR	2.5
1	С	438	THR	2.5
1	С	182	PRO	2.5
1	С	174	ILE	2.5
1	С	414	ILE	2.5
1	А	553	LYS	2.5
1	С	939	SER	2.5
1	А	551	ALA	2.5
1	С	118 ASP		2.5
1	С	909	ALA	2.4
1	С	929	ALA	2.4
1	А	93 LYS		2.4
2	D	36 C		2.4
1	С	511 ILE		2.4
1	С	564	564 ARG	
1	С	680	ARG	2.4
1	С	816	ARG	2.4
1	А	100	LEU	2.4
1	А	323	LEU	2.4
1	С	635	LEU	2.4
1	С	754	LEU	2.4
1	А	713	PHE	2.4
1	А	854	ALA	2.4
1	А	1046	ASP	2.4
1	С	921	ARG	2.4
2	D	35	А	2.4
1	А	587	LYS	2.4
1	А	21	LEU	2.4
1	А	650	ALA	2.4
1	С	646	ALA	2.4
1	А	696	VAL	2.4



Mol	Chain	Res	Type	RSRZ	
1	А	778	VAL	2.4	
1	А	586	ARG 2.4		
1	А	174	ILE	2.4	
1	А	457	LEU	2.4	
1	С	833	LEU	2.4	
1	С	990 LEU		2.4	
1	С	362 ALA		2.4	
1	А	406	ARG	2.4	
1	А	675	ASP	2.4	
1	С	282	PRO	2.4	
1	С	307	LYS	2.4	
1	А	52	SER	2.4	
1	А	433	ILE	2.4	
1	А	905	TYR	2.4	
1	С	616	LEU	2.4	
1	А	390	ALA	2.4	
1	А	506	ALA	2.4	
1	С	405	ASP	2.4	
1	А	552	VAL	2.4	
1	А	655	VAL	2.4	
1	А	704 SER		2.4	
1	С	422 GLU		2.4	
1	С	537	537 SER		
1	А	772	772 TYR		
1	А	262	GLY	2.4	
1	А	896	LEU	2.4	
1	С	1013	ALA	2.4	
1	С	742	GLU	2.4	
1	А	963	ILE	2.3	
1	С	51	ILE	2.3	
1	A	43	PRO	2.3	
1	А	638	PRO	2.3	
1	А	965	PRO	2.3	
1	С	642	ALA	2.3	
1	А	470	LEU	2.3	
1	С	383 LEU		2.3	
1	С	568	LEU	2.3	
1	С	639 ALA		2.3	
1	А	716	ASN	2.3	
2	D	38	U	2.3	
1	С	1087	ARG	2.3	
1	С	497	HIS	2.3	



Mol	Iol   Chain		ChainResType		
1	А	730	ILE	2.3	
1	А	495	ALA	2.3	
1	А	796	796 LEU		
1	С	83	ALA	2.3	
1	С	619 TYR		2.3	
1	А	725	MET	2.3	
1	С	149	MET	2.3	
1	С	949	THR	2.3	
1	С	496	GLU	2.3	
1	А	1135	VAL	2.3	
1	С	368	LYS	2.3	
1	С	549	VAL	2.3	
1	А	212	ALA	2.3	
1	С	604	ASP	2.3	
1	А	365	THR	2.3	
1	А	831	LEU	2.3	
1	С	1096	LEU	2.3	
1	С	1104	LEU	2.3	
1	А	815	ARG	2.3	
1	С	894	ARG	2.3	
1	А	1086	LYS	2.3	
1	С	738	ILE	2.3	
1	С	1086	LYS	2.3	
1	А	747	ALA	2.3	
1	А	1142	THR	2.3	
1	С	302	LEU	2.3	
1	А	58	TYR	2.3	
1	А	936	GLN	2.3	
1	А	958	CYS	2.3	
1	А	1024	ASN	2.3	
1	А	780	ALA	2.3	
1	С	54	ILE	2.3	
1	С	258	SER	2.3	
1	С	1125	ILE	2.3	
2	D	45	С	2.3	
1	А	298	THR	2.2	
1	А	911	LEU	2.2	
1	С	10	THR	2.2	
1	С	519	LEU	2.2	
1	С	1061	LEU	2.2	
1	А	986	GLY	2.2	
1	С	48	GLY	2.2	



Mol	Chain	Res	Type	RSRZ
1	С	375	ARG	2.2
1	С	151	51 LYS	
1	С	938	LYS	2.2
1	С	1035	TRP	2.2
1	С	355	GLN	2.2
1	А	11	ILE	2.2
1	А	941	ILE	2.2
1	А	1052[A]	ARG	2.2
1	С	266	ALA	2.2
1	С	333	ARG	2.2
1	С	269	LEU	2.2
1	С	432	GLY	2.2
1	С	679	LEU	2.2
1	С	850	LYS	2.2
1	А	476	PHE	2.2
1	С	34	GLU	2.2
2	F	8	А	2.2
1	А	384	ALA	2.2
1	А	630	ILE	2.2
1	А	1051	THR	2.2
1	С	25	ILE	2.2
1	С	1031	ALA	2.2
1	С	1033	ALA	2.2
1	А	444	LEU	2.2
1	А	502	ASP	2.2
1	С	493	LYS	2.2
1	А	266	ALA	2.2
1	С	633	THR	2.2
1	С	685	ALA	2.2
1	A	706	ASN	2.2
1	C	746	THR	2.2
1	A	568	LEU	2.2
1	С	500	LEU	2.2
1	C	708	ARG	2.2
1	C	1098	MET	2.2
1	A	192	VAL	2.2
1	A	559	SER	2.2
1	С	498	VAL	2.2
1	A	165	GLU	2.2
1	А	360	THR	2.2
1	A	697	GLN	2.2
1	С	322	ALA	2.2



Mol	Chain	Res	Type	RSRZ	
1	С	487	THR	2.2	
1	А	50	TRP	2.2	
1	С	30	LYS	2.2	
1	С	377	TRP	2.2	
1	А	383	LEU	2.2	
1	С	586	ARG	2.2	
1	А	89	GLU	2.2	
1	А	557	GLU	2.2	
1	С	146	TYR	2.2	
1	С	1150	TYR	2.2	
1	С	453	VAL	2.2	
1	А	838	ALA	2.2	
1	С	101	ALA	2.2	
1	С	678	THR	2.2	
1	С	548	ILE	2.2	
1	А	145	TRP	2.2	
1	С	323	LEU	2.2	
1	А	96	SER	2.2	
1	А	1117	ASP	2.2	
1	С	853	ARG	2.1	
1	С	948	ARG	2.1	
1	С	625	ALA	2.1	
1	С	715	GLU	2.1	
1	А	456	LEU	2.1	
1	С	456 LEU		2.1	
1	С	477	477 LEU		
1	С	569	LEU	2.1	
1	С	675	ASP	2.1	
2	F	46	С	2.1	
1	А	600	PRO	2.1	
1	A	1150	TYR	2.1	
1	С	164	TYR	2.1	
1	С	905	TYR	2.1	
1	Α	453	VAL	2.1	
1	С	1135	VAL	2.1	
1	A	148	ALA	2.1	
1	A	636	ALA	2.1	
1	A	647	THR	2.1	
1	С	799	LYS	2.1	
1	A	548	ILE	2.1	
1	A	197	LEU	2.1	
1	А	420	ASN	2.1	



Mol	Chain	Res	s Type RS		
1	А	594 LEU		2.1	
1	А	786	LEU	2.1	
1	С	216	GLY	2.1	
1	С	285	GLY	2.1	
1	А	776	HIS	2.1	
1	С	290	ALA	2.1	
1	С	499	VAL	2.1	
1	С	507	ALA	2.1	
1	С	516	ALA	2.1	
1	С	925	VAL	2.1	
1	С	724	PHE	2.1	
1	А	1085	ARG	2.1	
1	С	195	ARG	2.1	
1	С	582	LEU	2.1	
1	С	540	HIS	2.1	
1	А	463	CYS	2.1	
1	С	502	ASP	2.1	
1	А	14	PHE	2.1	
1	С	840	PHE	2.1	
1	А	143	GLY	2.1	
1	С	613	ILE	2.1	
1	А	183	LYS	2.1	
1	А	771	LEU	2.1	
1	С	1069	ASP	2.1	
1	А	861	THR	2.1	
1	С	982	ARG	2.1	
1	А	1155	ALA	2.1	
1	С	384	ALA	2.1	
1	С	893	ALA	2.1	
1	A	581	GLY	2.1	
1	А	842	GLY	2.1	
1	С	110	LYS	2.1	
1	А	167	LEU	2.1	
1	С	1105	THR	2.1	
1	A	1047	ALA	2.1	
1	С	751	ALA	2.1	
2	F	53	U	2.1	
1	С	342	VAL	2.1	
1	А	729	TYR	2.1	
1	А	102	GLN	2.0	
1	С	534	HIS	2.0	
1	А	718	ARG	2.0	



Mol	Chain	Res	Type	RSRZ
1	С	93	LYS	2.0
1	С	297	297 LYS	
1	А	438	THR	2.0
1	А	487	THR	2.0
1	А	614	ALA	2.0
1	А	342	VAL	2.0
1	С	697	GLN	2.0
1	С	822	VAL	2.0
1	С	985	VAL	2.0
1	А	220	ILE	2.0
1	С	47	ILE	2.0
2	F	19	G	2.0
1	А	966	GLU	2.0
1	А	1013	1013 ALA	
1	С	230	ALA	2.0
1	С	605	ASP	2.0
1	А	6	VAL	2.0
1	С	1111 LYS		2.0
1	С	588	588 HIS	
1	А	1035	TRP	2.0
1	С	476	PHE	2.0
1	А	460	LEU	2.0
1	А	984	LEU	2.0
1	А	1007	LEU	2.0
1	С	741	ILE	2.0
1	С	773	LEU	2.0
1	С	956	MET	2.0
1	А	415	ARG	2.0
1	А	473	ARG	2.0
1	С	343	SER	2.0
1	С	1047	ALA	2.0

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#### 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	EDO	С	1403	4/4	0.47	0.33	78,78,80,82	0
3	EDO	D	102	4/4	0.56	0.50	67,74,77,80	0
3	EDO	A	1404	4/4	0.61	0.41	85,85,89,92	0
3	EDO	А	1402	4/4	0.69	0.24	63,64,69,70	0
3	EDO	С	1401	4/4	0.76	0.31	51,52,56,59	0
3	EDO	С	1402	4/4	0.80	0.19	61,66,68,69	0
4	BME	С	1405	4/4	0.80	0.24	95,96,96,96	0
3	EDO	А	1401	4/4	0.82	0.22	52,52,53,55	0
3	EDO	A	1403	4/4	0.90	0.18	64,70,71,75	0
3	EDO	F	101	4/4	0.91	0.26	43,45,45,46	0
3	EDO	D	101	4/4	0.91	0.29	$49,\!50,\!52,\!52$	0
4	BME	D	103	4/4	0.91	0.23	68,68,73,74	0
3	EDO	C	1404	4/4	0.93	0.24	68,68,70,71	0
4	BME	A	1405	4/4	0.94	0.17	74,76,76,81	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

