



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:10 pm BST

PDB ID : 5VW1  
Title : Crystal structure of SpyCas9-sgRNA-AcrIIA4 ternary complex  
Authors : Yang, H.; Patel, D.J.  
Deposited on : 2017-05-21  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

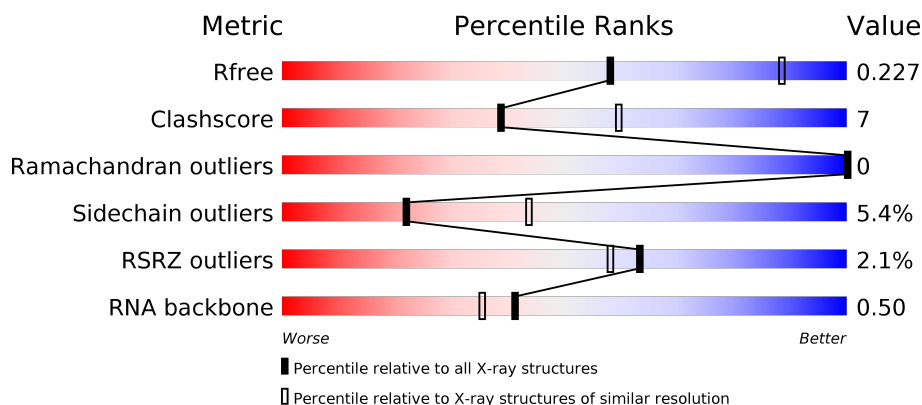
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1370	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
2	C	85	<div> <div>47%</div> <div>27%</div> <div>9%</div> <div>14%</div> <div>.</div> </div>
3	B	89	<div> <div>81%</div> <div>15%</div> <div>..</div> </div>

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
4	PEG	A	1402	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13410 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1362	Total	C	N	O	S	0	0	0
			10910	6943	1887	2056	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q99ZW2
A	0	SER	-	expression tag	UNP Q99ZW2
A	10	ALA	ASP	engineered mutation	UNP Q99ZW2
A	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	73	Total	C	N	O	P	0	0	0
			1562	701	286	502	73			

- Molecule 3 is a protein called anti-CRISPR protein AcrIIA4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	86	Total	C	N	O	S	0	0	0
			703	435	113	153	2			

There are 18 discrepancies between the modelled and reference sequences:

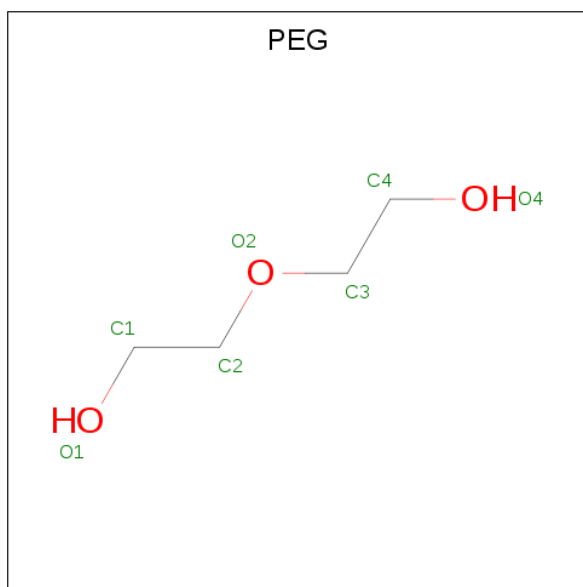
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A0E0UT28
B	0	SER	-	expression tag	UNP A0A0E0UT28
B	4	ASN	SER	see REMARK 999	UNP A0A0E0UT28
B	5	ASP	GLU	see REMARK 999	UNP A0A0E0UT28
B	16	THR	ALA	see REMARK 999	UNP A0A0E0UT28
B	18	LYS	ARG	see REMARK 999	UNP A0A0E0UT28

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	GLU	see REMARK 999	UNP A0A0E0UT28
B	24	SER	ASP	see REMARK 999	UNP A0A0E0UT28
B	29	GLN	LYS	see REMARK 999	UNP A0A0E0UT28
B	33	ARG	ASP	see REMARK 999	UNP A0A0E0UT28
B	35	ASN	ASP	see REMARK 999	UNP A0A0E0UT28
B	47	GLU	LYS	see REMARK 999	UNP A0A0E0UT28
B	52	VAL	ALA	see REMARK 999	UNP A0A0E0UT28
B	56	ILE	ALA	see REMARK 999	UNP A0A0E0UT28
B	58	ALA	THR	see REMARK 999	UNP A0A0E0UT28
B	65	GLN	LYS	see REMARK 999	UNP A0A0E0UT28
B	79	THR	SER	see REMARK 999	UNP A0A0E0UT28
B	81	THR	ILE	see REMARK 999	UNP A0A0E0UT28

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



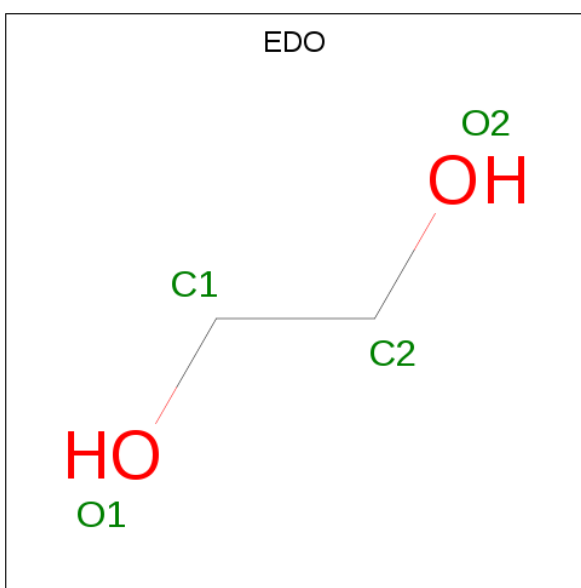
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Mg 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	140	Total 140	O 140	0	0
8	C	30	Total 30	O 30	0	0
8	B	20	Total 20	O 20	0	0

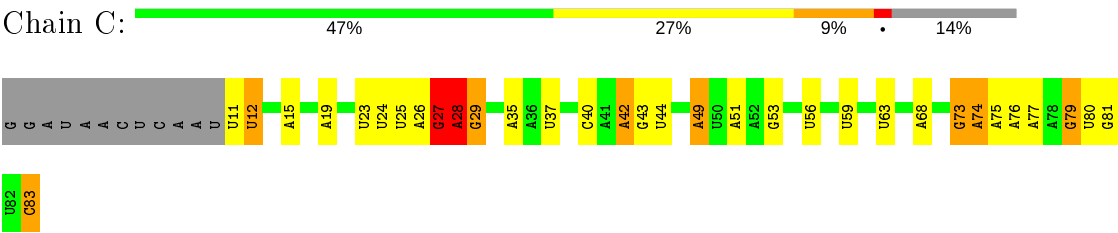
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Chain A:

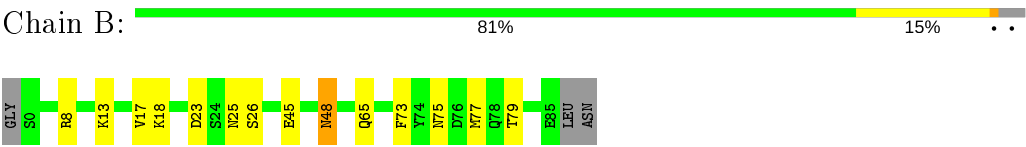
The figure displays a detailed view of Chain A, showing 1000 amino acid residues arranged in a grid. The residues are color-coded by type: Glycine (grey), Serine (orange), Aspartate (green), Glutamate (yellow), Asparagine (light green), Glutamine (light yellow), Lysine (dark green), Arginine (dark yellow), Histidine (light orange), Proline (light green), Alanine (yellow), Valine (light green), Leucine (light yellow), Isoleucine (light green), Methionine (light yellow), Cysteine (light green), Phenylalanine (light yellow), Tyrosine (light green), Tryptophan (light yellow), and Nucleic acids (grey). The grid is labeled with residue numbers 1 to 1000 on the left and right sides.



● Molecule 2: sgRNA



● Molecule 3: anti-CRISPR protein AcrIIA4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.19Å 101.24Å 303.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.60 48.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.02-2.60) 94.2 (48.02-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.178 , 0.226 0.178 , 0.227	Depositor DCC
$R_{free}$ test set	3301 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: PG4, PEG, MG, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/11102	0.60	3/14966 (0.0%)
2	C	0.87	6/1751 (0.3%)	1.15	7/2726 (0.3%)
3	B	0.45	0/711	0.60	0/958
All	All	0.52	6/13564 (0.0%)	0.71	10/18650 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	26	A	O3'-P	-8.72	1.50	1.61
2	C	80	U	O3'-P	-7.58	1.52	1.61
2	C	79	G	O3'-P	-7.42	1.52	1.61
2	C	28	A	O3'-P	-6.89	1.52	1.61
2	C	27	G	O3'-P	-6.57	1.53	1.61
2	C	28	A	P-OP2	-5.29	1.40	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	63	U	C5-C4-O4	-7.87	121.18	125.90
2	C	63	U	N1-C2-O2	-7.76	117.37	122.80
2	C	63	U	N3-C2-O2	7.02	127.11	122.20
1	A	419	LEU	CA-CB-CG	6.65	130.60	115.30
2	C	63	U	C2-N3-C4	-6.51	123.10	127.00
1	A	502	LEU	CA-CB-CG	6.05	129.23	115.30
2	C	49	A	N1-C6-N6	-5.89	115.07	118.60
2	C	28	A	C2'-C3'-O3'	5.55	122.58	113.70
1	A	282	ILE	C-N-CA	-5.42	110.92	122.30
2	C	42	A	P-O3'-C3'	5.39	126.17	119.70

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	10910	0	10851	171	0
2	C	1562	0	783	17	0
3	B	703	0	664	9	0
4	A	14	0	20	6	0
5	A	13	0	18	2	0
5	C	13	0	18	3	0
6	A	4	0	6	1	0
7	C	1	0	0	0	0
8	A	140	0	0	7	1
8	B	20	0	0	0	0
8	C	30	0	0	0	0
All	All	13410	0	12360	191	1

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 7.

All (191) 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)
2:C:27:G:H5''	2:C:27:G:H8	1.13	1.09
2:C:27:G:H5''	2:C:27:G:C8	2.00	0.97
1:A:249:THR:HG22	1:A:265:GLN:HB2	1.53	0.90
1:A:554:LYS:NZ	1:A:608:ASP:OD2	2.03	0.89
1:A:253:LYS:HB2	1:A:261:ASP:HA	1.59	0.84
1:A:116:HIS:HB3	1:A:125:GLU:HG3	1.59	0.82
1:A:70:ARG:NH1	2:C:15:A:OP1	2.11	0.82
1:A:531:THR:HG21	1:A:575:PHE:CE1	2.15	0.81
1:A:761:ILE:HD11	1:A:935:LEU:HD12	1.63	0.80
2:C:73:G:H21	2:C:76:A:H2	1.27	0.80
1:A:627:GLU:HG2	1:A:655:ARG:HD2	1.62	0.79
1:A:781:MET:HE2	1:A:803:ASN:HB3	1.66	0.76
1:A:601:ILE:HD11	1:A:643:PHE:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:HG2	1:A:476:TRP:CD1	2.23	0.74
1:A:28:PRO:HG2	1:A:47:LEU:HD12	1.69	0.74
1:A:893:THR:HG23	1:A:896:LYS:H	1.52	0.73
1:A:1110:ILE:HG23	1:A:1122:ARG:HD2	1.72	0.71
1:A:870:VAL:HG21	1:A:902:LYS:HB3	1.72	0.71
1:A:30:LYS:NZ	8:A:1503:HOH:O	2.24	0.69
1:A:496:THR:HG21	1:A:506:LYS:HG2	1.75	0.69
1:A:708:ILE:O	1:A:711:ALA:HB3	1.92	0.69
1:A:158:LEU:HD22	1:A:419:LEU:HD22	1.78	0.66
1:A:661:ARG:NH2	8:A:1504:HOH:O	2.27	0.66
2:C:19:A:H61	5:C:102:PG4:H72	1.61	0.66
2:C:83:C:C6	2:C:83:C:H3'	2.31	0.66
1:A:158:LEU:HA	1:A:161:MET:HE2	1.78	0.66
3:B:23:ASP:HB3	3:B:25:ASN:H	1.60	0.66
1:A:1079:ASP:OD2	4:A:1401:PEG:H32	1.96	0.64
1:A:762:GLU:HG2	1:A:990:ASN:HD21	1.62	0.64
2:C:28:A:O2'	2:C:29:G:OP1	2.12	0.64
1:A:525:THR:HG23	1:A:526:LYS:HD3	1.80	0.63
1:A:1206:LEU:HD13	1:A:1345:ALA:HB2	1.81	0.63
1:A:251:ASN:HD21	1:A:261:ASP:HB2	1.62	0.63
1:A:682:PHE:HB2	1:A:696:LEU:HD21	1.81	0.63
1:A:1122:ARG:NH2	2:C:49:A:N3	2.46	0.62
1:A:161:MET:HE3	1:A:419:LEU:HA	1.81	0.62
2:C:83:C:H6	2:C:83:C:H3'	1.65	0.62
1:A:777:SER:OG	1:A:803:ASN:O	2.18	0.62
1:A:216:LEU:HD22	1:A:220:ARG:HG2	1.82	0.61
2:C:83:C:C6	2:C:83:C:C3'	2.83	0.61
1:A:175:ASN:HB2	1:A:176:PRO:HD2	1.81	0.60
1:A:569:PHE:HB3	1:A:578:VAL:HG21	1.83	0.60
1:A:502:LEU:HD21	1:A:665:LYS:HG2	1.83	0.60
1:A:718:ASP:OD2	1:A:718:ASP:N	2.33	0.60
1:A:776:ASN:HD21	1:A:807:GLN:HE22	1.50	0.60
1:A:1252:ASN:O	1:A:1256:GLN:HG3	2.02	0.59
1:A:1122:ARG:HG2	1:A:1134:PHE:CE1	2.37	0.59
1:A:781:MET:CE	1:A:801:VAL:HG23	2.33	0.59
1:A:1279:ARG:NH1	8:A:1508:HOH:O	2.36	0.58
1:A:601:ILE:HA	1:A:647:VAL:HG21	1.84	0.58
1:A:926:GLN:H	5:A:1403:PG4:H62	1.69	0.58
2:C:27:G:C8	2:C:27:G:C5'	2.83	0.58
1:A:1279:ARG:NH2	8:A:1502:HOH:O	2.17	0.57
1:A:731:PRO:HD2	8:A:1588:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:LYS:NZ	8:A:1509:HOH:O	2.36	0.57
1:A:1124:LYS:HE3	2:C:53:G:H5'	1.87	0.57
1:A:75:ARG:HD3	1:A:163:LYS:HG3	1.87	0.56
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.39	0.56
1:A:71:ARG:HH11	5:C:102:PG4:H32	1.70	0.56
1:A:1194:LEU:HD22	1:A:1365:LEU:HD22	1.87	0.56
1:A:492:ILE:HG12	1:A:625:LEU:HD13	1.88	0.56
1:A:762:GLU:HG2	1:A:990:ASN:ND2	2.21	0.56
1:A:609:ASN:C	1:A:611:GLU:H	2.08	0.56
1:A:1292:SER:O	1:A:1296:LYS:HG3	2.06	0.55
1:A:853:ASP:OD2	1:A:893:THR:HG21	2.06	0.55
1:A:519:THR:HG23	1:A:589:ALA:HB1	1.87	0.55
1:A:1207:GLU:OE2	1:A:1210:ARG:NH1	2.40	0.55
1:A:654:ARG:HD2	1:A:656:TYR:CZ	2.43	0.54
1:A:415:HIS:CE1	4:A:1402:PEG:H32	2.43	0.54
1:A:415:HIS:HE1	4:A:1402:PEG:H32	1.73	0.54
1:A:784:ILE:HD12	1:A:806:LEU:HD21	1.90	0.53
1:A:1143:VAL:HG12	1:A:1145:VAL:HG23	1.91	0.53
1:A:768:GLN:O	1:A:771:GLN:NE2	2.41	0.53
1:A:136:TYR:OH	4:A:1402:PEG:H31	2.09	0.53
3:B:75:ASN:O	3:B:79:THR:HG23	2.09	0.52
1:A:880:LYS:HZ1	1:A:884:ARG:HH11	1.56	0.52
1:A:846:PHE:O	1:A:1040:SER:HB3	2.10	0.52
1:A:675:SER:HB3	1:A:677:LYS:HG3	1.92	0.52
3:B:48:ASN:N	3:B:48:ASN:OD1	2.31	0.52
1:A:682:PHE:CB	1:A:696:LEU:HD21	2.40	0.51
1:A:1295:ASN:HA	1:A:1298:ARG:HG3	1.92	0.51
1:A:556:ASN:O	1:A:595:HIS:NE2	2.44	0.51
1:A:1179:ILE:H	1:A:1179:ILE:HD12	1.75	0.51
1:A:400:ARG:NH1	1:A:406:ASP:OD1	2.40	0.50
1:A:665:LYS:O	1:A:669:GLY:HA3	2.11	0.50
1:A:1048:THR:HG22	1:A:1076:LYS:HD3	1.94	0.50
1:A:140:LYS:NZ	1:A:144:ASP:OD1	2.42	0.50
1:A:305:ILE:HD11	1:A:406:ASP:HB3	1.94	0.50
1:A:329:HIS:ND1	8:A:1507:HOH:O	2.35	0.50
1:A:829:ASP:CG	1:A:832:ARG:HG3	2.32	0.50
1:A:756:PRO:O	1:A:953:VAL:HG22	2.13	0.49
1:A:525:THR:OG1	1:A:545:LYS:NZ	2.41	0.49
1:A:524:LEU:O	1:A:527:VAL:HG12	2.13	0.49
1:A:600:ILE:HG22	1:A:647:VAL:HG23	1.94	0.49
1:A:963:VAL:HG21	1:A:990:ASN:OD1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:MET:HE1	1:A:467:ARG:HG3	1.94	0.48
1:A:820:ARG:NH2	1:A:825:ASP:OD1	2.47	0.48
1:A:251:ASN:ND2	1:A:261:ASP:HB2	2.28	0.48
1:A:343:LEU:HD13	1:A:346:LYS:HD2	1.95	0.48
1:A:313:THR:HB	1:A:315:ALA:H	1.79	0.48
1:A:788:ILE:HG23	1:A:793:SER:HB3	1.96	0.48
1:A:563:GLN:O	1:A:567:ASP:HB2	2.13	0.47
1:A:654:ARG:HD2	1:A:656:TYR:CE2	2.48	0.47
3:B:73:PHE:O	3:B:77:MET:HG2	2.14	0.47
2:C:23:U:H2'	2:C:24:U:C6	2.50	0.47
1:A:415:HIS:HE2	4:A:1402:PEG:H12	1.80	0.47
1:A:1179:ILE:HD11	1:A:1192:LYS:HE3	1.97	0.47
1:A:623:LEU:HD13	1:A:654:ARG:O	2.15	0.47
1:A:975:VAL:HB	1:A:978:ILE:HD12	1.97	0.47
1:A:273:ASP:HA	1:A:276:ASP:HB2	1.97	0.47
1:A:180:ASP:HB3	1:A:182:ASP:OD1	2.14	0.47
1:A:633:GLU:HA	1:A:652:LYS:HE2	1.97	0.46
1:A:1231:LYS:HE3	1:A:1232:TYR:CZ	2.50	0.46
1:A:160:HIS:CE1	4:A:1402:PEG:H42	2.50	0.46
2:C:11:U:O2'	2:C:12:U:OP2	2.29	0.46
1:A:182:ASP:N	1:A:182:ASP:OD1	2.48	0.46
1:A:497:ASN:O	1:A:507:VAL:HG22	2.16	0.46
1:A:539:PHE:HB3	1:A:690:ASN:ND2	2.30	0.46
1:A:1105:PHE:HB3	1:A:1169:MET:HE2	1.98	0.46
1:A:606:PHE:CD1	1:A:612:ASN:ND2	2.84	0.46
1:A:1308:ASN:HB3	1:A:1326:TYR:CD1	2.51	0.46
1:A:549:VAL:HA	1:A:553:PHE:HB2	1.98	0.46
3:B:8:ARG:HB2	3:B:8:ARG:CZ	2.46	0.46
1:A:269:ASP:OD2	1:A:269:ASP:N	2.49	0.46
2:C:74:A:H2'	2:C:75:A:C8	2.51	0.45
1:A:427:GLU:HB2	1:A:434:LYS:HB2	1.98	0.45
1:A:544:GLN:NE2	1:A:573:GLU:OE2	2.47	0.45
1:A:314:LYS:C	1:A:316:PRO:HD3	2.36	0.45
1:A:600:ILE:HG23	1:A:650:GLN:HB3	1.99	0.45
1:A:294:LYS:O	1:A:297:SER:HB3	2.17	0.45
1:A:502:LEU:HD21	1:A:665:LYS:HE2	1.99	0.45
1:A:560:THR:HA	1:A:586:ARG:HA	1.98	0.45
1:A:802:GLU:O	1:A:802:GLU:HG2	2.17	0.45
1:A:71:ARG:NH1	5:C:102:PG4:H32	2.31	0.45
1:A:439:LYS:HG2	1:A:476:TRP:NE1	2.31	0.45
1:A:531:THR:HG22	1:A:534:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:LEU:HD23	1:A:1019:ARG:HD3	1.99	0.44
1:A:680:LEU:HG	1:A:684:LYS:HE3	2.00	0.44
1:A:998:ILE:HA	1:A:998:ILE:HD12	1.82	0.44
1:A:148:LYS:HD2	1:A:429:PHE:HB3	1.99	0.44
1:A:632:ILE:HG22	1:A:652:LYS:HG2	2.00	0.44
1:A:397:ASP:O	6:A:1404:EDO:H12	2.18	0.44
1:A:847:LEU:HD13	1:A:916:PHE:HB3	1.99	0.44
1:A:510:LYS:HE2	1:A:510:LYS:HB3	1.74	0.44
1:A:1179:ILE:O	1:A:1183:GLU:HB2	2.17	0.44
1:A:1028:GLU:OE1	1:A:1035:LYS:CE	2.66	0.43
1:A:691:ARG:NH1	1:A:702:LEU:HD11	2.34	0.43
1:A:1205:GLU:OE2	1:A:1359:ARG:NH2	2.50	0.43
1:A:1274:SER:O	1:A:1278:LYS:HG3	2.18	0.43
1:A:665:LYS:O	1:A:669:GLY:CA	2.67	0.43
1:A:560:THR:HG22	1:A:563:GLN:OE1	2.19	0.43
1:A:974:LYS:HD3	1:A:982:HIS:HB2	2.00	0.43
1:A:306:LEU:O	1:A:308:VAL:N	2.52	0.43
1:A:654:ARG:HD3	1:A:655:ARG:N	2.33	0.43
1:A:764:ALA:HB2	3:B:25:ASN:ND2	2.34	0.43
1:A:708:ILE:O	1:A:712:GLN:HG3	2.18	0.43
1:A:641:HIS:CD2	1:A:642:LEU:HG	2.54	0.43
1:A:731:PRO:HD3	2:C:12:U:H5'	2.00	0.43
1:A:437:ARG:O	1:A:441:GLU:HG3	2.19	0.42
1:A:1321:PRO:O	1:A:1333:ARG:HD2	2.19	0.42
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.88	0.42
1:A:1036:TYR:HB2	1:A:1037:PHE:CD1	2.55	0.42
1:A:251:ASN:HD21	1:A:261:ASP:CB	2.28	0.42
1:A:529:TYR:HA	1:A:579:GLU:O	2.20	0.42
1:A:186:ILE:O	1:A:190:GLN:HG3	2.19	0.42
1:A:548:ILE:HG23	1:A:552:LEU:HD12	2.00	0.42
1:A:954:LYS:NZ	1:A:1005:GLU:OE2	2.41	0.41
1:A:266:LEU:HD23	1:A:271:TYR:CZ	2.54	0.41
1:A:226:ILE:HD13	1:A:226:ILE:HA	1.85	0.41
1:A:118:ILE:N	1:A:125:GLU:OE2	2.49	0.41
1:A:1215:ALA:HB2	1:A:1221:GLN:HG3	2.02	0.41
1:A:936:ASP:OD1	1:A:951:ARG:NH1	2.53	0.41
1:A:902:LYS:HG2	1:A:907:GLY:O	2.21	0.41
1:A:473:ILE:HG12	1:A:481:VAL:HG11	2.02	0.41
1:A:158:LEU:HD23	1:A:161:MET:CE	2.51	0.41
1:A:306:LEU:O	1:A:308:VAL:HG22	2.21	0.41
1:A:836:TYR:CD1	1:A:859:ARG:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HH21	1:A:307:ARG:HH11	1.69	0.41
1:A:706:GLU:H	1:A:706:GLU:HG3	1.60	0.41
1:A:735:LYS:O	1:A:739:GLN:HG2	2.20	0.41
3:B:23:ASP:HB2	3:B:26:SER:H	1.85	0.41
3:B:13:LYS:NZ	3:B:79:THR:OG1	2.52	0.41
1:A:526:LYS:HE2	1:A:690:ASN:O	2.21	0.41
1:A:641:HIS:NE2	1:A:642:LEU:HG	2.36	0.41
1:A:730:SER:O	1:A:733:ILE:HG22	2.21	0.41
1:A:1207:GLU:CD	1:A:1210:ARG:HH11	2.23	0.40
1:A:925:ARG:HA	5:A:1403:PG4:H71	2.03	0.40
1:A:104:SER:O	2:C:25:U:H1'	2.20	0.40
1:A:679:ILE:HG23	1:A:696:LEU:HD23	2.03	0.40
3:B:17:VAL:O	3:B:18:LYS:HD3	2.21	0.40
1:A:561:VAL:HG22	1:A:583:VAL:CG1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1610:HOH:O	8:A:1626:HOH:O[1_545]	2.19	0.01

## 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	
1	A	1354/1370 (99%)	1289 (95%)	65 (5%)	0	100	100
3	B	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
All	All	1438/1459 (99%)	1370 (95%)	68 (5%)	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	
1	A	1168/1226 (95%)	1103 (94%)	65 (6%)	21	42
3	B	81/84 (96%)	78 (96%)	3 (4%)	34	60
All	All	1249/1310 (95%)	1181 (95%)	68 (5%)	22	44

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	43	ILE
1	A	257	ASP
1	A	285	GLN
1	A	308	VAL
1	A	312	ILE
1	A	313	THR
1	A	320	SER
1	A	323	LYS
1	A	340	ARG
1	A	345	GLU
1	A	376	ILE
1	A	424	ARG
1	A	439	LYS
1	A	461	ARG
1	A	476	TRP
1	A	496	THR
1	A	519	THR
1	A	529	TYR
1	A	574	CYS
1	A	583	VAL
1	A	599	LYS
1	A	613	GLU
1	A	622	THR
1	A	629	ARG
1	A	633	GLU
1	A	696	LEU

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Mol	Chain	Res	Type
1	A	700	ASP
1	A	703	THR
1	A	706	GLU
1	A	718	ASP
1	A	762	GLU
1	A	770	THR
1	A	795	ILE
1	A	803	ASN
1	A	804	THR
1	A	806	LEU
1	A	809	GLU
1	A	834	SER
1	A	844	GLN
1	A	845	SER
1	A	850	ASP
1	A	853	ASP
1	A	869	ASN
1	A	911	LEU
1	A	937	SER
1	A	938	ARG
1	A	945	GLU
1	A	947	ASP
1	A	955	VAL
1	A	960	SER
1	A	964	SER
1	A	974	LYS
1	A	1004	LEU
1	A	1021	MET
1	A	1033	THR
1	A	1099	GLU
1	A	1157	LEU
1	A	1159	SER
1	A	1183	GLU
1	A	1206	LEU
1	A	1340	LYS
1	A	1342	VAL
1	A	1357	GLU
1	A	1368	ASP
3	B	45	GLU
3	B	48	ASN
3	B	65	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	803	ASN
1	A	807	GLN
1	A	844	GLN
1	A	982	HIS
1	A	983	HIS
1	A	1297	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	72/85 (84%)	19 (26%)	2 (2%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	12	U
2	C	27	G
2	C	28	A
2	C	29	G
2	C	35	A
2	C	37	U
2	C	40	C
2	C	43	G
2	C	44	U
2	C	51	A
2	C	56	U
2	C	59	U
2	C	68	A
2	C	73	G
2	C	74	A
2	C	77	A
2	C	79	G
2	C	81	G
2	C	83	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	28	A
2	C	42	A

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
4	PEG	A	1401	-	6,6,6	0.53	0	5,5,5	0.38	0
4	PEG	A	1402	-	6,6,6	0.50	0	5,5,5	0.26	0
5	PG4	A	1403	-	12,12,12	0.67	0	11,11,11	0.51	0
5	PG4	C	102	-	12,12,12	0.58	0	11,11,11	0.72	0
6	EDO	A	1404	-	3,3,3	0.48	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
4	PEG	A	1401	-	-	2/4/4/4	-
4	PEG	A	1402	-	-	3/4/4/4	-
5	PG4	A	1403	-	-	3/10/10/10	-
5	PG4	C	102	-	-	4/10/10/10	-
6	EDO	A	1404	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1401	PEG	O1-C1-C2-O2
5	C	102	PG4	O3-C5-C6-O4
4	A	1402	PEG	O2-C3-C4-O4
5	A	1403	PG4	O1-C1-C2-O2
5	C	102	PG4	O1-C1-C2-O2
5	C	102	PG4	O4-C7-C8-O5
4	A	1402	PEG	C4-C3-O2-C2
4	A	1401	PEG	O2-C3-C4-O4
4	A	1402	PEG	O1-C1-C2-O2
5	A	1403	PG4	C3-C4-O3-C5
5	A	1403	PG4	C1-C2-O2-C3
5	C	102	PG4	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1401	PEG	1	0
4	A	1402	PEG	5	0
5	A	1403	PG4	2	0
5	C	102	PG4	3	0
6	A	1404	EDO	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1362/1370 (99%)	-0.04	32 (2%) 60 54	30, 55, 101, 125	0
2	C	73/85 (85%)	-0.51	0 100 100	35, 51, 106, 112	0
3	B	86/89 (96%)	-0.20	0 100 100	34, 49, 79, 109	0
All	All	1521/1544 (98%)	-0.07	32 (2%) 63 58	30, 55, 101, 125	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	801	VAL	4.9
1	A	568	TYR	4.4
1	A	574	CYS	4.1
1	A	583	VAL	4.1
1	A	0	SER	4.1
1	A	310	THR	4.1
1	A	529	TYR	4.0
1	A	1157	LEU	3.6
1	A	527	VAL	3.3
1	A	688	PHE	3.1
1	A	640	ALA	2.9
1	A	1153	LYS	2.9
1	A	525	THR	2.7
1	A	580	ILE	2.6
1	A	943	TYR	2.5
1	A	769	THR	2.5
1	A	697	ILE	2.4
1	A	683	LEU	2.4
1	A	540	LEU	2.3
1	A	1115	ASN	2.3
1	A	1154	SER	2.2
1	A	658	GLY	2.2
1	A	575	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	ILE	2.1
1	A	531	THR	2.1
1	A	572	ILE	2.1
1	A	587	PHE	2.1
1	A	567	ASP	2.1
1	A	576	ASP	2.0
1	A	551	LEU	2.0
1	A	651	LEU	2.0
1	A	1034	ALA	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 carbohydrates 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<sup>th</sup> 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	PG4	A	1403	13/13	0.83	0.17	76,92,115,117	0
5	PG4	C	102	13/13	0.88	0.27	49,60,70,73	0
4	PEG	A	1401	7/7	0.93	0.23	47,62,63,63	0
6	EDO	A	1404	4/4	0.94	0.27	54,61,63,64	0
7	MG	C	101	1/1	0.97	0.45	43,43,43,43	0
4	PEG	A	1402	7/7	0.97	0.24	44,50,59,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.