



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 02:26 PM JST

PDB ID : 5B2R
Title : Crystal structure of the Streptococcus pyogenes Cas9 VQR variant in complex with sgRNA and target DNA (TGA PAM)
Authors : Hirano, S.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2016-02-02
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

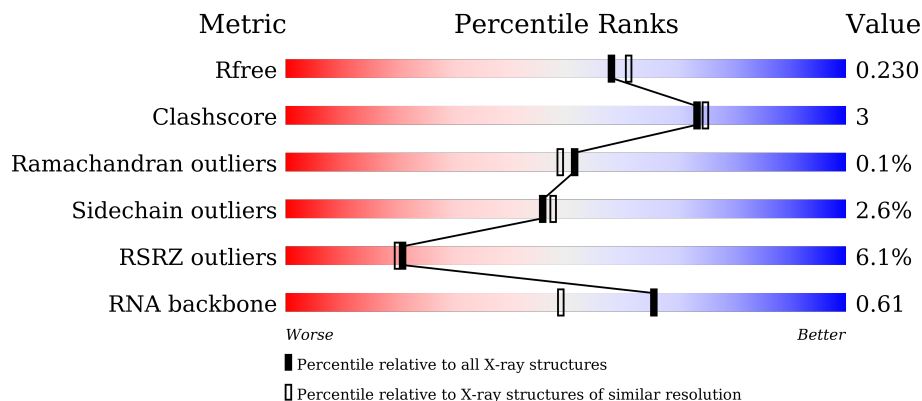
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)
RNA backbone	3102	1079 (2.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	81	 80% 15% 5%
2	B	1372	 87% 9% 6%
3	C	28	 71% 29%
4	D	8	 75% 25% 12%

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
5	K	B	1407	-	-	-	X

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 13799 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Guide RNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1319	10547	6734	1826	1967	20	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a DNA chain called Target DNA.

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

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

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

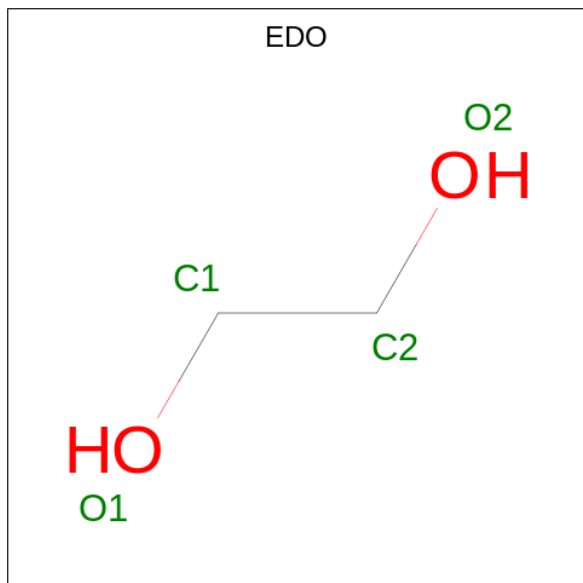
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	K	0	0
			4	4		
5	B	7	Total	K	0	0
			7	7		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



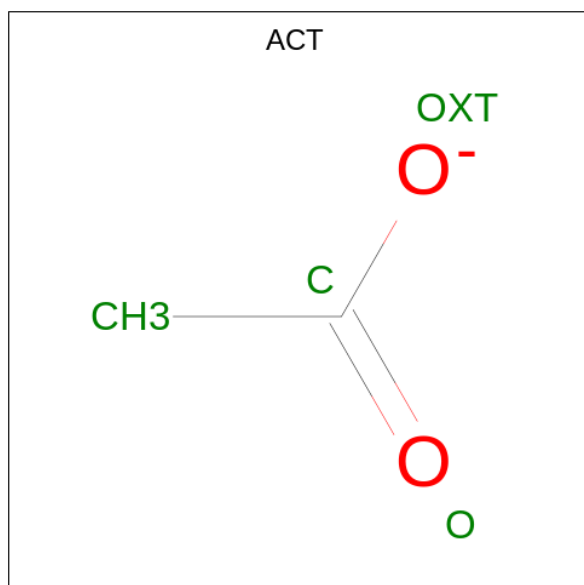
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

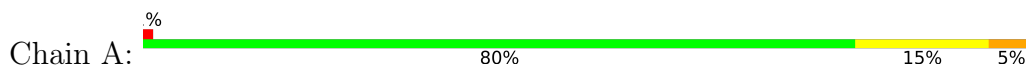
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	199	Total	O	0	0
			199	199		
9	B	492	Total	O	0	0
			492	492		
9	C	50	Total	O	0	0
			50	50		
9	D	13	Total	O	0	0
			13	13		

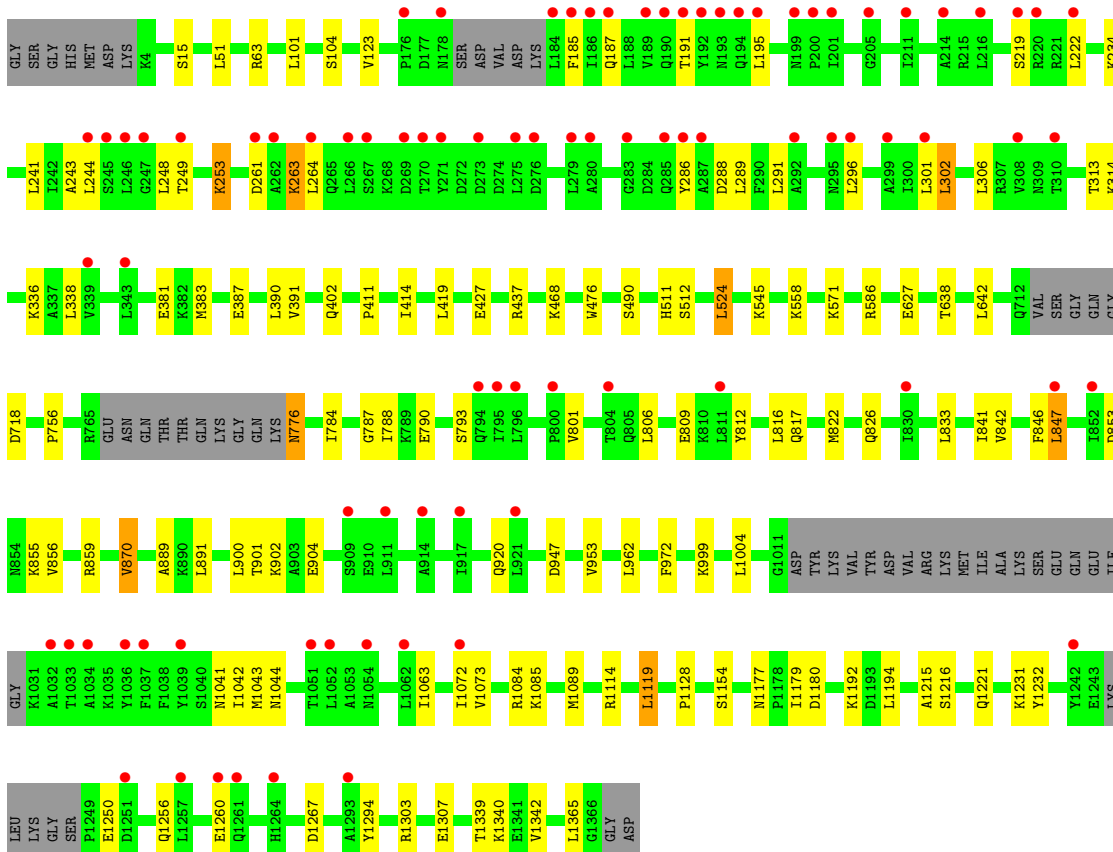
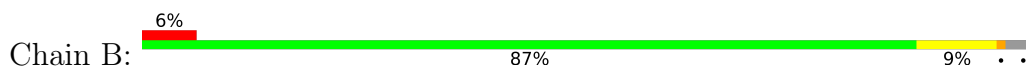
3 Residue-property plots [i](#)

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: Guide RNA



- Molecule 2: CRISPR-associated endonuclease Cas9




- Molecule 3: Target DNA

Chain C:  71% 29%



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

Chain D:  12% 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.76Å 67.74Å 187.59Å 90.00° 111.23° 90.00°	Depositor
Resolution (Å)	47.94 – 2.00 47.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.94-2.00) 97.3 (47.94-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.201 , 0.230 0.201 , 0.230	Depositor DCC
R_{free} test set	6818 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtrriage
Anisotropy	0.586	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13799	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/1949	0.90	0/3037
2	B	0.31	0/10738	0.47	0/14474
3	C	0.75	0/626	0.99	0/961
4	D	0.66	0/185	1.03	1/285 (0.4%)
All	All	0.37	0/13498	0.61	1/18757 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	7	DA	O4'-C1'-N9	5.54	111.88	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1739	0	870	5	0
2	B	10547	0	10509	69	0
3	C	560	0	316	7	0
4	D	165	0	93	1	0
5	A	4	0	0	0	0
5	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	6	0	0
7	B	12	0	18	0	0
8	A	4	0	3	0	0
9	A	199	0	0	0	0
9	B	492	0	0	6	0
9	C	50	0	0	2	0
9	D	13	0	0	0	0
All	All	13799	0	11815	79	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 (79) 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)
3:C:2:DA:H2'	3:C:3:DA:C8	2.19	0.78
3:C:19:DC:OP2	9:C:101:HOH:O	2.07	0.72
2:B:586:ARG:NH1	9:B:1501:HOH:O	2.26	0.67
2:B:558:LYS:HD2	2:B:586:ARG:HH21	1.62	0.64
2:B:241:LEU:O	2:B:244:LEU:N	2.24	0.64
2:B:222:LEU:HD23	2:B:234:LYS:HE3	1.83	0.61
2:B:253:LYS:NZ	2:B:261:ASP:OD1	2.30	0.59
1:A:71:U:H2'	1:A:72:U:C6	2.37	0.58
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.85	0.57
2:B:427:GLU:OE1	2:B:437[B]:ARG:NH1	2.37	0.57
2:B:842:VAL:HB	2:B:847:LEU:HD22	1.87	0.56
2:B:784:ILE:HD12	2:B:806:LEU:HD13	1.88	0.56
2:B:302:LEU:HD12	2:B:414:ILE:HD11	1.88	0.56
2:B:468:LYS:NZ	9:B:1504:HOH:O	2.32	0.56
3:C:19:DC:H5''	3:C:19:DC:H6	1.71	0.55
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.88	0.55
2:B:1267:ASP:OD1	2:B:1294:TYR:OH	2.22	0.54
2:B:1179:ILE:HD11	2:B:1192:LYS:HG3	1.90	0.53
2:B:1256:GLN:O	2:B:1260:GLU:HG2	2.08	0.53
2:B:1303:ARG:NH2	2:B:1307:GLU:OE2	2.42	0.53
2:B:999:LYS:HB3	2:B:1073:VAL:HG22	1.91	0.52
2:B:243:ALA:HB1	2:B:248:LEU:HB3	1.92	0.51
2:B:338:LEU:HB3	2:B:383:MET:HE1	1.92	0.51
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HD22	2:B:302:LEU:H	1.76	0.51
2:B:826:GLN:NE2	2:B:859:ARG:HD2	2.25	0.51
2:B:776:ASN:N	2:B:776:ASN:OD1	2.43	0.50
2:B:809:GLU:OE2	2:B:855:LYS:NZ	2.32	0.50
2:B:411:PRO:HD2	2:B:414:ILE:HG13	1.94	0.50
2:B:627:GLU:HG3	9:C:102:HOH:O	2.11	0.49
2:B:524:LEU:HD13	2:B:545:LYS:HG2	1.93	0.49
2:B:822:MET:HG3	2:B:856:VAL:HB	1.93	0.49
2:B:249:THR:HG22	2:B:263:LYS:HB2	1.93	0.49
2:B:846:PHE:O	2:B:920:GLN:NE2	2.44	0.48
2:B:1339:THR:O	2:B:1342:VAL:HG22	2.14	0.48
2:B:195:LEU:HD21	2:B:286:TYR:HA	1.94	0.48
3:C:1:DC:H2'	3:C:2:DA:C8	2.48	0.48
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.48	0.47
2:B:901:THR:O	2:B:904:GLU:HG2	2.16	0.46
2:B:336:LYS:NZ	9:B:1511:HOH:O	2.41	0.46
2:B:185:PHE:HD2	2:B:296:LEU:HD11	1.80	0.46
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.98	0.46
2:B:253:LYS:HG3	2:B:261:ASP:HA	1.97	0.46
2:B:302:LEU:HG	2:B:306:LEU:HD12	1.97	0.46
2:B:817:GLN:CD	2:B:822:MET:HG2	2.36	0.45
2:B:972:PHE:HE1	2:B:1084:ARG:HG2	1.81	0.45
2:B:1085:LYS:O	2:B:1089:MET:HG3	2.17	0.45
1:A:14:G:OP2	2:B:63:ARG:NH1	2.39	0.45
2:B:756:PRO:O	2:B:953:VAL:HG22	2.17	0.45
2:B:387:GLU:O	2:B:391:VAL:HG23	2.16	0.45
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.98	0.45
1:A:45:U:H5'	2:B:402:GLN:HE21	1.82	0.44
2:B:788:ILE:HG23	2:B:793:SER:HB3	2.00	0.44
2:B:511:HIS:HD2	9:B:1610:HOH:O	2.00	0.44
2:B:1194:LEU:HD13	2:B:1365:LEU:HD22	2.00	0.44
2:B:1340:LYS:NZ	9:B:1532:HOH:O	2.51	0.44
2:B:248:LEU:HD12	2:B:249:THR:H	1.83	0.43
2:B:288:ASP:HA	2:B:291:LEU:HB3	2.00	0.43
2:B:870:VAL:HG11	2:B:902:LYS:HB3	2.01	0.43
1:A:46:A:H2'	1:A:47:A:C8	2.54	0.43
2:B:1041:ASN:OD1	2:B:1044:ASN:ND2	2.49	0.43
2:B:187:GLN:O	2:B:191:THR:N	2.50	0.43
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.87	0.43
2:B:841:ILE:HD13	2:B:900:LEU:HG	2.01	0.43
2:B:1231:LYS:HE3	2:B:1232:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:A:H3'	1:A:75:A:H8	1.84	0.42
2:B:195:LEU:HD23	2:B:289:LEU:HB2	2.01	0.42
2:B:302:LEU:H	2:B:302:LEU:CD2	2.31	0.42
2:B:1063:ILE:HG23	2:B:1072:ILE:HG13	2.02	0.42
2:B:1119:LEU:HB3	2:B:1128:PRO:HB3	2.02	0.42
3:C:20:DC:H2''	3:C:21:DT:H5'	2.02	0.42
3:C:16:DG:H2'	3:C:17:DC:C6	2.54	0.42
2:B:381:GLU:HG2	2:B:390:LEU:HD11	2.02	0.41
2:B:15:SER:HA	2:B:51:LEU:O	2.21	0.41
2:B:962:LEU:HD11	2:B:1043:MET:CE	2.49	0.41
2:B:302:LEU:HG	2:B:306:LEU:CD1	2.50	0.41
3:C:2:DA:H2''	3:C:3:DA:O5'	2.20	0.41
2:B:812:TYR:CZ	2:B:816:LEU:HD11	2.55	0.41
2:B:104:SER:HA	9:B:1774:HOH:O	2.21	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
2	B	1308/1372 (95%)	1269 (97%)	38 (3%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1216	SER

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
2	B	1121/1227 (91%)	1092 (97%)	29 (3%)	46 48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	101	LEU
2	B	123	VAL
2	B	219	SER
2	B	253	LYS
2	B	263	LYS
2	B	264	LEU
2	B	301	LEU
2	B	302	LEU
2	B	313	THR
2	B	314	LYS
2	B	419	LEU
2	B	476	TRP
2	B	490	SER
2	B	512	SER
2	B	524	LEU
2	B	571	LYS
2	B	638	THR
2	B	642	LEU
2	B	718	ASP
2	B	776	ASN
2	B	801	VAL
2	B	833	LEU
2	B	847	LEU
2	B	853	ASP
2	B	870	VAL
2	B	947	ASP
2	B	1119	LEU
2	B	1154	SER
2	B	1250	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	402	GLN
2	B	412	HIS
2	B	511	HIS
2	B	726	ASN
2	B	926	GLN
2	B	1041	ASN
2	B	1044	ASN
2	B	1261	GLN
2	B	1295	ASN
2	B	1297	HIS
2	B	1317	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/81 (98%)	12 (15%)	1 (1%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	17	U
1	A	28	A
1	A	40	C
1	A	51	A
1	A	56	U
1	A	58	G
1	A	59	U
1	A	68	A
1	A	71	U
1	A	72	U
1	A	74	A
1	A	75	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	71	U

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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	1410	-	3,3,3	0.53	0	2,2,2	0.17	0
7	EDO	B	1409	-	3,3,3	0.57	0	2,2,2	0.16	0
7	EDO	A	106	-	3,3,3	0.47	0	2,2,2	0.25	0
8	ACT	A	107	-	3,3,3	0.76	0	3,3,3	1.31	0
7	EDO	B	1411	-	3,3,3	0.45	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	1409	-	-	0/1/1/1	-
7	EDO	B	1411	-	-	0/1/1/1	-
7	EDO	A	106	-	-	0/1/1/1	-
7	EDO	B	1410	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	81/81 (100%)	-0.58	1 (1%) 79 78	26, 41, 122, 188	0
2	B	1319/1372 (96%)	0.20	86 (6%) 18 18	24, 52, 95, 123	0
3	C	28/28 (100%)	-0.29	0 100 100	34, 48, 74, 84	0
4	D	8/8 (100%)	0.12	1 (12%) 3 3	37, 52, 98, 119	0
All	All	1436/1489 (96%)	0.15	88 (6%) 21 20	24, 51, 96, 188	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	186	ILE	8.0
2	B	247	GLY	6.2
2	B	264	LEU	6.0
2	B	292	ALA	5.5
2	B	244	LEU	5.3
2	B	262	ALA	5.0
2	B	245	SER	4.9
2	B	296	LEU	4.8
2	B	1033	THR	4.7
2	B	190	GLN	4.7
2	B	1039	TYR	4.5
2	B	275	LEU	4.5
2	B	1257	LEU	4.3
2	B	911	LEU	4.3
2	B	286	TYR	4.3
2	B	266	LEU	4.2
2	B	193	ASN	4.0
2	B	194	GLN	3.9
2	B	1052	LEU	3.8
2	B	189	VAL	3.8
2	B	216	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	1054	ASN	3.7
2	B	267	SER	3.7
2	B	1036	TYR	3.7
2	B	847	LEU	3.7
2	B	200	PRO	3.7
2	B	287	ALA	3.6
2	B	271	TYR	3.6
2	B	1072	ILE	3.5
2	B	804	THR	3.5
2	B	276	ASP	3.3
2	B	184	LEU	3.3
2	B	178	ASN	3.3
2	B	1034	ALA	3.3
2	B	192	TYR	3.2
2	B	270	THR	3.1
1	A	74	A	3.1
2	B	295	ASN	3.1
2	B	299	ALA	3.1
2	B	301	LEU	3.0
2	B	917	ILE	2.9
2	B	201	ILE	2.9
2	B	222	LEU	2.9
2	B	280	ALA	2.9
2	B	195	LEU	2.9
2	B	1062	LEU	2.9
2	B	279	LEU	2.8
2	B	1032	ALA	2.8
2	B	795	ILE	2.8
2	B	249	THR	2.7
2	B	205	GLY	2.7
2	B	220	ARG	2.7
2	B	187	GLN	2.7
2	B	214	ALA	2.7
2	B	269	ASP	2.6
2	B	1251	ASP	2.5
2	B	191	THR	2.5
2	B	796	LEU	2.5
2	B	310	THR	2.5
2	B	211	ILE	2.5
2	B	800	PRO	2.4
2	B	273	ASP	2.4
2	B	219	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	308	VAL	2.4
2	B	283	GLY	2.4
2	B	909	SER	2.3
2	B	914	ALA	2.3
2	B	176	PRO	2.3
2	B	921	LEU	2.3
2	B	794	GLN	2.3
2	B	830	ILE	2.3
4	D	12	DG	2.3
2	B	1264	HIS	2.3
2	B	261	ASP	2.3
2	B	199	ASN	2.3
2	B	1242	TYR	2.2
2	B	343	LEU	2.2
2	B	185	PHE	2.2
2	B	246	LEU	2.1
2	B	285	GLN	2.1
2	B	1051	THR	2.1
2	B	339	VAL	2.1
2	B	852	ILE	2.1
2	B	1037	PHE	2.1
2	B	1261	GLN	2.0
2	B	1293	ALA	2.0
2	B	811	LEU	2.0
2	B	1260	GLU	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 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, 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(\AA^2)	Q<0.9
5	K	B	1407	1/1	-0.48	0.64	210,210,210,210	0
5	K	A	108	1/1	0.77	0.32	114,114,114,114	0
5	K	B	1406	1/1	0.82	0.61	118,118,118,118	0
5	K	B	1405	1/1	0.85	0.07	83,83,83,83	0
7	EDO	B	1410	4/4	0.88	0.14	45,47,47,48	0
8	ACT	A	107	4/4	0.88	0.17	49,52,53,55	0
7	EDO	B	1411	4/4	0.95	0.16	34,41,45,48	0
7	EDO	A	106	4/4	0.95	0.13	33,34,34,37	0
7	EDO	B	1409	4/4	0.96	0.10	33,34,35,35	0
6	MG	A	104	1/1	0.96	0.07	42,42,42,42	0
6	MG	B	1408	1/1	0.96	0.11	46,46,46,46	0
5	K	B	1404	1/1	0.96	0.14	94,94,94,94	0
5	K	B	1403	1/1	0.97	0.09	58,58,58,58	0
6	MG	A	105	1/1	0.97	0.10	46,46,46,46	0
5	K	B	1402	1/1	0.98	0.12	48,48,48,48	0
5	K	B	1401	1/1	0.98	0.05	39,39,39,39	0
5	K	A	102	1/1	0.99	0.09	34,34,34,34	0
5	K	A	103	1/1	0.99	0.08	34,34,34,34	0
5	K	A	101	1/1	0.99	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.