



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:08 PM UTC

PDB ID : 5B43 / pdb_00005b43
Title : Crystal structure of Acidaminococcus sp. Cpf1 in complex with crRNA and target DNA
Authors : Yamano, T.; Nishimasu, H.; Hirano, H.; Nakane, T.; Ishitani, R.; Nureki, O.
Deposited on : 2016-03-30
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

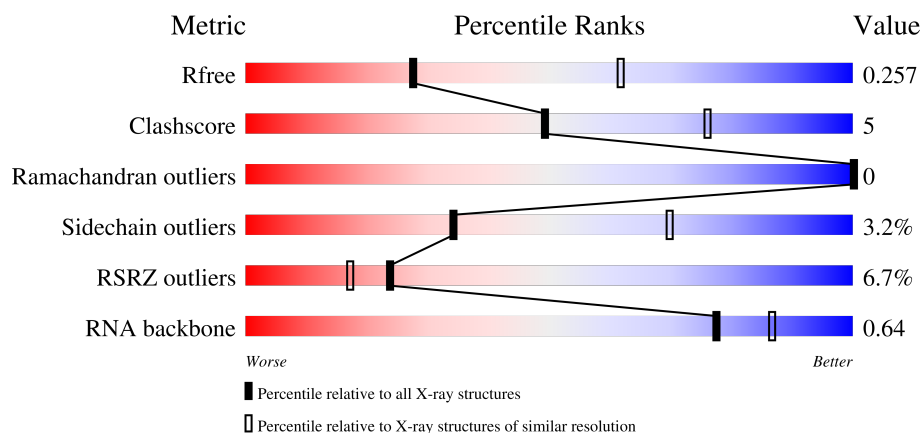
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	1310	7% 82% 14% ••
2	B	43	58% 30% 5% 7%
3	C	34	3% 76% 12% 12%
4	D	10	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11852 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 Cpf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1272	Total	C	N	O	S	0	0	0
			10157	6522	1709	1901	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP U2UMQ6
A	-1	SER	-	expression tag	UNP U2UMQ6
A	0	HIS	-	expression tag	UNP U2UMQ6

- Molecule 2 is a RNA chain called RNA (43-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	P	0	0	0
			847	380	146	282	39			

- Molecule 3 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			612	291	114	177	30			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*CP*CP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			198	97	32	60	9			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

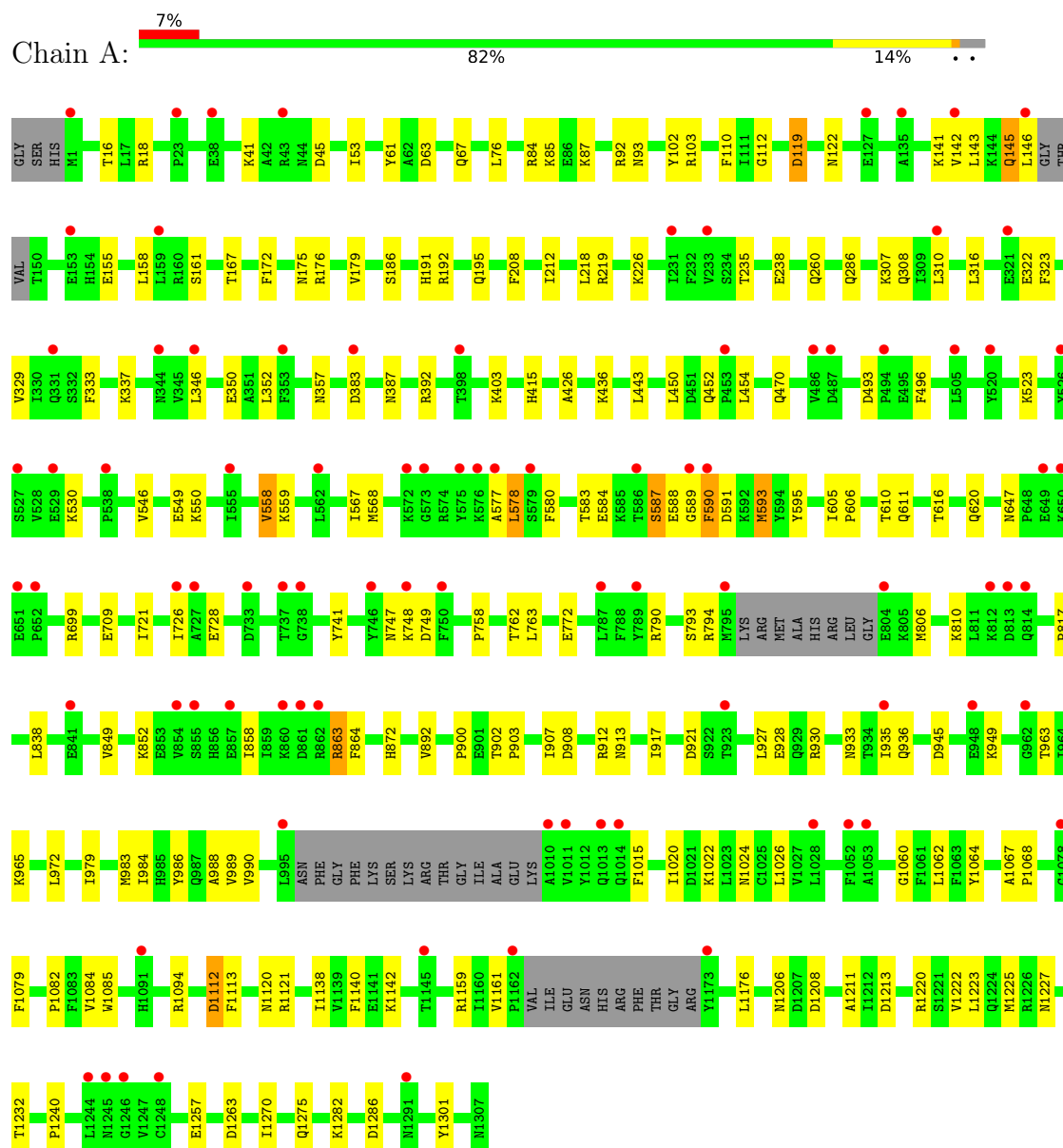
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	B	1	Total	O	0	0
			1	1		

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: CRISPR-associated endonuclease Cpf1



• Molecule 2: RNA (43-MER)

Chain B:

58%

30%

5%

7%



● Molecule 3: DNA (34-MER)

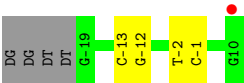
Chain C:

3%

76%

12%

12%

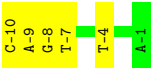


● Molecule 4: DNA (5'-D(*CP*AP*GP*TP*CP*CP*TP*TP*TP*A)-3')

Chain D:

50%

50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.52Å 136.73Å 196.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.16 – 2.80 56.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (56.16-2.80) 98.7 (56.16-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.220 , 0.257 0.227 , 0.257	Depositor DCC
R_{free} test set	2658 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11852	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: EDO, NA

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	0.09	0/10389	0.26	0/14086
2	B	0.08	0/946	0.23	0/1472
3	C	0.16	0/686	0.31	0/1055
4	D	0.23	0/220	0.45	0/337
All	All	0.10	0/12241	0.26	0/16950

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10157	0	9875	110	0
2	B	847	0	428	14	0
3	C	612	0	337	3	0
4	D	198	0	116	4	0
5	A	12	0	18	1	0
6	A	1	0	0	0	0
7	A	24	0	0	0	0
7	B	1	0	0	0	0
All	All	11852	0	10774	120	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 5.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:SER:HB3	1:A:864:PHE:HB3	1.69	0.73
2:B:-8:U:O2	2:B:-6:G:O2'	2.07	0.69
1:A:357:ASN:OD1	1:A:436:LYS:NZ	2.29	0.66
1:A:928:GLU:OE2	1:A:930:ARG:NH2	2.28	0.66
1:A:984:ILE:HD11	1:A:1026:LEU:HD21	1.80	0.64
1:A:53:ILE:HD13	1:A:155:GLU:HG2	1.82	0.62
1:A:945:ASP:OD2	1:A:949:LYS:NZ	2.31	0.62
1:A:593:MET:HE3	1:A:595:TYR:HB2	1.82	0.62
1:A:1113:PHE:HB2	1:A:1140:PHE:HB2	1.83	0.60
1:A:1159:ARG:NH1	1:A:1222:VAL:O	2.32	0.60
1:A:337:LYS:NZ	1:A:452:GLN:O	2.34	0.60
1:A:903:PRO:HG2	1:A:988:ALA:HB2	1.84	0.58
1:A:337:LYS:NZ	1:A:470:GLN:OE1	2.37	0.58
1:A:578:LEU:H	1:A:578:LEU:HD23	1.68	0.58
1:A:699:ARG:NH1	1:A:709:GLU:OE2	2.38	0.57
1:A:322:GLU:OE2	1:A:523:LYS:NZ	2.37	0.57
1:A:112:GLY:O	1:A:122:ASN:ND2	2.40	0.55
1:A:748:LYS:N	2:B:-16:U:OP1	2.39	0.55
2:B:0:G:H1'	2:B:1:G:C8	2.42	0.55
1:A:383:ASP:O	1:A:387:ASN:ND2	2.35	0.54
1:A:1082:PRO:HB3	5:A:1403:EDO:H12	1.88	0.54
1:A:1275:GLN:NE2	1:A:1301:TYR:OH	2.41	0.54
1:A:1206:ASN:HD21	1:A:1208:ASP:HB2	1.73	0.54
1:A:1094:ARG:NE	1:A:1213:ASP:OD1	2.40	0.53
1:A:747:ASN:ND2	1:A:749:ASP:H	2.06	0.53
1:A:900:PRO:HG3	1:A:1282:LYS:HE3	1.91	0.52
1:A:1067:ALA:N	1:A:1068:PRO:HD2	2.23	0.52
1:A:84:ARG:O	1:A:87:LYS:NZ	2.40	0.52
1:A:260:GLN:HE22	1:A:316:LEU:H	1.58	0.52
1:A:41:LYS:NZ	1:A:45:ASP:OD1	2.43	0.52
1:A:226:LYS:NZ	1:A:235:THR:O	2.39	0.51
1:A:286:GLN:NE2	2:B:17:G:O2'	2.44	0.51
1:A:584:GLU:O	1:A:587:SER:OG	2.28	0.51
1:A:590:PHE:O	1:A:726:ILE:HG22	2.11	0.51
1:A:186:SER:HA	1:A:191:HIS:CD2	2.46	0.51
1:A:530:LYS:HB3	1:A:790:ARG:HB3	1.93	0.51
1:A:1112:ASP:HB3	1:A:1142:LYS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:ND2	2:B:3:A:O2'	2.44	0.51
1:A:103:ARG:NH1	1:A:195:GLN:OE1	2.43	0.51
1:A:1161:VAL:HG21	1:A:1176:LEU:HD12	1.93	0.51
1:A:907:ILE:HD13	1:A:990:VAL:HG13	1.94	0.50
1:A:493:ASP:HB3	1:A:496:PHE:HB3	1.93	0.50
1:A:568:MET:HE2	1:A:580:PHE:HE2	1.76	0.50
1:A:1225:MET:HG2	1:A:1240:PRO:HD3	1.93	0.50
1:A:810:LYS:HA	1:A:817:PRO:HA	1.94	0.49
1:A:212:ILE:HG23	1:A:219:ARG:HB2	1.95	0.49
1:A:921:ASP:HB3	1:A:927:LEU:HD11	1.94	0.49
1:A:558:VAL:HG13	1:A:591:ASP:HB2	1.94	0.49
1:A:92:ARG:NH2	1:A:93:ASN:OD1	2.45	0.49
1:A:1138:ILE:HD13	1:A:1223:LEU:HD21	1.94	0.49
2:B:6:U:H2'	2:B:7:A:C8	2.48	0.49
1:A:141:LYS:O	1:A:145:GLN:HG2	2.13	0.49
1:A:907:ILE:HG13	1:A:917:ILE:HG22	1.95	0.49
1:A:350:GLU:HG2	1:A:443:LEU:HD13	1.95	0.49
1:A:790:ARG:NH1	2:B:-15:U:OP1	2.32	0.48
1:A:119:ASP:N	1:A:119:ASP:OD1	2.46	0.48
1:A:167:THR:OG1	4:D:-4:DT:OP2	2.22	0.48
1:A:16:THR:HG21	2:B:1:G:H1'	1.96	0.48
1:A:333:PHE:O	1:A:337:LYS:N	2.42	0.48
1:A:794:ARG:HG2	1:A:864:PHE:HB2	1.96	0.48
1:A:219:ARG:NE	1:A:238:GLU:OE1	2.46	0.48
4:D:-10:DC:H2''	4:D:-9:DA:C8	2.49	0.48
1:A:18:ARG:HG2	1:A:872:HIS:CD2	2.50	0.47
1:A:179:VAL:HG11	1:A:310:LEU:HD12	1.96	0.47
1:A:913:ASN:HA	1:A:933:ASN:HD21	1.78	0.47
1:A:1206:ASN:ND2	1:A:1208:ASP:HB2	2.30	0.47
1:A:307:LYS:NZ	1:A:308:GLN:O	2.42	0.47
1:A:1208:ASP:HB3	1:A:1211:ALA:HB3	1.98	0.46
1:A:392:ARG:HD3	1:A:426:ALA:HB2	1.98	0.45
1:A:567:ILE:HB	1:A:741:TYR:HB2	1.98	0.45
3:C:-2:DT:H2'	3:C:-1:DC:C6	2.51	0.45
1:A:559:LYS:NZ	1:A:728:GLU:OE2	2.48	0.45
3:C:-13:DC:H2'	3:C:-12:DG:C8	2.51	0.45
1:A:172:PHE:HA	1:A:175:ASN:HD22	1.82	0.45
1:A:192:ARG:HH22	2:B:6:U:H4'	1.81	0.44
1:A:747:ASN:HD21	1:A:762:THR:HG21	1.83	0.44
1:A:806:MET:HE1	1:A:858:ILE:HB	1.98	0.44
1:A:1022:LYS:HD3	2:B:-1:U:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:O	1:A:67:GLN:HG3	2.18	0.44
1:A:908:ASP:HB2	1:A:1270:ILE:HD12	2.00	0.44
1:A:1225:MET:O	1:A:1227:ASN:ND2	2.50	0.44
1:A:892:VAL:HG21	1:A:1060:GLY:HA2	1.99	0.43
2:B:-8:U:O2	2:B:-8:U:H2'	2.17	0.43
1:A:852:LYS:HZ1	2:B:-9:C:P	2.42	0.43
4:D:-9:DA:H4'	4:D:-8:DG:OP1	2.19	0.43
1:A:913:ASN:ND2	1:A:1263:ASP:OD2	2.44	0.43
1:A:142:VAL:HA	1:A:145:GLN:HG3	2.00	0.43
1:A:1120:ASN:HD21	1:A:1121:ARG:NH2	2.17	0.42
1:A:972:LEU:HD22	1:A:1015:PHE:HB2	2.00	0.42
1:A:546:VAL:HA	1:A:549:GLU:HG3	2.00	0.42
1:A:588:GLU:HG2	1:A:728:GLU:HB2	2.01	0.42
1:A:337:LYS:HE3	1:A:450:LEU:HA	2.02	0.42
1:A:145:GLN:HE21	1:A:145:GLN:HB3	1.54	0.42
3:C:-13:DC:H2'	3:C:-12:DG:H8	1.84	0.42
1:A:208:PHE:O	1:A:212:ILE:HG12	2.19	0.42
1:A:323:PHE:CD2	1:A:329:VAL:HG12	2.54	0.42
1:A:415:HIS:O	1:A:415:HIS:ND1	2.51	0.42
1:A:863:ARG:HG3	2:B:-17:U:OP2	2.20	0.42
1:A:605:ILE:HB	1:A:606:PRO:HD3	2.02	0.41
1:A:1085:TRP:CE2	1:A:1220:ARG:HG3	2.56	0.41
1:A:550:LYS:HB2	1:A:577:ALA:HB2	2.02	0.41
1:A:903:PRO:HG2	1:A:986:TYR:HB3	2.01	0.41
1:A:76:LEU:HB2	1:A:102:TYR:CE1	2.56	0.41
1:A:16:THR:H	2:B:0:G:H5''	1.86	0.41
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.94	0.41
1:A:589:GLY:HA3	1:A:726:ILE:O	2.20	0.41
1:A:747:ASN:ND2	1:A:749:ASP:OD1	2.53	0.41
1:A:917:ILE:HG21	1:A:979:ILE:HD11	2.03	0.41
1:A:963:THR:HG23	1:A:965:LYS:HG2	2.02	0.41
1:A:1020:ILE:HD11	1:A:1064:TYR:OH	2.21	0.41
1:A:749:ASP:OD2	1:A:758:PRO:HA	2.21	0.41
1:A:61:TYR:OH	1:A:110:PHE:O	2.39	0.40
1:A:176:ARG:HA	1:A:176:ARG:HD3	1.86	0.40
1:A:616:THR:O	1:A:620:GLN:HG2	2.21	0.40
1:A:1159:ARG:HD3	1:A:1159:ARG:HA	1.77	0.40
1:A:852:LYS:HD3	1:A:852:LYS:HA	1.92	0.40
1:A:158:LEU:O	1:A:161:SER:OG	2.31	0.40
1:A:611:GLN:OE1	1:A:647:ASN:ND2	2.48	0.40
1:A:1079:PHE:O	1:A:1225:MET:HE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:-8:DG:H2'	4:D:-7:DT:H71	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1262/1310 (96%)	1220 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	1081/1172 (92%)	1046 (97%)	35 (3%)	34	70

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	119	ASP
1	A	143	LEU
1	A	145	GLN
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	346	LEU
1	A	403	LYS
1	A	454	LEU
1	A	558	VAL
1	A	578	LEU
1	A	583	THR
1	A	587	SER
1	A	590	PHE
1	A	593	MET
1	A	610	THR
1	A	721	ILE
1	A	763	LEU
1	A	772	GLU
1	A	838	LEU
1	A	849	VAL
1	A	863	ARG
1	A	902	THR
1	A	912	ARG
1	A	935	ILE
1	A	936	GLN
1	A	983	MET
1	A	989	VAL
1	A	1024	ASN
1	A	1062	LEU
1	A	1084	VAL
1	A	1112	ASP
1	A	1232	THR
1	A	1257	GLU
1	A	1286	ASP

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

Mol	Chain	Res	Type
1	A	70	GLN
1	A	145	GLN
1	A	175	ASN
1	A	191	HIS
1	A	206	HIS
1	A	224	ASN
1	A	286	GLN
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	445	HIS
1	A	552	ASN
1	A	560	ASN
1	A	666	GLN
1	A	747	ASN
1	A	890	GLN
1	A	974	GLN
1	A	987	GLN
1	A	1013	GLN
1	A	1014	GLN
1	A	1096	HIS
1	A	1120	ASN
1	A	1206	ASN
1	A	1245	ASN
1	A	1275	GLN
1	A	1291	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/43 (90%)	4 (10%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-7	U
2	B	-6	G
2	B	0	G
2	B	20	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
5	EDO	A	1402	-	3,3,3	0.43	0	2,2,2	0.34	0
5	EDO	A	1401	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	A	1403	-	3,3,3	0.43	0	2,2,2	0.38	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
5	EDO	A	1402	-	-	0/1/1/1	-
5	EDO	A	1401	-	-	0/1/1/1	-
5	EDO	A	1403	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1403	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1272/1310 (97%)	0.65	89 (6%) 22 16	33, 69, 113, 146	0
2	B	40/43 (93%)	0.04	0 100 100	44, 58, 107, 120	0
3	C	30/34 (88%)	0.08	1 (3%) 49 39	44, 57, 130, 189	0
4	D	10/10 (100%)	0.42	0 100 100	66, 81, 143, 146	0
All	All	1352/1397 (96%)	0.62	90 (6%) 24 17	33, 68, 114, 189	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	804	GLU	4.7
1	A	1010	ALA	4.2
1	A	861	ASP	4.1
1	A	995	LEU	3.9
1	A	854	VAL	3.8
1	A	750	PHE	3.5
1	A	231	ILE	3.5
1	A	331	GLN	3.4
1	A	43	ARG	3.4
1	A	649	GLU	3.3
1	A	650	LYS	3.3
1	A	346	LEU	3.3
1	A	1173	TYR	3.2
1	A	146	LEU	3.2
1	A	321	GLU	3.2
1	A	652	PRO	3.2
1	A	579	SER	3.1
1	A	486	VAL	3.1
1	A	353	PHE	3.1
1	A	383	ASP	3.0
1	A	153	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1162	PRO	3.0
1	A	855	SER	3.0
1	A	1145	THR	3.0
1	A	862	ARG	2.9
1	A	487	ASP	2.9
1	A	135	ALA	2.9
1	A	795	MET	2.8
3	C	10	DG	2.8
1	A	1053	ALA	2.7
1	A	572	LYS	2.7
1	A	737	THR	2.7
1	A	1291	ASN	2.7
1	A	505	LEU	2.6
1	A	1246	GLY	2.6
1	A	127	GLU	2.6
1	A	538	PRO	2.5
1	A	529	GLU	2.5
1	A	555	ILE	2.5
1	A	1011	VAL	2.4
1	A	159	LEU	2.4
1	A	726	ILE	2.4
1	A	142	VAL	2.4
1	A	575	TYR	2.4
1	A	1	MET	2.4
1	A	787	LEU	2.4
1	A	1245	ASN	2.3
1	A	577	ALA	2.3
1	A	1248	CYS	2.3
1	A	233	VAL	2.3
1	A	738	GLY	2.3
1	A	948	GLU	2.3
1	A	1013	GLN	2.3
1	A	23	PRO	2.3
1	A	962	GLY	2.3
1	A	727	ALA	2.3
1	A	576	LYS	2.3
1	A	1078	GLY	2.3
1	A	860	LYS	2.2
1	A	526	TYR	2.2
1	A	590	PHE	2.2
1	A	344	ASN	2.2
1	A	562	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1014	GLN	2.2
1	A	494	PRO	2.2
1	A	527	SER	2.2
1	A	589	GLY	2.2
1	A	310	LEU	2.2
1	A	1091	HIS	2.2
1	A	1028	LEU	2.1
1	A	789	TYR	2.1
1	A	453	PRO	2.1
1	A	398	THR	2.1
1	A	733	ASP	2.1
1	A	812	LYS	2.1
1	A	1244	LEU	2.1
1	A	573	GLY	2.1
1	A	935	ILE	2.1
1	A	38	GLU	2.1
1	A	841	GLU	2.1
1	A	520	TYR	2.1
1	A	586	THR	2.0
1	A	923	THR	2.0
1	A	813	ASP	2.0
1	A	814	GLN	2.0
1	A	1052	PHE	2.0
1	A	651	GLU	2.0
1	A	748	LYS	2.0
1	A	857	GLU	2.0
1	A	746	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1401	4/4	0.79	0.29	75,75,76,76	0
5	EDO	A	1402	4/4	0.84	0.18	69,70,70,70	0
5	EDO	A	1403	4/4	0.88	0.25	59,61,61,61	0
6	NA	A	1404	1/1	0.92	0.21	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.