



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:09 AM UTC

PDB ID : 9MK3 / pdb_00009mk3
Title : Engineered AsCas12a (M537R, F870L)
Authors : Dementiev, A.; White, A.; Olland, A.M.; Suto, R.K.
Deposited on : 2024-12-16
Resolution : 2.70 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

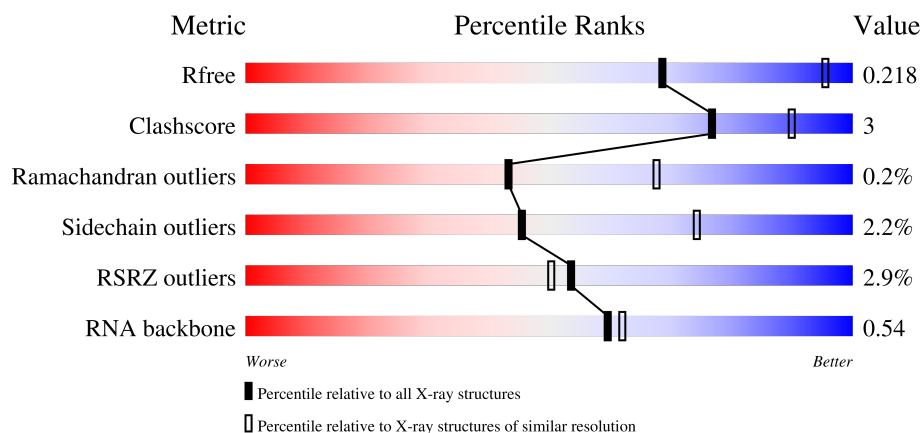
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



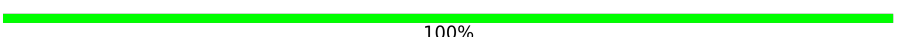
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	1307	2% 89% 9% •
1	E	1307	4% 89% 10% •
2	B	44	70% 23% 7%
2	F	44	73% 18% 7% •

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Mol	Chain	Length	Quality of chain
3	C	34	 6% 71% 21% 9%
3	G	34	 76% 12% 12%
4	D	10	 90% 10%
4	H	10	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24407 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 Cas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1292	Total	C	N	O	S	0	4	0
			10430	6684	1764	1958	24			
1	E	1295	Total	C	N	O	S	0	6	0
			10436	6681	1769	1962	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	ARG	MET	engineered mutation	UNP U2UMQ6
A	870	LEU	PHE	engineered mutation	UNP U2UMQ6
E	537	ARG	MET	engineered mutation	UNP U2UMQ6
E	870	LEU	PHE	engineered mutation	UNP U2UMQ6

- Molecule 2 is a RNA chain called gRNA (41-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	P	0	0	0
			867	389	148	290	40			
2	F	41	Total	C	N	O	P	0	0	0
			849	379	143	287	40			

- Molecule 3 is a DNA chain called TS DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	P	0	0	0
			633	301	119	182	31			
3	G	30	Total	C	N	O	P	0	0	0
			613	291	117	175	30			

- Molecule 4 is a DNA chain called NTS DNA (5'-D(*CP*AP*GP*TP*CP*CP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			197	97	29	62	9			
4	H	10	Total	C	N	O	P	0	0	0
			197	97	29	62	9			

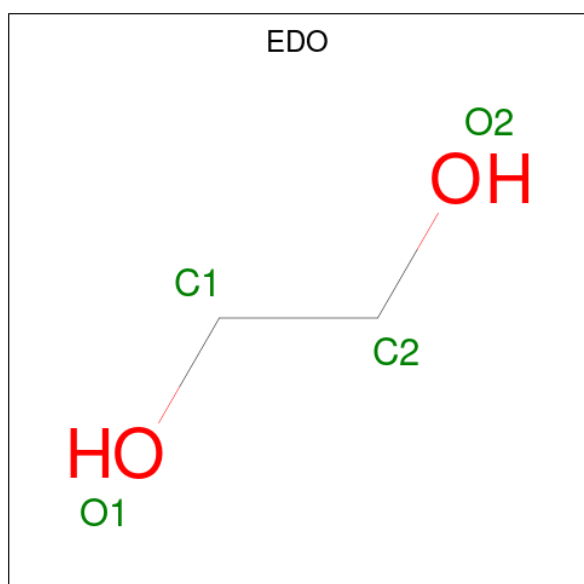
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

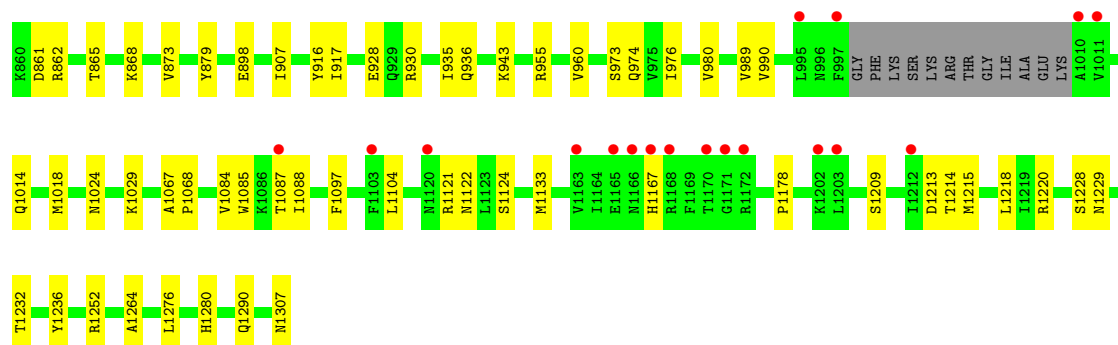
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0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

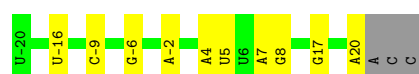
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	34	Total O 34 34	0	0
8	B	17	Total O 17 17	0	0
8	C	5	Total O 5 5	0	0
8	E	51	Total O 51 51	0	0
8	F	21	Total O 21 21	0	0
8	G	9	Total O 9 9	0	0



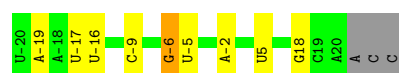
- Molecule 2: gRNA (41-MER)

Chain B: 70% 23% 7%



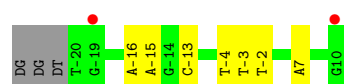
- Molecule 2: gRNA (41-MER)

Chain F: 73% 18% 7%



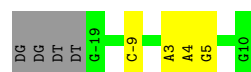
- Molecule 3: TS DNA (31-MER)

Chain C: 6% 71% 21% 9%



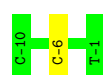
- Molecule 3: TS DNA (31-MER)

Chain G: 76% 12% 12%



- Molecule 4: NTS DNA (5'-D(*CP*AP*GP*TP*CP*CP*TP*TP*TP*T)-3')

Chain D: 90% 10%



- Molecule 4: NTS DNA (5'-D(*CP*AP*GP*TP*CP*CP*TP*TP*TP*T)-3')

Chain H: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.92Å 198.59Å 140.36Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	49.28 – 2.70 49.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.28-2.70) 98.2 (49.28-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.82)	Depositor
R, R_{free}	0.196 , 0.240 (Not available) , 0.218	Depositor DCC
R_{free} test set	6068 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24407	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/10676	0.93	3/14453 (0.0%)
1	E	0.47	0/10688	0.93	1/14475 (0.0%)
2	B	0.49	0/968	1.00	1/1506 (0.1%)
2	F	0.49	0/947	1.07	4/1474 (0.3%)
3	C	0.37	0/710	0.90	2/1092 (0.2%)
3	G	0.38	0/688	0.91	0/1058
4	D	0.36	0/218	1.04	1/334 (0.3%)
4	H	0.36	0/218	0.99	0/334
All	All	0.46	0/25113	0.94	12/34726 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	18	G	O3'-P-O5'	-6.01	94.99	104.00
2	F	5	U	O3'-P-O5'	-5.78	95.32	104.00
2	F	-17	U	O3'-P-O5'	-5.69	95.47	104.00
2	F	-19	A	O3'-P-O5'	-5.64	95.54	104.00
4	D	-6	DC	O3'-P-O5'	-5.49	95.77	104.00
2	B	17	G	O3'-P-O5'	-5.28	96.07	104.00
1	A	1208	ASP	CA-CB-CG	5.21	117.81	112.60
3	C	7	DA	O3'-P-O5'	-5.20	96.19	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1047	ASP	CA-CB-CG	5.14	117.74	112.60
3	C	-4	DT	O3'-P-O5'	-5.14	96.30	104.00
1	A	963	THR	CA-CB-OG1	-5.04	102.04	109.60
1	E	595	TYR	N-CA-CB	-5.02	102.14	110.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	947	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10430	0	10241	57	0
1	E	10436	0	10210	72	0
2	B	867	0	438	3	0
2	F	849	0	426	2	0
3	C	633	0	348	3	0
3	G	613	0	336	4	0
4	D	197	0	117	0	0
4	H	197	0	117	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	28	0	42	0	0
7	E	12	0	18	0	0
7	G	4	0	6	0	0
8	A	34	0	0	1	0
8	B	17	0	0	1	0
8	C	5	0	0	0	0
8	E	51	0	0	0	0
8	F	21	0	0	0	0
8	G	9	0	0	0	0
All	All	24407	0	22299	136	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 (136) 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:1100:GLY:HA3	1:A:1122:ASN:OD1	1.90	0.72
1:A:587:SER:O	1:A:725:ARG:HD3	1.93	0.68
1:E:1280:HIS:ND1	1:E:1290:GLN:OE1	2.23	0.67
1:E:1133:MET:HE3	1:E:1307:ASN:CB	2.27	0.65
1:A:1120:ASN:O	1:A:1123:LEU:HD21	1.97	0.65
1:A:152:THR:OG1	1:A:155:GLU:HG3	1.98	0.64
1:E:1133:MET:HE3	1:E:1307:ASN:HB2	1.79	0.63
1:E:907:ILE:HG12	1:E:917:ILE:HG22	1.81	0.62
1:A:1116:HIS:ND1	1:A:1137:ASP:OD1	2.31	0.62
1:E:231:ILE:HD11	1:E:261:LEU:HB2	1.83	0.59
1:E:229:ILE:HG23	1:E:265:ILE:HD11	1.85	0.59
1:E:1088:ILE:HG22	1:E:1088:ILE:O	2.02	0.59
1:A:118:THR:OG1	1:A:121:ILE:HD12	2.03	0.59
1:E:928:GLU:OE1	1:E:930:ARG:NH1	2.31	0.58
1:E:1087:THR:O	1:E:1088:ILE:HD12	2.04	0.57
1:A:321:GLU:O	1:A:516:LYS:HD2	2.04	0.56
1:A:1084:VAL:HG22	1:A:1127:ARG:HG3	1.87	0.56
1:A:834:LEU:O	1:A:835:SER:HB3	2.06	0.56
1:A:170:SER:HA	1:A:173:TYR:CD2	2.40	0.56
1:E:229:ILE:HG22	1:E:231:ILE:HG23	1.89	0.55
1:E:1229:ASN:ND2	1:E:1232:THR:HG22	2.22	0.55
1:E:1236:TYR:CD2	1:E:1252:ARG:HD3	2.42	0.55
1:E:1229:ASN:HD22	1:E:1232:THR:HG22	1.71	0.54
1:E:641:GLU:O	1:E:645:LEU:HD23	2.07	0.54
3:G:4:DA:H2''	3:G:5:DG:H5'	1.89	0.54
1:A:721:ILE:HG22	1:A:774:LEU:HD22	1.90	0.54
1:E:677:ILE:O	1:E:681:ARG:HG2	2.07	0.53
1:A:359:ILE:O	1:A:361:LEU:HD22	2.08	0.53
1:A:605:ILE:HB	1:A:606:PRO:HD3	1.90	0.53
2:B:4:A:H2'	2:B:5:U:O4'	2.08	0.53
1:E:732:MET:HA	1:E:732:MET:HE2	1.90	0.53
1:E:758:PRO:HG2	1:E:763:LEU:HD13	1.91	0.53
1:A:86:GLU:HG3	1:A:91:THR:HG21	1.91	0.52
1:E:599:PRO:O	1:E:600:ASP:C	2.52	0.52
1:E:256:ASP:OD2	1:E:314[A]:ASN:OD1	2.27	0.52
1:E:1097:PHE:HA	1:E:1122:ASN:ND2	2.25	0.52
1:E:348:THR:O	1:E:352:LEU:HD23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:LEU:HD22	1:A:1200:LEU:HD22	1.92	0.50
1:E:831:ASN:O	1:E:833:ARG:HG3	2.11	0.50
1:E:1214:THR:O	1:E:1218:LEU:HD23	2.11	0.50
1:A:103:ARG:NH1	1:A:195:GLN:OE1	2.44	0.50
1:A:1020:ILE:HD13	1:A:1055:MET:HE1	1.94	0.50
1:E:935:ILE:HG22	1:E:936:GLN:HG2	1.94	0.49
1:A:327:GLU:O	1:A:331:GLN:HG2	2.13	0.49
1:A:599:PRO:O	1:A:600:ASP:C	2.55	0.49
1:A:201:PHE:CE2	1:A:246:TYR:HB2	2.48	0.49
1:E:955:ARG:NH2	3:G:-9:DC:O2	2.46	0.49
1:A:51:LYS:HB3	1:A:52:PRO:HD3	1.95	0.48
1:E:1067:ALA:N	1:E:1068:PRO:CD	2.76	0.48
1:E:20:GLU:CD	1:E:868[B]:LYS:HE3	2.38	0.48
1:E:347:GLU:N	1:E:347:GLU:OE1	2.46	0.48
2:B:7:A:H2'	2:B:8:G:O4'	2.14	0.48
1:E:790:ARG:NH2	1:E:868[B]:LYS:HD3	2.29	0.48
1:E:935:ILE:HG21	1:E:974:GLN:HB3	1.96	0.47
1:E:375:SER:O	1:E:379:CYS:HB2	2.14	0.47
1:A:633:ILE:HD11	1:A:691:THR:OG1	2.14	0.47
1:E:313:ARG:HG3	1:E:313:ARG:HH11	1.80	0.47
1:E:339:LEU:C	1:E:339:LEU:HD23	2.39	0.47
1:A:1208:ASP:O	1:A:1212:ILE:HG12	2.15	0.47
1:E:699:ARG:NH2	1:E:709:GLU:OE1	2.48	0.47
1:A:309:ILE:O	1:A:310:LEU:HB2	2.14	0.47
1:E:548:LYS:CE	3:G:3:DA:N7	2.78	0.46
1:E:226:LYS:NZ	1:E:235:THR:O	2.40	0.46
1:A:58:TYR:OH	1:A:137:LEU:HD11	2.16	0.46
1:E:768:LEU:C	1:E:768:LEU:HD23	2.40	0.46
2:B:-2:A:OP1	8:B:101:HOH:O	2.21	0.46
1:E:446:ALA:O	1:E:450:LEU:HD12	2.16	0.46
1:A:76:LEU:HB2	1:A:102:TYR:CE1	2.52	0.45
1:A:955:ARG:HH11	1:A:955:ARG:HG2	1.80	0.45
1:A:1123:LEU:H	1:A:1123:LEU:HD22	1.81	0.45
1:E:1276:LEU:C	1:E:1276:LEU:HD23	2.41	0.45
1:A:620:GLN:HG2	1:A:621:THR:HG23	1.99	0.45
1:A:26:LYS:HE2	1:A:736:GLU:OE1	2.16	0.45
1:E:486:VAL:HG21	1:E:501:THR:OG1	2.17	0.45
1:E:548:LYS:HE2	3:G:3:DA:N7	2.32	0.45
1:E:1104:LEU:HD22	1:E:1215:MET:HE2	1.99	0.45
1:A:508:GLU:N	1:A:509:PRO:CD	2.79	0.45
1:E:1085:TRP:CD2	1:E:1220:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:GLN:O	1:E:670:ARG:HG2	2.16	0.45
1:E:780:LYS:HD3	1:E:879:TYR:CE1	2.52	0.45
1:E:385:LEU:HD21	1:E:431:LEU:CD1	2.47	0.45
1:E:627:LEU:HD23	1:E:637:GLU:HA	1.98	0.45
1:E:337:LYS:HE3	1:E:450:LEU:HA	1.99	0.44
1:E:361:LEU:HB2	1:E:421:GLN:HG2	2.00	0.44
1:A:207:ILE:HG12	1:A:299:PRO:HB2	1.98	0.44
1:A:1032:PRO:HD2	1:A:1035:LYS:HD3	1.98	0.44
1:A:307:LYS:HE2	1:A:308:GLN:O	2.18	0.44
1:A:352:LEU:O	1:A:355:GLU:HB2	2.17	0.44
1:A:903:PRO:HG2	1:A:986:TYR:HB3	1.98	0.44
1:A:651:GLU:HB3	1:A:652:PRO:HD3	1.99	0.44
1:A:1014:GLN:HG2	1:A:1018:MET:HE3	2.00	0.44
1:A:1067:ALA:N	1:A:1068:PRO:CD	2.80	0.44
1:E:806:MET:O	1:E:851:THR:HA	2.18	0.44
1:A:1029:LYS:NZ	8:A:1502:HOH:O	2.45	0.44
1:A:512:SER:O	1:A:516:LYS:HG3	2.18	0.43
1:E:1209:SER:O	1:E:1213:ASP:CG	2.61	0.43
1:A:1146:GLN:O	1:A:1153:PRO:HA	2.18	0.43
1:E:1014:GLN:HE21	1:E:1018:MET:CE	2.32	0.43
1:A:158:LEU:O	1:A:161:SER:OG	2.26	0.43
1:A:1161:VAL:HB	1:A:1162:PRO:HD2	2.00	0.43
1:A:189:ILE:HB	1:A:190:PRO:HD3	2.00	0.43
1:A:1113:PHE:HB2	1:A:1140:PHE:HB2	2.01	0.43
1:A:393:ARG:HD2	1:A:413:LEU:HD21	2.01	0.43
1:A:394:ILE:HD12	1:A:406:LYS:HG2	2.01	0.42
1:E:371:LEU:HD21	1:E:389:LEU:HD12	2.02	0.42
1:E:861:ASP:O	1:E:865:THR:HG23	2.19	0.42
1:A:141:LYS:O	1:A:145:GLN:HG3	2.19	0.42
1:E:198:PHE:HB3	1:E:199:PRO:HD3	2.02	0.42
1:A:768:LEU:HD23	1:A:768:LEU:O	2.20	0.42
1:E:508:GLU:N	1:E:509:PRO:CD	2.83	0.42
1:E:1088:ILE:O	1:E:1088:ILE:CG2	2.67	0.42
1:E:916:TYR:CZ	1:E:1264:ALA:HB2	2.55	0.42
1:A:229:ILE:HG23	1:A:265:ILE:HD11	2.01	0.41
2:F:-6:G:C2	2:F:-5:U:C5	3.07	0.41
1:E:605:ILE:HB	1:E:606:PRO:HD3	2.02	0.41
3:C:-3:DT:H2'	3:C:-2:DT:C6	2.55	0.41
1:E:693:ILE:O	1:E:695:LEU:HD22	2.20	0.41
1:E:859:ILE:HD13	1:E:862:ARG:HG3	2.02	0.41
1:E:907:ILE:HD12	1:E:990:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1014:GLN:HG2	1:E:1018:MET:HE3	2.03	0.41
1:A:715:ASN:N	1:A:716:PRO:CD	2.83	0.41
1:A:768:LEU:HD23	1:A:768:LEU:C	2.45	0.41
1:E:43[A]:ARG:HD2	1:E:168:TYR:CE2	2.55	0.41
1:E:325:SER:OG	1:E:328:GLU:HB2	2.21	0.41
1:A:243:PHE:N	1:A:244:PRO:CD	2.84	0.41
1:E:768:LEU:HD23	1:E:768:LEU:O	2.21	0.41
1:E:243:PHE:N	1:E:244:PRO:CD	2.84	0.41
1:E:1029:LYS:HE3	2:F:-2:A:OP2	2.21	0.41
1:E:1121:ARG:O	1:E:1122:ASN:C	2.64	0.40
1:E:1178:PRO:HA	1:E:1218:LEU:CD1	2.51	0.40
1:A:801:ARG:O	1:A:802:LEU:CB	2.69	0.40
3:C:-16:DA:H2'	3:C:-15:DA:C8	2.57	0.40
1:E:2:THR:OG1	1:E:898:GLU:OE1	2.40	0.40
1:A:927:LEU:HD13	1:A:986:TYR:CE1	2.56	0.40
1:A:266:SER:HB2	3:C:-13:DC:H2''	2.03	0.40

There are no symmetry-related clashes.

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	1290/1307 (99%)	1245 (96%)	42 (3%)	3 (0%)	43	68
1	E	1297/1307 (99%)	1254 (97%)	42 (3%)	1 (0%)	48	73
All	All	2587/2614 (99%)	2499 (97%)	84 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	LEU
1	E	1167	HIS

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Mol	Chain	Res	Type
1	A	600	ASP
1	A	310	LEU

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	1124/1170 (96%)	1103 (98%)	21 (2%)	50	77
1	E	1120/1170 (96%)	1091 (97%)	29 (3%)	40	70
All	All	2244/2340 (96%)	2194 (98%)	50 (2%)	45	74

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	143	LEU
1	A	251	THR
1	A	288	ASN
1	A	314	ASN
1	A	354	ASN
1	A	402	THR
1	A	437	GLN
1	A	454	LEU
1	A	487	ASP
1	A	550	LYS
1	A	633	ILE
1	A	721	ILE
1	A	729	LYS
1	A	792	LYS
1	A	856	HIS
1	A	976	ILE
1	A	980	VAL
1	A	995	LEU
1	A	1105	HIS
1	A	1213	ASP

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Mol	Chain	Res	Type
1	E	2	THR
1	E	3	GLN
1	E	165	PHE
1	E	314[A]	ASN
1	E	314[B]	ASN
1	E	338	THR
1	E	354	ASN
1	E	358	SER
1	E	380	ASP
1	E	429	LYS
1	E	442	ILE
1	E	526	TYR
1	E	620	GLN
1	E	633	ILE
1	E	695	LEU
1	E	697	SER
1	E	763	LEU
1	E	858	ILE
1	E	873	VAL
1	E	943	LYS
1	E	960	VAL
1	E	973	SER
1	E	976	ILE
1	E	980	VAL
1	E	989	VAL
1	E	1024	ASN
1	E	1084	VAL
1	E	1124	SER
1	E	1228	SER

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	93	ASN
1	A	104	ASN
1	A	145	GLN
1	A	419	ASN
1	A	534	ASN
1	A	832	HIS
1	A	1041	ASN
1	A	1295	ASN
1	E	9	ASN

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Mol	Chain	Res	Type
1	E	145	GLN
1	E	354	ASN
1	E	437	GLN
1	E	551	ASN
1	E	560	ASN
1	E	611	GLN
1	E	647	ASN
1	E	724	GLN
1	E	880	GLN
1	E	1014	GLN
1	E	1048	GLN
1	E	1105	HIS
1	E	1210	HIS
1	E	1229	ASN
1	E	1307	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	40/44 (90%)	4 (10%)	0
2	F	39/44 (88%)	3 (7%)	0
All	All	79/88 (89%)	7 (8%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-16	U
2	B	-9	C
2	B	-6	G
2	B	20	A
2	F	-16	U
2	F	-9	C
2	F	-6	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	A	1409	-	3,3,3	0.14	0	2,2,2	0.33	0
7	EDO	G	101	-	3,3,3	0.25	0	2,2,2	0.37	0
7	EDO	A	1407	-	3,3,3	0.10	0	2,2,2	0.10	0
7	EDO	A	1408	-	3,3,3	0.09	0	2,2,2	0.17	0
7	EDO	A	1405	-	3,3,3	0.09	0	2,2,2	0.13	0
7	EDO	A	1403	-	3,3,3	0.08	0	2,2,2	0.14	0
7	EDO	E	1405	-	3,3,3	0.18	0	2,2,2	0.27	0
7	EDO	E	1403	-	3,3,3	0.10	0	2,2,2	0.23	0
7	EDO	A	1404	-	3,3,3	0.11	0	2,2,2	0.20	0
7	EDO	E	1404	-	3,3,3	0.08	0	2,2,2	0.13	0
7	EDO	A	1406	-	3,3,3	0.12	0	2,2,2	0.24	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	A	1409	-	-	0/1/1/1	-
7	EDO	G	101	-	-	1/1/1/1	-
7	EDO	A	1407	-	-	1/1/1/1	-
7	EDO	A	1408	-	-	0/1/1/1	-
7	EDO	A	1405	-	-	0/1/1/1	-
7	EDO	A	1403	-	-	0/1/1/1	-
7	EDO	E	1405	-	-	1/1/1/1	-
7	EDO	E	1403	-	-	1/1/1/1	-
7	EDO	A	1404	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	1404	-	-	1/1/1/1	-
7	EDO	A	1406	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	1405	EDO	O1-C1-C2-O2
7	E	1403	EDO	O1-C1-C2-O2
7	E	1404	EDO	O1-C1-C2-O2
7	A	1407	EDO	O1-C1-C2-O2
7	G	101	EDO	O1-C1-C2-O2
7	A	1404	EDO	O1-C1-C2-O2
7	A	1406	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

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	1292/1307 (98%)	0.13	32 (2%) 58 55	32, 67, 105, 153	4 (0%)
1	E	1295/1307 (99%)	0.13	46 (3%) 46 42	30, 64, 110, 168	6 (0%)
2	B	41/44 (93%)	-0.88	0 100 100	43, 52, 79, 145	0
2	F	41/44 (93%)	-0.95	0 100 100	38, 49, 81, 102	0
3	C	31/34 (91%)	-0.39	2 (6%) 25 22	48, 56, 124, 145	0
3	G	30/34 (88%)	-0.50	0 100 100	42, 53, 96, 128	0
4	D	10/10 (100%)	-0.12	0 100 100	56, 67, 119, 125	0
4	H	10/10 (100%)	-0.43	0 100 100	49, 60, 113, 121	0
All	All	2750/2790 (98%)	0.08	80 (2%) 53 50	30, 65, 108, 168	10 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1007	ALA	7.1
1	A	1008	GLU	5.4
1	A	1164	ILE	5.2
1	A	149	VAL	4.6
1	E	1010	ALA	4.3
1	E	801	ARG	4.2
1	E	1011	VAL	4.1
1	E	1167	HIS	3.9
1	A	1011	VAL	3.9
1	E	486	VAL	3.9
1	A	997	PHE	3.8
1	E	800	HIS	3.7
1	E	149	VAL	3.7
1	E	663	THR	3.5
1	E	997	PHE	3.5
1	E	995	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	856	HIS	3.3
3	C	10	DG	3.2
1	A	2	THR	3.2
1	E	2	THR	3.1
1	A	294	ILE	3.1
1	A	798	MET	3.1
1	E	526	TYR	3.0
1	E	1120	ASN	3.0
1	E	485	ALA	3.0
1	E	799	ALA	3.0
1	E	797	ARG	2.8
1	E	492	VAL	2.8
1	E	802	LEU	2.7
1	E	1166	ASN	2.7
1	A	222	PHE	2.7
1	A	1165	GLU	2.7
1	E	1	MET	2.7
1	E	1168	ARG	2.7
1	E	1172	ARG	2.7
1	E	764	TYR	2.6
1	E	803	GLY	2.6
1	E	1087	THR	2.6
1	E	1163	VAL	2.6
1	E	1165	GLU	2.6
1	E	1171	GLY	2.5
1	E	794[A]	ARG	2.4
1	E	1203	LEU	2.4
1	A	1009	LYS	2.4
1	E	1202	LYS	2.3
1	A	485	ALA	2.3
1	A	799	ALA	2.3
1	E	150	THR	2.3
1	A	1	MET	2.3
1	E	798	MET	2.3
1	E	401	ILE	2.3
1	A	801	ARG	2.3
1	A	995	LEU	2.3
1	A	649	GLU	2.3
1	A	486	VAL	2.3
1	A	800	HIS	2.2
1	E	1170	THR	2.2
1	A	760	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	854	VAL	2.2
1	A	642	ILE	2.2
1	E	621	THR	2.2
1	A	650	LYS	2.2
1	E	487	ASP	2.2
1	E	1103	PHE	2.2
1	A	526	TYR	2.2
1	A	1173	TYR	2.2
1	A	854	VAL	2.2
1	E	1212	ILE	2.2
1	A	142	VAL	2.1
3	C	-19	DG	2.1
1	A	852	LYS	2.1
1	E	662	LYS	2.1
1	A	320	LEU	2.1
1	E	528	VAL	2.1
1	E	858	ILE	2.1
1	E	649	GLU	2.1
1	A	121	ILE	2.1
1	E	856	HIS	2.0
1	E	431	LEU	2.0
1	A	229	ILE	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
7	EDO	E	1404	4/4	0.72	0.25	80,80,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	1406	4/4	0.85	0.17	71,75,76,77	0
7	EDO	E	1405	4/4	0.85	0.23	64,68,68,70	0
7	EDO	A	1403	4/4	0.88	0.17	81,81,81,81	0
7	EDO	A	1409	4/4	0.88	0.16	64,66,67,68	0
7	EDO	E	1403	4/4	0.90	0.14	69,70,70,71	0
7	EDO	A	1408	4/4	0.90	0.18	80,80,80,82	0
7	EDO	A	1407	4/4	0.90	0.18	78,81,82,83	0
7	EDO	G	101	4/4	0.90	0.15	59,63,65,65	0
7	EDO	A	1404	4/4	0.92	0.16	72,72,74,74	0
5	NA	E	1401	1/1	0.96	0.09	54,54,54,54	0
7	EDO	A	1405	4/4	0.96	0.09	63,64,64,64	0
6	CL	E	1402	1/1	0.98	0.06	77,77,77,77	0
6	CL	A	1402	1/1	0.98	0.04	66,66,66,66	0
5	NA	A	1401	1/1	0.99	0.03	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.