



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 06:07 PM EST

PDB ID : 9DEN
Title : USP7 in complex with macrocycle MC07
Authors : Ultsch, M.; Tenorio, C.A.; Dueber, E.C.; Harris, S.F.
Deposited on : 2024-08-29
Resolution : 2.93 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

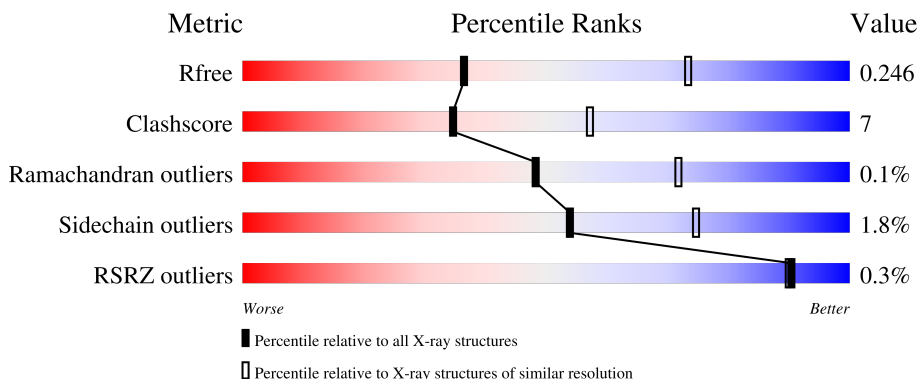
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




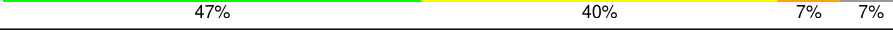
The reported resolution of this entry is 2.93 Å.

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}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	368	 74% 16% • 9%
1	B	368	 72% 18% • 10%
2	C	15	 53% 47%
2	D	15	 47% 40% 7% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5689 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	333	Total	C	N	O	S	0	0	0
			2700	1708	458	518	16			
1	A	334	Total	C	N	O	S	0	0	0
			2716	1717	465	518	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	187	MET	-	initiating methionine	UNP Q93009
B	188	GLY	-	expression tag	UNP Q93009
B	189	SER	-	expression tag	UNP Q93009
B	190	SER	-	expression tag	UNP Q93009
B	191	HIS	-	expression tag	UNP Q93009
B	192	HIS	-	expression tag	UNP Q93009
B	193	HIS	-	expression tag	UNP Q93009
B	194	HIS	-	expression tag	UNP Q93009
B	195	HIS	-	expression tag	UNP Q93009
B	196	HIS	-	expression tag	UNP Q93009
B	197	SER	-	expression tag	UNP Q93009
B	198	SER	-	expression tag	UNP Q93009
B	199	GLY	-	expression tag	UNP Q93009
B	200	LEU	-	expression tag	UNP Q93009
B	201	VAL	-	expression tag	UNP Q93009
B	202	PRO	-	expression tag	UNP Q93009
B	203	ARG	-	expression tag	UNP Q93009
B	204	GLY	-	expression tag	UNP Q93009
B	205	SER	-	expression tag	UNP Q93009
B	206	HIS	-	expression tag	UNP Q93009
B	207	MET	-	expression tag	UNP Q93009
A	187	MET	-	initiating methionine	UNP Q93009
A	188	GLY	-	expression tag	UNP Q93009
A	189	SER	-	expression tag	UNP Q93009
A	190	SER	-	expression tag	UNP Q93009

Continued on next page...

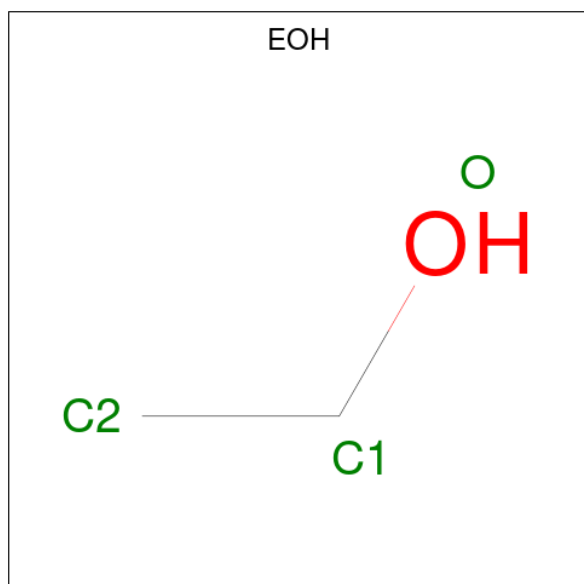
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	HIS	-	expression tag	UNP Q93009
A	192	HIS	-	expression tag	UNP Q93009
A	193	HIS	-	expression tag	UNP Q93009
A	194	HIS	-	expression tag	UNP Q93009
A	195	HIS	-	expression tag	UNP Q93009
A	196	HIS	-	expression tag	UNP Q93009
A	197	SER	-	expression tag	UNP Q93009
A	198	SER	-	expression tag	UNP Q93009
A	199	GLY	-	expression tag	UNP Q93009
A	200	LEU	-	expression tag	UNP Q93009
A	201	VAL	-	expression tag	UNP Q93009
A	202	PRO	-	expression tag	UNP Q93009
A	203	ARG	-	expression tag	UNP Q93009
A	204	GLY	-	expression tag	UNP Q93009
A	205	SER	-	expression tag	UNP Q93009
A	206	HIS	-	expression tag	UNP Q93009
A	207	MET	-	expression tag	UNP Q93009

- Molecule 2 is a protein called Macrocycle peptide MC07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	S	0	0	0
			126	86	22	17	1			
2	C	15	Total	C	N	O	S	0	0	0
			135	92	24	18	1			

- Molecule 3 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	2	1		

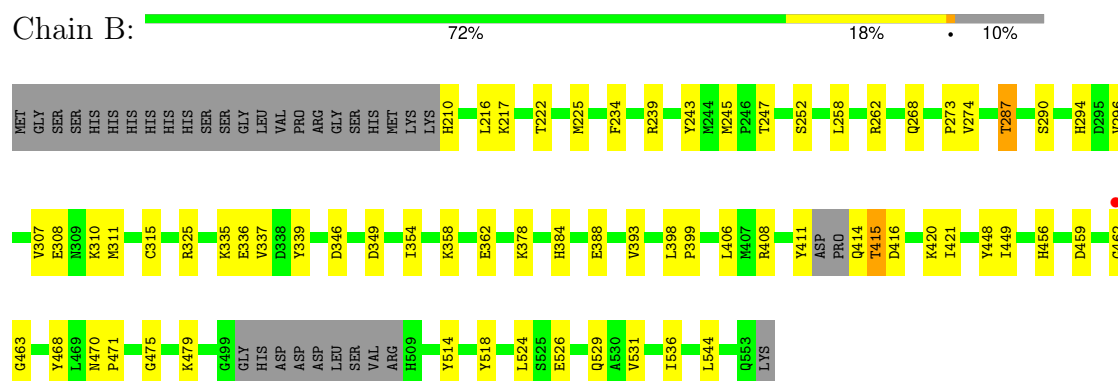
- Molecule 4 is water.

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

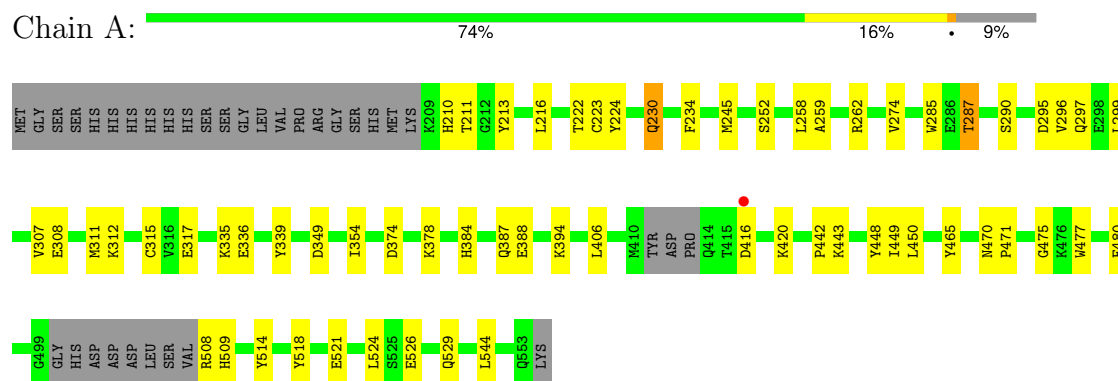
3 Residue-property plots

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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 2: Macrocycle peptide MC07



- Molecule 2: Macrocycle peptide MC07



ACE0
F1
F2
N3
F4
F5
N6
D187
K14

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.36Å 69.67Å 77.62Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	41.66 – 2.93 41.66 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.66-2.93) 97.0 (41.66-2.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.224 , 0.250 0.225 , 0.246	Depositor DCC
R_{free} test set	908 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5689	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4126e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EOH, DI8, ACE, MEA

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	0.27	0/2771	0.52	0/3734
1	B	0.27	0/2756	0.51	0/3719
2	C	0.30	0/96	0.59	0/120
2	D	0.31	0/87	0.57	0/109
All	All	0.27	0/5710	0.52	0/7682

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	6	ASN	Mainchain

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	2716	0	2659	40	1
1	B	2700	0	2620	40	1
2	C	135	0	130	6	0
2	D	126	0	117	5	0
3	A	3	0	6	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
All	All	5689	0	5532	83	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 (83) 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:354:ILE:HD11	1:A:406:LEU:HB3	1.56	0.84
1:B:287:THR:HG23	1:B:290:SER:HB3	1.63	0.80
1:B:354:ILE:HD11	1:B:406:LEU:HB3	1.64	0.79
1:A:335:LYS:HG3	1:A:336:GLU:HG3	1.70	0.74
1:A:296:VAL:HG13	2:C:2:MEA:HC1	1.73	0.71
1:B:415:THR:HG22	1:B:416:ASP:H	1.55	0.71
1:B:459:ASP:OD1	1:B:462:GLY:HA3	1.91	0.70
1:A:252:SER:HA	1:A:258:LEU:HD23	1.75	0.68
1:A:216:LEU:HD23	1:A:274:VAL:HB	1.76	0.68
1:B:262:ARG:HA	1:B:544:LEU:HD21	1.77	0.66
1:B:378:LYS:HD3	1:B:388:GLU:HG3	1.79	0.65
1:B:247:THR:HG22	1:B:310:LYS:HE2	1.81	0.62
1:A:287:THR:HG23	1:A:290:SER:HB3	1.80	0.62
1:B:296:VAL:HG13	2:D:2:MEA:HC1	1.83	0.60
1:B:216:LEU:HD23	1:B:274:VAL:HB	1.83	0.59
1:B:411:TYR:HA	1:B:414:GLN:NE2	2.16	0.59
1:A:378:LYS:HG2	1:A:388:GLU:HG3	1.83	0.59
1:B:234:PHE:CD1	1:B:471:PRO:HB3	2.39	0.58
1:B:335:LYS:HG3	1:B:336:GLU:HG3	1.86	0.58
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.85	0.57
1:B:449:ILE:HD12	1:B:524:LEU:HD22	1.87	0.57
1:A:234:PHE:CD1	1:A:471:PRO:HB3	2.39	0.57
1:B:217:LYS:HG3	1:B:273:PRO:HB2	1.87	0.56
1:B:217:LYS:HE3	1:B:273:PRO:HB2	1.88	0.56
1:A:296:VAL:HG11	1:A:514:TYR:HE2	1.71	0.56
1:B:290:SER:O	1:B:294:HIS:ND1	2.37	0.56
1:B:349:ASP:N	1:B:349:ASP:OD1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ILE:HD12	1:A:524:LEU:HD22	1.88	0.55
1:A:470:ASN:HD22	1:A:475:GLY:H	1.56	0.54
1:B:411:TYR:HD1	1:B:414:GLN:HE21	1.56	0.54
1:A:211:THR:HG23	1:A:213:TYR:H	1.73	0.54
1:A:349:ASP:N	1:A:349:ASP:OD1	2.41	0.54
1:B:526:GLU:O	1:B:529:GLN:HG3	2.08	0.53
1:B:415:THR:HG22	1:B:416:ASP:N	2.23	0.53
1:B:222:THR:HB	1:B:225:MET:HB3	1.91	0.52
1:A:335:LYS:HE2	1:A:388:GLU:HB3	1.91	0.51
1:A:295:ASP:HB3	1:A:297:GLN:OE1	2.10	0.51
1:A:384:HIS:O	1:A:387:GLN:NE2	2.35	0.50
1:A:508:ARG:HG3	1:A:509:HIS:ND1	2.27	0.50
1:A:312:LYS:HA	1:A:317:GLU:HG3	1.95	0.49
1:A:374:ASP:HA	1:A:388:GLU:HG2	1.93	0.48
2:D:10:ARG:HA	2:D:13:LYS:HD2	1.95	0.48
1:B:339:TYR:HB2	1:B:384:HIS:CE1	2.48	0.48
1:B:468:TYR:CZ	1:B:479:LYS:HD3	2.48	0.48
1:B:245:MET:SD	1:B:307:VAL:HG13	2.54	0.48
1:A:449:ILE:HD11	1:A:521:GLU:HG3	1.95	0.48
1:B:296:VAL:HG11	1:B:514:TYR:HE2	1.78	0.47
1:B:408:ARG:O	2:D:2:MEA:HE1	2.14	0.47
1:B:358:LYS:HG2	1:B:362:GLU:OE1	2.14	0.47
1:A:223:CYS:HA	1:A:465:TYR:CE1	2.50	0.46
1:A:262:ARG:HA	1:A:544:LEU:HD21	1.96	0.46
1:A:526:GLU:O	1:A:529:GLN:HG3	2.16	0.46
1:B:252:SER:HA	1:B:258:LEU:HD23	1.96	0.45
1:B:325:ARG:HD2	1:B:346:ASP:HB3	1.98	0.45
1:B:456:HIS:CE1	1:B:463:GLY:HA2	2.51	0.45
1:B:308:GLU:HA	1:B:311:MET:HE2	1.98	0.45
1:A:308:GLU:HA	1:A:311:MET:HE2	1.97	0.45
1:A:450:LEU:HG	1:A:477:TRP:HH2	1.81	0.45
1:B:243:TYR:CD2	1:B:536:ILE:HG12	2.52	0.45
1:A:307:VAL:O	1:A:311:MET:HG3	2.17	0.45
1:B:315:CYS:HB3	1:A:315:CYS:O	2.17	0.45
1:B:337:VAL:HG11	1:B:384:HIS:CG	2.51	0.45
1:B:420:LYS:HG3	2:D:4:MEA:HB2	1.98	0.45
2:C:1:PHE:HA	2:C:2:MEA:HA	1.62	0.44
1:A:295:ASP:HA	2:C:1:PHE:O	2.18	0.44
1:A:378:LYS:CG	1:A:388:GLU:HG3	2.47	0.44
1:A:224:TYR:HD2	2:C:3:ASN:HD21	1.63	0.44
1:A:308:GLU:O	1:A:312:LYS:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:HG2	2:C:2:MEA:HZ	1.99	0.44
1:B:408:ARG:NH1	1:B:421:ILE:O	2.50	0.43
2:D:1:PHE:HA	2:D:2:MEA:HA	1.63	0.43
1:A:339:TYR:HB2	1:A:384:HIS:CE1	2.54	0.42
1:A:245:MET:HG2	1:A:311:MET:HG2	2.01	0.42
1:B:239:ARG:NH1	1:B:268:GLN:OE1	2.52	0.42
1:B:398:LEU:HA	1:B:399:PRO:HD3	1.90	0.42
1:A:442:PRO:O	1:A:443:LYS:HG2	2.20	0.41
2:C:14:LYS:HD3	2:C:14:LYS:HA	1.76	0.41
1:A:259:ALA:HA	1:A:262:ARG:NH1	2.36	0.41
1:A:285:TRP:CZ3	1:A:299:LEU:HD13	2.55	0.41
1:B:470:ASN:HD22	1:B:475:GLY:H	1.69	0.40
1:A:245:MET:SD	1:A:307:VAL:HG13	2.61	0.40
1:A:230:GLN:HG2	1:A:480:PHE:CD2	2.56	0.40
1:A:448:TYR:HB3	1:A:518:TYR:HB3	2.03	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)
1:B:217:LYS:NZ	1:A:416:ASP:OD2[1_554]	2.17	0.03

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	328/368 (89%)	313 (95%)	15 (5%)	0	100	100
1	B	327/368 (89%)	311 (95%)	15 (5%)	1 (0%)	37	60
2	C	10/15 (67%)	8 (80%)	2 (20%)	0	100	100
2	D	9/15 (60%)	7 (78%)	2 (22%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	674/766 (88%)	639 (95%)	34 (5%)	1 (0%)	48 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	415	THR

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	302/332 (91%)	297 (98%)	5 (2%)	56 76
1	B	299/332 (90%)	295 (99%)	4 (1%)	65 80
2	C	10/10 (100%)	10 (100%)	0	100 100
2	D	9/10 (90%)	7 (78%)	2 (22%)	1 1
All	All	620/684 (91%)	609 (98%)	11 (2%)	54 75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	210	HIS
1	B	287	THR
1	B	393	VAL
1	B	531	VAL
1	A	210	HIS
1	A	222	THR
1	A	230	GLN
1	A	287	THR
1	A	394	LYS
2	D	9	ARG
2	D	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	414	GLN
1	A	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	DI8	C	7	2	11,13,14	2.25	4 (36%)	13,17,19	2.08	2 (15%)
2	MEA	C	4	2	11,12,13	0.33	0	13,14,16	1.00	1 (7%)
2	MEA	C	2	2	11,12,13	0.49	0	13,14,16	0.78	0
2	DI8	D	7	2	11,13,14	2.21	4 (36%)	13,17,19	2.03	1 (7%)
2	MEA	D	4	2	11,12,13	0.30	0	13,14,16	0.95	0
2	MEA	D	2	2	11,12,13	0.44	0	13,14,16	0.77	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
2	DI8	C	7	2	-	0/1/11/13	0/2/2/2
2	MEA	C	4	2	-	2/5/8/10	0/1/1/1
2	MEA	C	2	2	-	0/5/8/10	0/1/1/1
2	DI8	D	7	2	-	0/1/11/13	0/2/2/2
2	MEA	D	4	2	-	0/5/8/10	0/1/1/1
2	MEA	D	2	2	-	1/5/8/10	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	DI8	O-C	5.27	1.40	1.20
2	D	7	DI8	O-C	5.25	1.39	1.20
2	C	7	DI8	C6-C7	2.96	1.44	1.39
2	D	7	DI8	C6-C7	2.83	1.44	1.39
2	C	7	DI8	C7-C2	-2.76	1.35	1.40
2	C	7	DI8	C1-C2	2.74	1.56	1.51
2	D	7	DI8	C1-C2	2.71	1.56	1.51
2	D	7	DI8	C7-C2	-2.61	1.35	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	DI8	O-C-CA	-6.68	107.59	124.77
2	D	7	DI8	O-C-CA	-6.56	107.90	124.77
2	C	4	MEA	CG-CB-CA	-2.28	110.28	113.51
2	C	7	DI8	C7-C8-N	2.11	118.28	113.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	MEA	O-C-CA-CB
2	C	4	MEA	CA-CB-CG-CD2
2	C	4	MEA	CA-CB-CG-CD1

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	MEA	3	0
2	D	4	MEA	1	0
2	D	2	MEA	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
3	EOH	A	601	-	2,2,2	0.46	0	1,1,1	0.17	0

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	334/368 (90%)	-0.35	1 (0%) 90 90	54, 75, 107, 156	0
1	B	333/368 (90%)	-0.18	1 (0%) 90 90	66, 83, 121, 157	0
2	C	11/15 (73%)	-0.11	0 100 100	66, 80, 95, 102	0
2	D	10/15 (66%)	-0.12	0 100 100	73, 91, 99, 99	0
All	All	688/766 (89%)	-0.26	2 (0%) 90 90	54, 80, 115, 157	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	ASP	3.0
1	B	462	GLY	2.8

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	DI8	D	7	12/13	0.89	0.12	90,97,100,101	0
2	MEA	C	4	12/13	0.91	0.10	71,74,77,78	0
2	DI8	C	7	12/13	0.92	0.13	84,87,88,89	0
2	MEA	D	4	12/13	0.94	0.09	71,78,89,90	0
2	MEA	D	2	12/13	0.94	0.12	63,70,75,77	0
2	MEA	C	2	12/13	0.98	0.08	65,67,68,70	0

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
3	EOH	A	601	3/3	0.86	0.16	59,59,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.