



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:44 PM UTC

PDB ID : 9DEK / pdb_00009dek
Title : USP7 in complex with macrocycle inhibitor MC02
Authors : Rouge, L.; Ultsch, M.; Holden, J.K.; Dueber, E.C.; Harris, S.F.
Deposited on : 2024-08-29
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 : 4-5-2 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

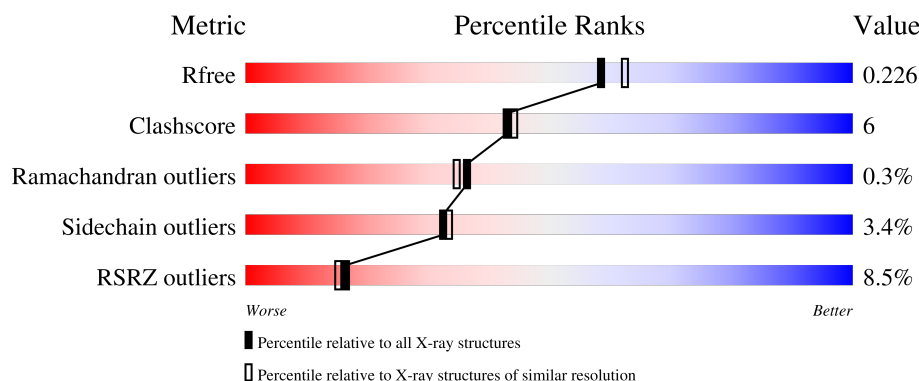
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	8% 79% 11% • 10%
1	B	368	8% 72% 16% • 11%
2	C	16	81% 19%
2	D	16	75% 19% 6%

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
2	KCJ	C	11	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6155 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	A	333	Total	C	N	O	S	0	3	0
			2723	1722	460	524	17			
1	B	329	Total	C	N	O	S	0	1	0
			2673	1693	449	514	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

Continued on next page...

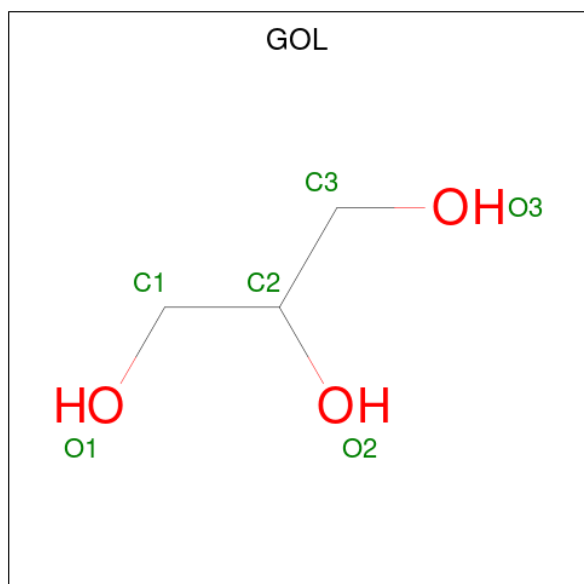
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Macrocycle peptide MC02.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total 130	C 85	N 23	O 19	S 3	0	0	0
2	D	16	Total 130	C 85	N 23	O 19	S 3	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

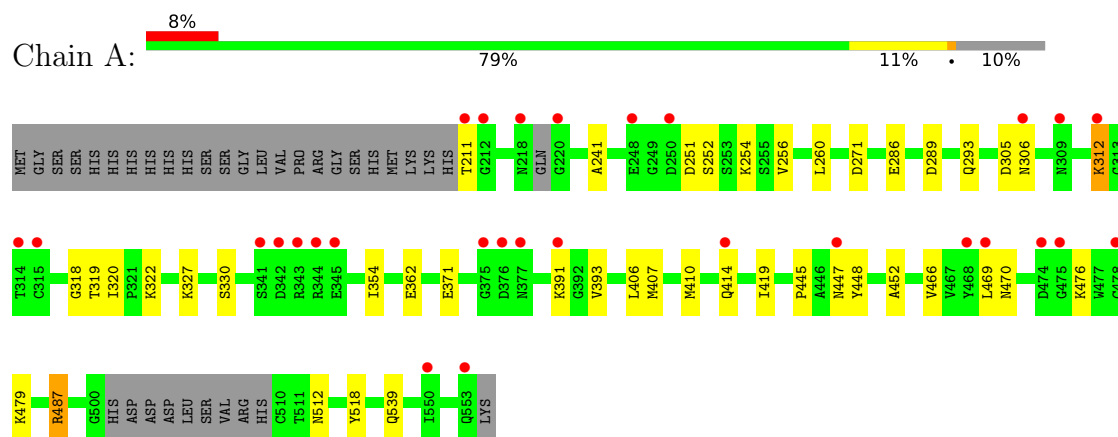
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	239	Total	O	0	0
			239	239		
4	B	213	Total	O	0	0
			213	213		
4	C	18	Total	O	0	0
			18	18		
4	D	17	Total	O	0	0
			17	17		

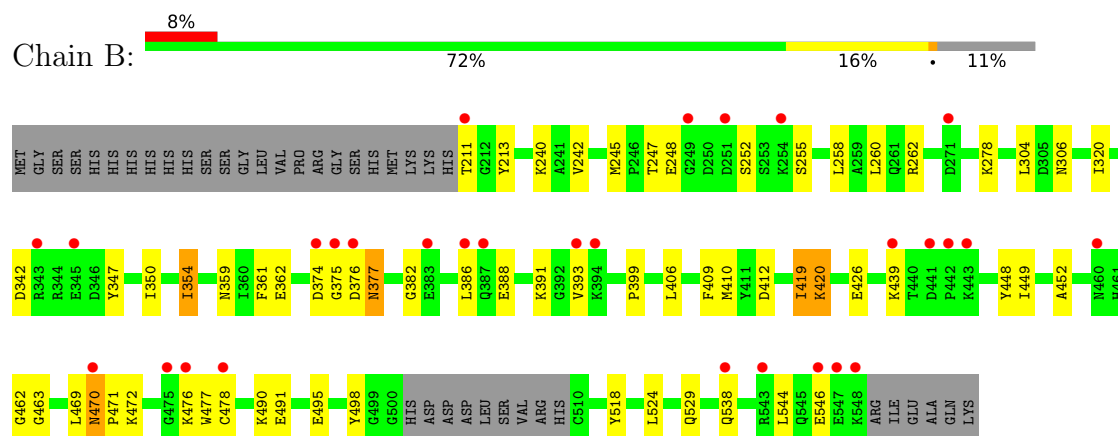
3 Residue-property plots [i](#)

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.

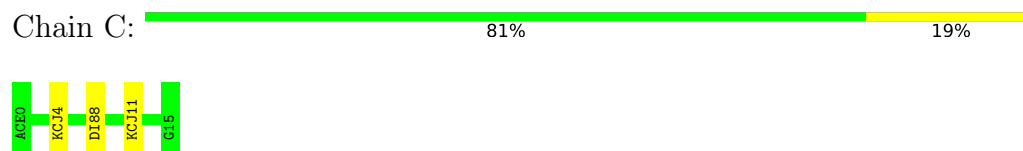
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 2: Macrocycle peptide MC02



- Molecule 2: Macrocycle peptide MC02

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.18Å 62.72Å 84.31Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	41.98 – 2.00 41.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.98-2.00) 99.7 (41.98-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.194 , 0.225 0.195 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.8	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	6155	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: ACE, DI8, SAR, GOL, KCJ

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	0.67	1/2778 (0.0%)	0.93	2/3746 (0.1%)
1	B	0.68	2/2729 (0.1%)	0.95	4/3682 (0.1%)
2	C	0.53	0/89	0.78	0/114
2	D	0.38	0/89	0.80	0/114
All	All	0.67	3/5685 (0.1%)	0.94	6/7656 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	VAL	CA-CB	7.29	1.58	1.54
1	B	342	ASP	C-O	-6.43	1.16	1.23
1	B	399	PRO	CA-C	-6.03	1.46	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASN	CB-CA-C	8.27	119.25	110.65
1	B	362	GLU	CA-CB-CG	-5.64	102.82	114.10
1	A	271	ASP	N-CA-C	-5.37	106.40	113.17
1	B	391	LYS	CB-CG-CD	-5.25	99.23	111.30
1	B	470	ASN	CB-CA-C	5.17	120.35	110.17
1	B	376	ASP	N-CA-C	-5.06	106.53	113.56

There are no chirality outliers.

There are no planarity outliers.

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	2723	0	2654	27	1
1	B	2673	0	2608	41	0
2	C	130	0	109	0	0
2	D	130	0	109	1	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
4	A	239	0	0	2	0
4	B	213	0	0	4	0
4	C	18	0	0	0	0
4	D	17	0	0	0	0
All	All	6155	0	5496	69	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 6.

All (69) 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:539:GLN:HG2	4:A:880:HOH:O	1.43	1.16
1:B:452:ALA:HB2	1:B:469:LEU:CD2	2.15	0.76
1:A:466:VAL:HG21	1:A:479:LYS:HE3	1.68	0.74
1:B:491:GLU:HA	1:B:495:GLU:OE1	1.88	0.73
1:B:382:GLY:O	4:B:701:HOH:O	2.07	0.71
1:A:445:PRO:HB2	1:A:447[A]:ASN:OD1	1.92	0.70
1:A:452:ALA:CB	1:A:469:LEU:CD2	2.70	0.70
1:B:452:ALA:CB	1:B:469:LEU:CD2	2.69	0.69
1:B:247:THR:HB	1:B:258:LEU:HD23	1.76	0.67
1:B:211:THR:CG2	1:B:213:TYR:H	2.09	0.66
1:A:452:ALA:HB2	1:A:469:LEU:CD2	2.27	0.65
1:B:452:ALA:CB	1:B:469:LEU:HD23	2.29	0.63
1:A:406:LEU:O	3:A:601:GOL:H12	1.98	0.63
1:A:286:GLU:HA	4:A:734:HOH:O	2.01	0.60
1:A:211:THR:HG22	1:A:487:ARG:HG2	1.82	0.60
1:B:470:ASN:OD1	1:B:470:ASN:O	2.21	0.58
1:B:242:VAL:HG13	1:B:245:MET:HE2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:HE3	1:B:529:GLN:HE21	1.69	0.57
1:A:251:ASP:HB3	1:A:254:LYS:HG3	1.87	0.57
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.87	0.55
1:A:476:LYS:C	1:A:487:ARG:NH1	2.64	0.55
1:A:318:GLY:O	1:A:322:LYS:HG3	2.06	0.55
1:B:211:THR:HG23	1:B:213:TYR:H	1.72	0.54
1:A:452:ALA:CB	1:A:469:LEU:HD23	2.38	0.52
1:A:476:LYS:C	1:A:487:ARG:HH12	2.17	0.52
1:B:452:ALA:HA	1:B:469:LEU:HD23	1.92	0.51
1:A:407:MET:HA	3:A:601:GOL:H11	1.92	0.51
1:B:347:TYR:CE2	1:B:350:ILE:HD11	2.45	0.51
1:B:211:THR:HG22	1:B:213:TYR:H	1.76	0.50
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.95	0.49
1:A:452:ALA:HB1	1:A:469:LEU:CD2	2.42	0.48
1:B:426:GLU:HG2	1:B:498:TYR:CD2	2.50	0.47
1:A:330:SER:HB3	1:A:393:VAL:HG12	1.97	0.47
1:B:469:LEU:O	1:B:471:PRO:HD3	2.14	0.47
1:B:412:ASP:HB2	1:B:419:ILE:HG12	1.98	0.46
1:B:449:ILE:HG13	1:B:524:LEU:HD11	1.98	0.46
1:B:374:ASP:CG	1:B:388:GLU:OE2	2.59	0.46
1:B:240:LYS:HE3	1:B:529:GLN:NE2	2.31	0.46
1:A:289:ASP:O	1:A:293:GLN:HG3	2.15	0.46
1:A:312:LYS:HA	1:A:312:LYS:HD3	1.64	0.46
1:B:247:THR:HB	1:B:258:LEU:CD2	2.45	0.45
1:A:327:LYS:HB2	1:A:327:LYS:HE2	1.82	0.45
1:B:410:MET:HE2	1:B:410:MET:HB3	1.84	0.44
1:B:359:ASN:OD1	1:B:361:PHE:HB2	2.16	0.44
1:B:252:SER:HB2	1:B:278:LYS:HD3	1.98	0.44
1:A:452:ALA:HB1	1:A:469:LEU:HD21	1.99	0.43
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.92	0.43
1:B:452:ALA:CA	1:B:469:LEU:HD23	2.48	0.43
1:B:240:LYS:CE	1:B:529:GLN:NE2	2.82	0.43
1:A:452:ALA:HA	1:A:469:LEU:HD23	2.00	0.42
1:B:262:ARG:HG3	1:B:544:LEU:HD22	2.01	0.42
1:B:452:ALA:CB	1:B:469:LEU:HD21	2.48	0.42
1:B:255:SER:OG	1:B:258:LEU:HG	2.19	0.42
1:A:241:ALA:CB	1:A:319:THR:HG21	2.50	0.42
1:B:320:ILE:HD13	1:B:320:ILE:HA	1.74	0.41
1:B:470:ASN:ND2	4:B:704:HOH:O	2.38	0.41
1:B:462:GLY:HA3	4:B:711:HOH:O	2.20	0.41
1:B:477:TRP:CD1	1:B:490:LYS:HG2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LYS:HA	1:B:476:LYS:HD3	1.72	0.41
2:D:7:LEU:HA	2:D:8:DI8:H8	1.88	0.41
1:B:469:LEU:C	1:B:471:PRO:HD3	2.46	0.41
1:B:354:ILE:HD11	1:B:406:LEU:HD22	2.03	0.40
1:B:260:LEU:HA	1:B:260:LEU:HD23	1.77	0.40
1:B:463:GLY:N	4:B:703:HOH:O	2.35	0.40
1:A:251:ASP:OD1	1:A:252:SER:N	2.54	0.40
1:A:320:ILE:HD13	1:A:320:ILE:HA	1.86	0.40
1:A:371:GLU:HB3	1:A:391:LYS:HB3	2.03	0.40
1:B:409:PHE:CZ	1:B:420:LYS:HE3	2.57	0.40
1:B:304:LEU:HD23	1:B:304:LEU:HA	1.76	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:A:305:ASP:OD2	1:A:362:GLU:OE2[2_655]	2.07	0.13

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	330/368 (90%)	319 (97%)	11 (3%)	0	100	100
1	B	326/368 (89%)	312 (96%)	12 (4%)	2 (1%)	21	17
2	C	10/16 (62%)	10 (100%)	0	0	100	100
2	D	10/16 (62%)	10 (100%)	0	0	100	100
All	All	676/768 (88%)	651 (96%)	23 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	GLY
1	B	377	ASN

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	303/332 (91%)	295 (97%)	8 (3%)	40	44
1	B	298/332 (90%)	285 (96%)	13 (4%)	25	24
2	C	10/10 (100%)	10 (100%)	0	100	100
2	D	10/10 (100%)	10 (100%)	0	100	100
All	All	621/684 (91%)	600 (97%)	21 (3%)	32	33

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	312	LYS
1	A	354	ILE
1	A	410	MET
1	A	414	GLN
1	A	419	ILE
1	A	487	ARG
1	A	512	ASN
1	B	248	GLU
1	B	306	ASN
1	B	354	ILE
1	B	377	ASN
1	B	386	LEU
1	B	393	VAL
1	B	419	ILE
1	B	420	LYS
1	B	439	LYS
1	B	472	LYS
1	B	478	CYS
1	B	538	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	546	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	351	GLN
1	A	438	GLN
1	A	496	HIS
1	B	372	GLN
1	B	430	GLN
1	B	447	ASN
1	B	470	ASN
1	B	529	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	KCJ	C	11	2	9,10,11	2.47	5 (55%)	7,12,14	3.67	4 (57%)
2	KCJ	D	4	2	9,10,11	2.42	5 (55%)	7,12,14	3.81	3 (42%)
2	SAR	C	5	2	3,4,5	0.61	0	1,3,5	1.50	0
2	DI8	C	8	2	11,13,14	1.17	1 (9%)	13,17,19	1.48	3 (23%)
2	SAR	D	5	2	3,4,5	0.91	0	1,3,5	1.77	0
2	KCJ	D	11	2	9,10,11	2.50	5 (55%)	7,12,14	3.55	3 (42%)
2	KCJ	C	4	2	9,10,11	2.47	5 (55%)	7,12,14	3.53	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DI8	D	8	2	11,13,14	1.23	1 (9%)	13,17,19	1.42	3 (23%)

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	KCJ	C	11	2	-	4/5/6/8	0/1/1/1
2	KCJ	D	4	2	-	0/5/6/8	0/1/1/1
2	SAR	C	5	2	-	1/1/2/3	-
2	DI8	C	8	2	-	1/1/11/13	0/2/2/2
2	SAR	D	5	2	-	1/1/2/3	-
2	KCJ	D	11	2	-	2/5/6/8	0/1/1/1
2	KCJ	C	4	2	-	0/5/6/8	0/1/1/1
2	DI8	D	8	2	-	1/1/11/13	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	KCJ	C15-N16	3.52	1.39	1.30
2	C	11	KCJ	C13-C12	3.51	1.42	1.35
2	D	11	KCJ	C13-C12	3.49	1.42	1.35
2	D	11	KCJ	C15-N16	3.42	1.39	1.30
2	D	4	KCJ	C13-C12	3.39	1.42	1.35
2	D	4	KCJ	C13-S14	-3.33	1.60	1.70
2	D	11	KCJ	C13-S14	-3.33	1.60	1.70
2	C	4	KCJ	C13-S14	-3.30	1.60	1.70
2	D	4	KCJ	C15-N16	3.28	1.38	1.30
2	C	4	KCJ	C13-C12	3.26	1.42	1.35
2	D	11	KCJ	C12-N16	3.21	1.46	1.38
2	C	11	KCJ	C15-N16	3.18	1.38	1.30
2	C	11	KCJ	C13-S14	-3.17	1.60	1.70
2	C	4	KCJ	C12-N16	3.12	1.46	1.38
2	C	4	KCJ	C15-S14	-3.09	1.62	1.70
2	C	11	KCJ	C15-S14	-3.07	1.62	1.70
2	D	4	KCJ	C12-N16	3.05	1.46	1.38
2	D	4	KCJ	C15-S14	-3.01	1.62	1.70
2	D	11	KCJ	C15-S14	-2.93	1.63	1.70
2	C	11	KCJ	C12-N16	2.87	1.46	1.38
2	D	8	DI8	C8-N	2.10	1.49	1.46
2	C	8	DI8	C8-N	2.08	1.49	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	KCJ	C13-S14-C15	8.70	100.21	89.47
2	C	11	KCJ	C13-S14-C15	8.37	99.81	89.47
2	D	11	KCJ	C13-S14-C15	8.13	99.52	89.47
2	C	4	KCJ	C13-S14-C15	8.12	99.50	89.47
2	D	4	KCJ	S14-C15-N16	-3.98	109.35	115.58
2	D	11	KCJ	S14-C15-N16	-3.58	109.97	115.58
2	C	11	KCJ	S14-C15-N16	-3.56	110.01	115.58
2	C	4	KCJ	S14-C15-N16	-3.53	110.05	115.58
2	D	11	KCJ	C13-C12-N16	-2.76	110.98	115.13
2	C	4	KCJ	C13-C12-N16	-2.59	111.23	115.13
2	D	4	KCJ	C13-C12-N16	-2.46	111.43	115.13
2	C	8	DI8	O-C-CA	-2.42	118.55	124.77
2	C	8	DI8	C2-C1-CA	2.41	114.20	111.17
2	D	8	DI8	C2-C1-CA	2.36	114.13	111.17
2	D	8	DI8	O-C-CA	-2.22	119.07	124.77
2	C	11	KCJ	C13-C12-N16	-2.18	111.85	115.13
2	D	8	DI8	C1-C2-C7	-2.11	115.83	120.33
2	C	11	KCJ	C12-C13-S14	-2.09	107.86	110.56
2	C	8	DI8	C1-C2-C7	-2.03	116.01	120.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	SAR	C-CA-N-CN
2	D	5	SAR	C-CA-N-CN
2	D	8	DI8	O-C-CA-C1
2	C	11	KCJ	C12-C11-CA-C
2	C	11	KCJ	CA-C11-C12-C13
2	C	11	KCJ	CA-C11-C12-N16
2	D	11	KCJ	CA-C11-C12-C13
2	D	11	KCJ	CA-C11-C12-N16
2	C	11	KCJ	C12-C11-CA-N
2	C	8	DI8	O-C-CA-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	8	DI8	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands 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	$\# Z > 2$
3	GOL	B	601	-	5,5,5	0.40	0	5,5,5	0.50	0
3	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.54	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
3	GOL	B	601	-	-	0/4/4/4	-
3	GOL	A	601	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	333/368 (90%)	0.17	29 (8%) 16 15	12, 25, 45, 62	3 (0%)
1	B	329/368 (89%)	0.28	29 (8%) 15 14	13, 27, 52, 69	1 (0%)
2	C	11/16 (68%)	-0.15	0 100 100	16, 23, 30, 40	0
2	D	11/16 (68%)	0.10	0 100 100	20, 25, 34, 37	0
All	All	684/768 (89%)	0.22	58 (8%) 16 15	12, 26, 48, 69	4 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	4.5
1	B	546	GLU	4.3
1	A	478	CYS	4.2
1	B	387	GLN	4.1
1	A	342	ASP	3.9
1	A	312	LYS	3.7
1	B	547	GLU	3.7
1	B	538	GLN	3.6
1	A	377	ASN	3.5
1	A	341	SER	3.4
1	B	393	VAL	3.2
1	B	442	PRO	3.2
1	A	218	ASN	3.2
1	B	394	LYS	3.1
1	B	343	ARG	3.1
1	B	345	GLU	3.1
1	A	211	THR	3.1
1	B	271	ASP	3.0
1	B	376	ASP	3.0
1	B	478	CYS	3.0
1	B	548	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	376	ASP	2.9
1	A	345	GLU	2.9
1	A	309	ASN	2.8
1	B	441	ASP	2.8
1	B	374	ASP	2.8
1	B	386	LEU	2.8
1	A	447[A]	ASN	2.7
1	A	250	ASP	2.7
1	B	375	GLY	2.7
1	A	343	ARG	2.7
1	A	306	ASN	2.6
1	B	251	ASP	2.6
1	A	220	GLY	2.6
1	A	344	ARG	2.6
1	B	443	LYS	2.5
1	A	248	GLU	2.5
1	B	476	LYS	2.4
1	A	414	GLN	2.3
1	B	439	LYS	2.3
1	A	550	ILE	2.2
1	A	391	LYS	2.2
1	A	475	GLY	2.2
1	B	211	THR	2.2
1	A	212	GLY	2.2
1	A	474	ASP	2.2
1	B	543	ARG	2.2
1	A	314	THR	2.2
1	B	383	GLU	2.1
1	B	249	GLY	2.1
1	B	475	GLY	2.1
1	B	254	LYS	2.1
1	A	315	CYS	2.1
1	A	468	TYR	2.1
1	A	553	GLN	2.1
1	B	460	ASN	2.1
1	A	375	GLY	2.1
1	B	470	ASN	2.0

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

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	SAR	D	5	5/6	0.91	0.10	30,32,34,36	0
2	DI8	D	8	12/13	0.94	0.07	16,19,21,21	0
2	KCJ	C	4	10/11	0.95	0.07	23,24,28,31	0
2	KCJ	D	4	10/11	0.95	0.07	22,27,31,37	0
2	DI8	C	8	12/13	0.97	0.05	13,16,17,19	0
2	SAR	C	5	5/6	0.97	0.06	21,22,23,26	0
2	KCJ	C	11	10/11	0.98	0.05	19,21,24,25	0
2	KCJ	D	11	10/11	0.98	0.05	17,19,22,23	0

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(Å ²)	Q<0.9
3	GOL	A	601	6/6	0.88	0.11	19,19,21,24	0
3	GOL	B	601	6/6	0.96	0.07	16,20,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.