



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:56 AM UTC

PDB ID : 8OYP / pdb_00008oyp
Title : Crystal structure of Ubiquitin specific protease 11 (USP11) in complex with a substrate mimetic
Authors : Maurer, S.K.; Caulton, S.G.; Ward, S.J.; Emsley, J.; Dreveny, I.
Deposited on : 2023-05-05
Resolution : 2.44 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

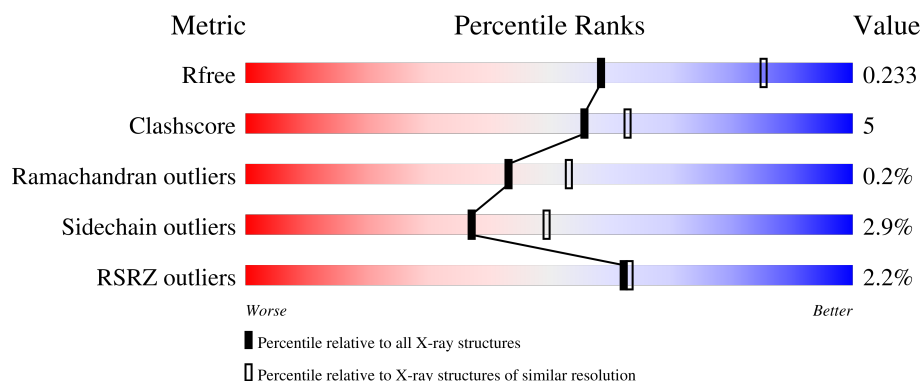
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

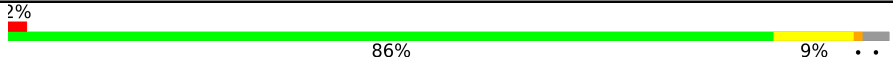
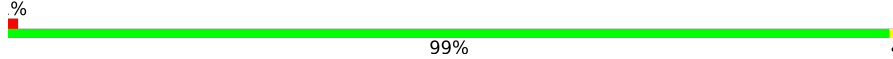
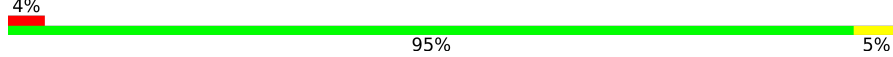
The reported resolution of this entry is 2.44 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	485	
1	B	485	
2	C	79	
2	D	79	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9397 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 11, Response regulator FrzS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	7	0
			3805	2404	662	722	17			
1	B	474	Total	C	N	O	S	0	5	0
			3810	2408	659	726	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	SER	CYS	engineered mutation	UNP P51784
A	490	GLY	-	linker	UNP P51784
A	491	ALA	-	linker	UNP P51784
A	583	ALA	LYS	conflict	UNP Q1D4U9
A	585	SER	LYS	conflict	UNP Q1D4U9
A	607	ALA	-	linker	UNP Q1D4U9
A	608	LEU	-	linker	UNP Q1D4U9
A	609	ILE	-	linker	UNP Q1D4U9
A	610	GLY	-	linker	UNP Q1D4U9
A	611	PHE	-	linker	UNP Q1D4U9
A	612	PRO	-	linker	UNP Q1D4U9
A	938	GLU	-	expression tag	UNP P51784
A	939	HIS	-	expression tag	UNP P51784
A	940	HIS	-	expression tag	UNP P51784
A	941	HIS	-	expression tag	UNP P51784
A	942	HIS	-	expression tag	UNP P51784
A	943	HIS	-	expression tag	UNP P51784
A	944	HIS	-	expression tag	UNP P51784
B	318	SER	CYS	engineered mutation	UNP P51784
B	490	GLY	-	linker	UNP P51784
B	491	ALA	-	linker	UNP P51784
B	583	ALA	LYS	conflict	UNP Q1D4U9
B	585	SER	LYS	conflict	UNP Q1D4U9
B	607	ALA	-	linker	UNP Q1D4U9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	608	LEU	-	linker	UNP Q1D4U9
B	609	ILE	-	linker	UNP Q1D4U9
B	610	GLY	-	linker	UNP Q1D4U9
B	611	PHE	-	linker	UNP Q1D4U9
B	612	PRO	-	linker	UNP Q1D4U9
B	938	GLU	-	expression tag	UNP P51784
B	939	HIS	-	expression tag	UNP P51784
B	940	HIS	-	expression tag	UNP P51784
B	941	HIS	-	expression tag	UNP P51784
B	942	HIS	-	expression tag	UNP P51784
B	943	HIS	-	expression tag	UNP P51784
B	944	HIS	-	expression tag	UNP P51784

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	79	Total	C	N	O	S	0	1	0
			622	389	109	123	1			
2	D	79	Total	C	N	O	S	0	0	0
			613	384	108	120	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	77	GLY	-	expression tag	UNP P0CG47
C	78	GLY	-	expression tag	UNP P0CG47
C	79	GLY	-	expression tag	UNP P0CG47
D	77	GLY	-	expression tag	UNP P0CG47
D	78	GLY	-	expression tag	UNP P0CG47
D	79	GLY	-	expression tag	UNP P0CG47

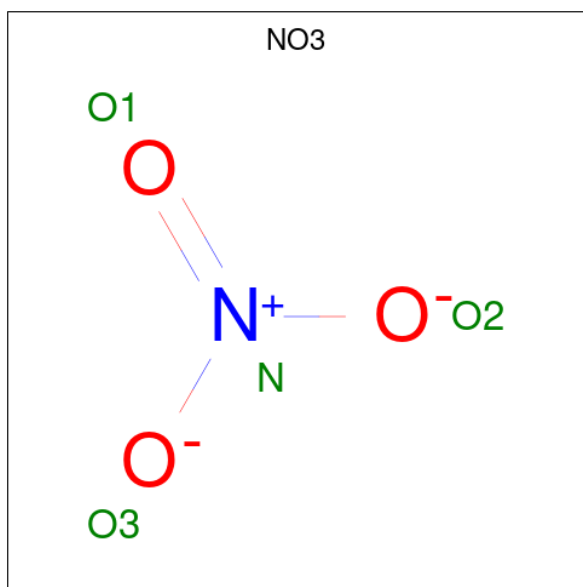
- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cd	0	0
			1	1		
3	B	1	Total	Cd	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

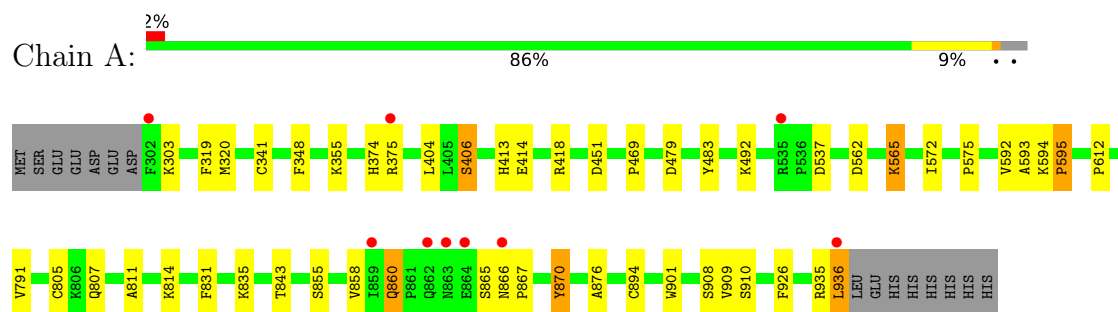
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	232	Total 232	O 232	0	0
8	B	193	Total 193	O 193	0	0
8	C	42	Total 42	O 42	0	0
8	D	38	Total 38	O 38	0	0

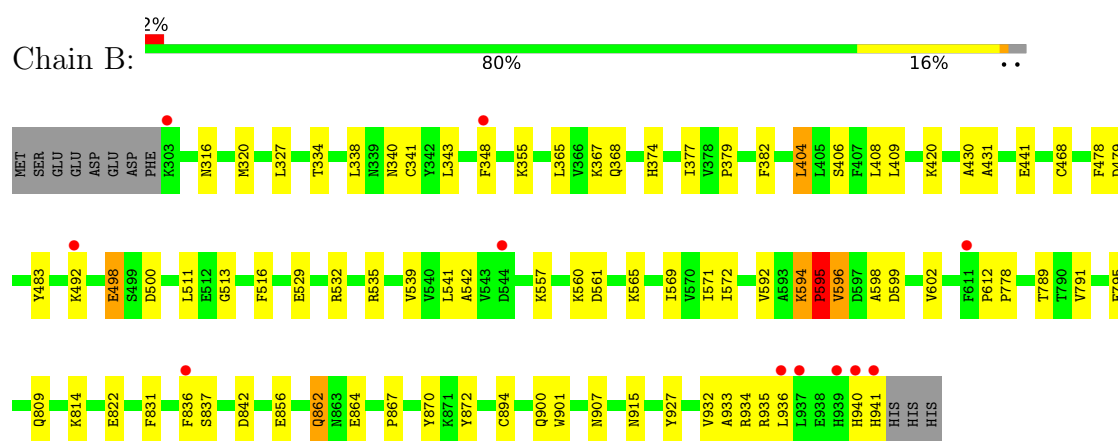
3 Residue-property plots

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.

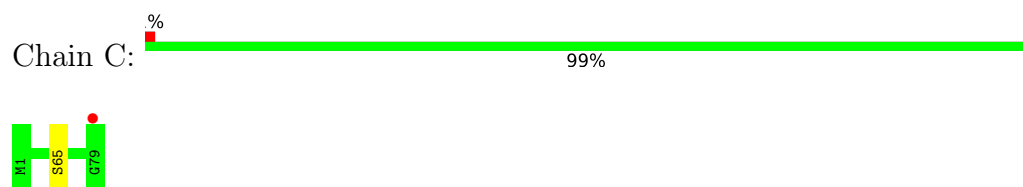
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 11, Response regulator FrzS



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 11, Response regulator FrzS

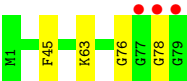


- Molecule 2: Polyubiquitin-B



- Molecule 2: Polyubiquitin-B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.32Å 186.10Å 75.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.44 48.00 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.00-2.44) 99.9 (48.00-2.44)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.170 , 0.235 0.175 , 0.233	Depositor DCC
R_{free} test set	2520 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	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	9397	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: CD, CL, GOL, PO4, NO3, CSU

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	0.71	7/3880 (0.2%)	0.72	2/5258 (0.0%)
1	B	0.58	1/3886 (0.0%)	0.78	5/5269 (0.1%)
2	C	0.58	0/628	0.65	0/843
2	D	0.61	0/619	0.66	0/831
All	All	0.64	8/9013 (0.1%)	0.74	7/12201 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	595	PRO	N-CA	12.34	1.68	1.47
1	B	867	PRO	C-O	-6.82	1.15	1.24
1	A	413	HIS	CE1-NE2	-6.15	1.26	1.32
1	A	612	PRO	C-O	-5.55	1.18	1.24
1	A	413	HIS	C-O	-5.43	1.17	1.24
1	A	594	LYS	C-N	5.27	1.44	1.34
1	A	909	VAL	C-O	-5.25	1.18	1.24
1	A	908	SER	C-O	-5.17	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	595	PRO	CB-CA-C	13.72	134.20	111.56
1	B	595	PRO	CA-N-CD	-9.64	98.50	112.00
1	A	595	PRO	CA-N-CD	-7.41	101.12	111.50
1	B	595	PRO	N-CA-C	-7.12	97.80	112.47
1	B	594	LYS	CB-CA-C	6.26	123.21	110.31
1	B	599	ASP	CB-CA-C	5.52	119.55	110.88
1	A	595	PRO	N-CA-C	-5.34	98.22	112.10

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	3805	0	3695	35	0
1	B	3810	0	3683	45	0
2	C	622	0	643	1	0
2	D	613	0	638	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	B	6	0	8	3	0
7	C	6	0	8	2	0
8	A	232	0	0	2	0
8	B	193	0	0	3	0
8	C	42	0	0	0	0
8	D	38	0	0	1	0
All	All	9397	0	8675	83	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 (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:595:PRO:N	1:A:595:PRO:CA	1.68	1.42
1:A:320:MET:HA	1:A:404:LEU:CD2	1.87	1.05
1:B:479:ASP:OD1	7:B:1005:GOL:O1	1.83	0.97
1:A:320:MET:HA	1:A:404:LEU:HD22	1.44	0.97
1:A:479:ASP:OD1	7:C:101:GOL:O1	1.99	0.79
1:A:595:PRO:N	1:A:595:PRO:C	2.42	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PHE:HE2	1:A:404:LEU:HD13	1.55	0.72
1:A:562[A]:ASP:HA	1:A:565:LYS:HE3	1.72	0.70
1:B:340:ASN:HB3	1:B:343:LEU:HD12	1.74	0.70
2:C:65:SER:OG	7:C:101:GOL:O1	2.08	0.69
1:B:498:GLU:HG2	1:B:542:ALA:HB2	1.74	0.69
1:B:862:GLN:HG3	1:B:870:TYR:CZ	2.28	0.68
1:B:320:MET:HA	1:B:404:LEU:HD22	1.77	0.66
1:A:936:LEU:O	1:A:936:LEU:HD23	1.97	0.65
1:A:867:PRO:HA	1:A:870:TYR:CE1	2.33	0.64
1:B:933:ALA:HA	1:B:936:LEU:HD12	1.80	0.64
1:A:320:MET:CA	1:A:404:LEU:HD22	2.25	0.63
1:B:529:GLU:OE2	1:B:532:ARG:NH2	2.32	0.61
1:B:594:LYS:HB3	1:B:595:PRO:HD2	1.83	0.60
1:A:855:SER:HB3	1:A:870:TYR:CD1	2.37	0.59
1:A:858:VAL:O	1:A:860:GLN:HG3	2.03	0.58
1:B:316:ASN:HA	2:D:76:GLY:O	2.04	0.58
1:B:492:LYS:HB3	1:B:516:PHE:HA	1.85	0.58
1:A:320:MET:HG3	1:A:404:LEU:HD21	1.86	0.58
1:A:562[B]:ASP:HA	1:A:565:LYS:HE3	1.86	0.58
1:B:872:TYR:HB3	1:B:927:TYR:HB3	1.87	0.57
1:B:511:LEU:HD23	1:B:602:VAL:HG13	1.86	0.56
1:A:492:LYS:N	1:A:537:ASP:OD2	2.37	0.56
1:A:414:GLU:HA	1:A:414:GLU:OE1	2.06	0.55
1:B:406:SER:HA	1:B:483:TYR:OH	2.07	0.55
2:D:63:LYS:NZ	8:D:302:HOH:O	2.41	0.54
1:A:575:PRO:HG3	1:A:593:ALA:HB1	1.89	0.54
1:B:348:PHE:O	1:B:355:LYS:HD3	2.08	0.53
1:A:320:MET:HA	1:A:404:LEU:HD21	1.85	0.53
1:B:557:LYS:HA	1:B:560:LYS:HE3	1.92	0.51
1:B:561:ASP:O	1:B:565:LYS:HB3	2.11	0.50
1:A:936:LEU:CD2	1:A:936:LEU:N	2.74	0.50
1:A:936:LEU:HD23	1:A:936:LEU:H	1.77	0.50
1:A:319:PHE:CE2	1:A:404:LEU:HD13	2.40	0.50
1:B:374:HIS:CG	1:B:377:ILE:HD11	2.48	0.49
1:A:791:VAL:HG22	1:A:814:LYS:HD2	1.94	0.49
1:A:406:SER:HA	1:A:483:TYR:OH	2.13	0.49
1:A:348:PHE:O	1:A:355:LYS:HD3	2.14	0.48
1:B:940:HIS:CG	1:B:941:HIS:H	2.32	0.48
1:A:374:HIS:HE1	8:A:1291:HOH:O	1.97	0.47
1:B:498:GLU:OE1	1:B:500:ASP:HB3	2.15	0.47
1:A:894:CYS:HB2	1:A:901:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:VAL:HG22	1:B:596:VAL:O	2.14	0.47
7:B:1005:GOL:H2	2:D:45:PHE:HZ	1.80	0.46
1:B:478:PHE:O	7:B:1005:GOL:H12	2.15	0.46
1:B:836:PHE:CD2	1:B:837:SER:HB3	2.50	0.45
1:A:936:LEU:CD2	1:A:936:LEU:H	2.28	0.45
1:B:789:THR:O	1:B:814:LYS:NZ	2.45	0.44
1:B:822:GLU:HB3	1:B:932:VAL:HG21	2.00	0.43
1:B:468:CYS:SG	1:B:809:GLN:HG3	2.58	0.43
1:A:805:CYS:SG	1:A:807:GLN:HG2	2.59	0.43
1:B:441:GLU:HB2	8:B:1105:HOH:O	2.19	0.43
1:B:795:GLU:OE1	8:B:1101:HOH:O	2.21	0.43
1:B:365:LEU:HD21	1:B:379:PRO:HB3	2.01	0.43
1:B:541:LEU:O	1:B:571:ILE:HA	2.17	0.43
1:A:572:ILE:HA	1:A:592:VAL:O	2.19	0.42
1:B:327:LEU:HD12	1:B:408:LEU:HD23	2.01	0.42
1:B:368:GLN:NE2	8:B:1118:HOH:O	2.53	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.91	0.42
1:B:612:PRO:HA	1:B:778:PRO:HD3	1.87	0.42
1:A:876:ALA:HB3	1:A:926:PHE:HB2	2.02	0.42
1:B:338:LEU:CD2	1:B:367:LYS:HA	2.50	0.41
1:B:791:VAL:HG22	1:B:814:LYS:HD2	2.02	0.41
1:A:375[A]:ARG:N	8:A:1116:HOH:O	2.48	0.41
1:B:894:CYS:HB2	1:B:901:TRP:CE2	2.56	0.41
1:B:382:PHE:HZ	1:B:408:LEU:HD13	1.86	0.41
1:B:430:ALA:O	1:B:431:ALA:C	2.64	0.41
1:B:539:VAL:HB	1:B:569:ILE:HD13	2.03	0.41
1:A:418:ARG:HG3	1:A:451:ASP:O	2.21	0.41
1:B:511:LEU:C	1:B:513:GLY:H	2.28	0.41
1:B:572:ILE:HA	1:B:592:VAL:O	2.20	0.41
1:B:598:ALA:O	1:B:602:VAL:HG23	2.21	0.41
1:A:575:PRO:HG3	1:A:593:ALA:CB	2.52	0.40
1:B:862:GLN:CG	1:B:870:TYR:CZ	3.01	0.40
1:A:303:LYS:HD3	1:A:303:LYS:HA	1.87	0.40
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.92	0.40
1:A:469:PRO:HD3	1:A:811:ALA:HA	2.03	0.40
1:B:377:ILE:HA	1:B:377:ILE:HD13	1.81	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	474/485 (98%)	468 (99%)	6 (1%)	0	100	100
1	B	476/485 (98%)	469 (98%)	6 (1%)	1 (0%)	43	53
2	C	78/79 (99%)	75 (96%)	3 (4%)	0	100	100
2	D	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	9	9
All	All	1105/1128 (98%)	1085 (98%)	18 (2%)	2 (0%)	43	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	595	PRO
2	D	78	GLY

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	415/425 (98%)	403 (97%)	12 (3%)	37	49
1	B	415/425 (98%)	398 (96%)	17 (4%)	27	38
2	C	69/68 (102%)	69 (100%)	0	100	100
2	D	68/68 (100%)	68 (100%)	0	100	100
All	All	967/986 (98%)	938 (97%)	29 (3%)	37	48

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

Mol	Chain	Res	Type
1	A	406	SER
1	A	565	LYS
1	A	831	PHE
1	A	835	LYS
1	A	843	THR
1	A	860	GLN
1	A	865	SER
1	A	866	ASN
1	A	870	TYR
1	A	910	SER
1	A	935	ARG
1	A	936	LEU
1	B	334	THR
1	B	404	LEU
1	B	420	LYS
1	B	498	GLU
1	B	535	ARG
1	B	596	VAL
1	B	831	PHE
1	B	842	ASP
1	B	856[A]	GLU
1	B	856[B]	GLU
1	B	862	GLN
1	B	864	GLU
1	B	900	GLN
1	B	907	ASN
1	B	915	ASN
1	B	934	ARG
1	B	935	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	HIS
1	A	388	HIS
1	A	440	GLN
1	A	444	GLN
1	A	900	GLN
1	B	392	GLN
2	D	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
1	CSU	B	341	1	7,9,10	1.50	1 (14%)	4,12,14	1.42	1 (25%)
1	CSU	A	341	1	7,9,10	1.50	1 (14%)	4,12,14	1.50	1 (25%)

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
1	CSU	B	341	1	-	4/4/8/10	-
1	CSU	A	341	1	-	0/4/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	CSU	OD3-S	3.13	1.54	1.45
1	A	341	CSU	OD3-S	2.60	1.53	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	CSU	OD2-S-OD1	2.29	120.37	112.74
1	B	341	CSU	OD2-S-OD1	2.27	120.32	112.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	341	CSU	N-CA-CB-SG
1	B	341	CSU	OD1-S-SG-CB
1	B	341	CSU	OD2-S-SG-CB
1	B	341	CSU	OD3-S-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	GOL	B	1005	-	5,5,5	0.14	0	5,5,5	0.63	0
5	NO3	B	1004	-	1,3,3	0.48	0	0,3,3	-	-
5	NO3	B	1003	-	1,3,3	0.54	0	0,3,3	-	-
5	NO3	A	1004	-	1,3,3	0.58	0	0,3,3	-	-
6	PO4	A	1005	-	4,4,4	0.71	0	6,6,6	0.46	0
7	GOL	C	101	-	5,5,5	0.28	0	5,5,5	0.67	0
6	PO4	D	201	-	4,4,4	0.83	0	6,6,6	0.69	0
5	NO3	A	1003	-	1,3,3	0.48	0	0,3,3	-	-

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	GOL	C	101	-	-	3/4/4/4	-
7	GOL	B	1005	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1005	GOL	C1-C2-C3-O3
7	C	101	GOL	C1-C2-C3-O3
7	B	1005	GOL	O2-C2-C3-O3
7	C	101	GOL	O2-C2-C3-O3
7	C	101	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1005	GOL	3	0
7	C	101	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	469/485 (96%)	-0.33	9 (1%) 66 67	15, 37, 64, 115	7 (1%)
1	B	473/485 (97%)	-0.07	11 (2%) 61 62	23, 45, 93, 130	5 (1%)
2	C	79/79 (100%)	-0.47	1 (1%) 75 77	20, 33, 51, 75	1 (1%)
2	D	79/79 (100%)	-0.47	3 (3%) 44 42	28, 38, 60, 95	0
All	All	1100/1128 (97%)	-0.24	24 (2%) 62 63	15, 39, 84, 130	13 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	936	LEU	5.2
1	B	941	HIS	3.9
1	B	303	LYS	3.8
1	B	836	PHE	3.8
2	D	79	GLY	3.8
1	A	866	ASN	3.6
1	A	864	GLU	3.5
1	A	535[A]	ARG	3.2
1	A	859	ILE	3.2
1	A	302	PHE	3.1
1	B	940	HIS	2.9
2	D	78	GLY	2.8
2	D	77	GLY	2.6
1	B	544[A]	ASP	2.5
1	B	936	LEU	2.4
1	B	492	LYS	2.4
1	B	348	PHE	2.3
1	B	937	LEU	2.3
1	A	375[A]	ARG	2.2
1	B	939	HIS	2.2
1	B	611	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	862	GLN	2.1
1	A	863	ASN	2.0
2	C	79	GLY	2.0

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
1	CSU	B	341	10/11	0.85	0.12	44,59,75,77	0
1	CSU	A	341	10/11	0.95	0.07	35,45,60,66	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
7	GOL	C	101	6/6	0.79	0.16	27,34,42,56	0
5	NO3	A	1003	4/4	0.80	0.14	47,59,74,74	0
5	NO3	A	1004	4/4	0.88	0.10	54,63,69,74	0
7	GOL	B	1005	6/6	0.89	0.11	33,39,40,41	0
5	NO3	B	1003	4/4	0.92	0.09	51,54,61,69	0
5	NO3	B	1004	4/4	0.92	0.15	65,67,75,80	0
6	PO4	A	1005	5/5	0.97	0.07	25,35,40,50	0
4	CL	A	1002	1/1	0.98	0.10	34,34,34,34	0
6	PO4	D	201	5/5	0.98	0.08	31,39,50,57	0
3	CD	A	1001	1/1	0.99	0.03	43,43,43,43	0
4	CL	B	1002	1/1	0.99	0.05	32,32,32,32	0
3	CD	B	1001	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.