Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 12:52 pm GMT

PDB ID	:	9S2Z / pdb_00009s2z
Title	:	Crystal structure of Usp10 catalytic domain bound to Ub-PA
Authors	:	Misra, M.; Vollrath, J.; Vidov, A.; Dikic, I.
Deposited on	:	2025-07-23
Resolution	:	1.30 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 (i) 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 (i)) were used in the production of this report:

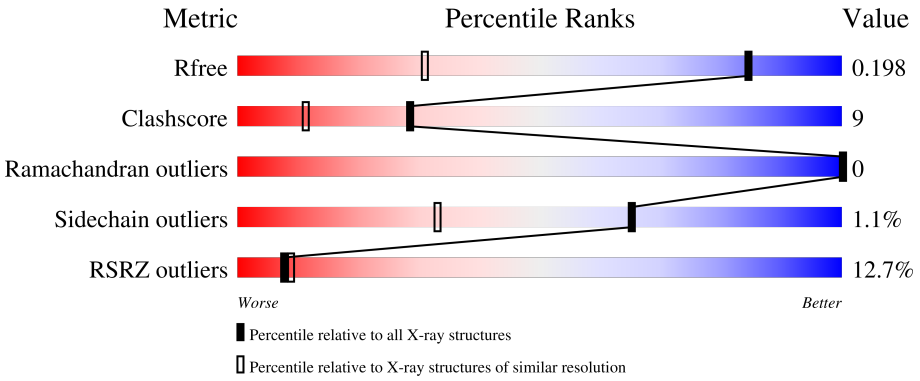
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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 <=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	394	13% 72% 13% • 13%
2	B	75	91% 9%

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
3	EDO	B	2303	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7864 atoms, of which 3708 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 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	20	0
			5856	1859	2955	494	534	14			

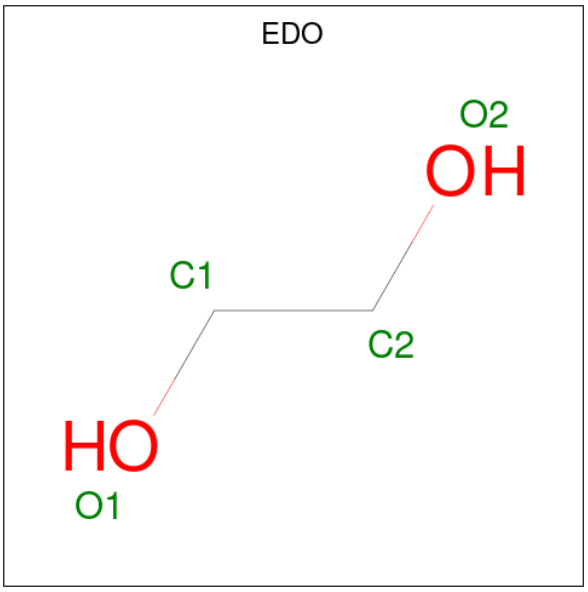
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	SER	-	expression tag	UNP Q14694
A	381	MET	-	expression tag	UNP Q14694
A	477	GLY	-	linker	UNP Q14694
A	478	SER	-	linker	UNP Q14694
A	479	GLY	-	linker	UNP Q14694
A	480	SER	-	linker	UNP Q14694
A	481	GLY	-	linker	UNP Q14694
A	572	GLY	-	linker	UNP Q14694
A	573	SER	-	linker	UNP Q14694
A	574	GLY	-	linker	UNP Q14694
A	575	SER	-	linker	UNP Q14694
A	576	SER	-	linker	UNP Q14694

- Molecule 2 is a protein called Polyubiquitin-B.

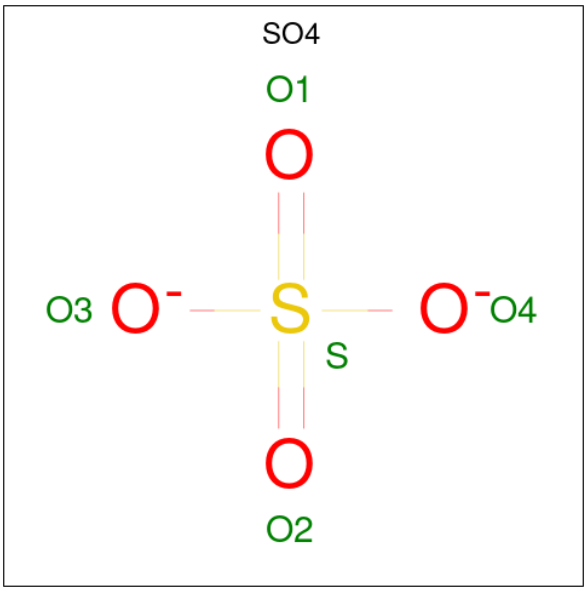
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	75	Total	C	H	N	O	S	0	3	0
			1267	390	650	108	118	1			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



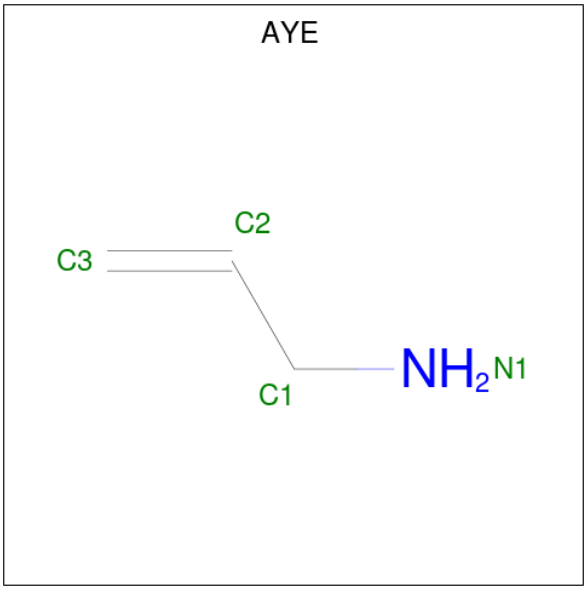
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

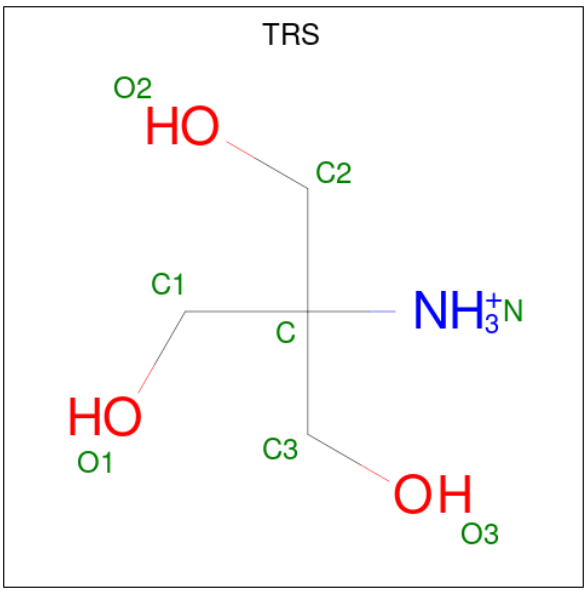
- Molecule 5 is prop-2-en-1-amine (CCD ID: AYE) (formula: C_3H_7N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H N 11 3 7 1	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
6	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

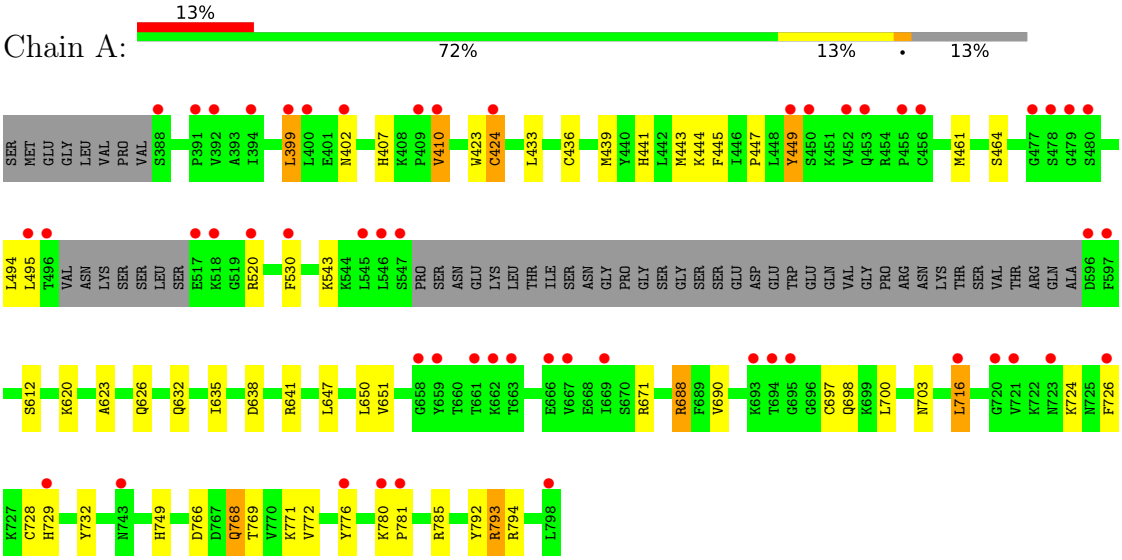
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	454	Total	O	0	0
			454	454		
7	B	106	Total	O	0	0
			106	106		

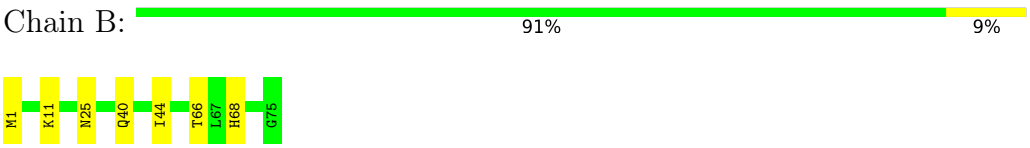
3 Residue-property plots (i)

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 10



• Molecule 2: Polyubiquitin-B



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.14Å 81.96Å 87.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.88 – 1.30 59.88 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (59.88-1.30) 99.1 (59.88-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.169 , 0.194 0.172 , 0.198	Depositor DCC
R_{free} test set	6453 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7864	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, TRS, EDO, AYE

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	0.93	6/2964 (0.2%)	1.24	13/4015 (0.3%)
2	B	0.70	0/630	1.08	0/848
All	All	0.90	6/3594 (0.2%)	1.22	13/4863 (0.3%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	MET	SD-CE	-6.19	1.64	1.79
1	A	793	ARG	NE-CZ	-5.86	1.26	1.33
1	A	423	TRP	C-O	5.85	1.31	1.24
1	A	441	HIS	CE1-NE2	-5.49	1.27	1.32
1	A	407	HIS	CG-CD2	5.40	1.41	1.35
1	A	423	TRP	C-N	5.03	1.40	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	793	ARG	CG-CD-NE	-10.24	89.47	112.00
1	A	444	LYS	CG-CD-CE	7.98	129.66	111.30
1	A	793	ARG	CB-CG-CD	-7.11	94.94	111.30
1	A	399	LEU	N-CA-CB	-6.74	100.19	110.16
1	A	443	MET	CG-SD-CE	-6.69	86.19	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	793	ARG	CA-CB-CG	6.58	127.26	114.10
1	A	688	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	785	ARG	CB-CG-CD	5.69	124.38	111.30
1	A	410	VAL	N-CA-CB	5.63	118.49	112.08
1	A	772[A]	VAL	N-CA-CB	5.29	118.38	110.13
1	A	772[B]	VAL	N-CA-CB	5.29	118.38	110.13
1	A	650	LEU	O-C-N	5.11	127.40	122.09
1	A	449	TYR	N-CA-CB	-5.06	103.39	111.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	ALA	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	2901	2955	2929	56	0
2	B	617	650	649	8	0
3	A	44	66	65	11	0
3	B	4	6	6	6	0
4	A	10	0	0	0	0
5	B	4	7	3	0	0
6	B	16	24	24	2	0
7	A	454	0	0	15	1
7	B	106	0	0	2	0
All	All	4156	3708	3676	64	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 9.

All (64) 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:436[B]:CYS:SG	1:A:439:MET:HB3	1.85	1.15
1:A:726:PHE:CE1	1:A:728[A]:CYS:SG	2.41	1.12
1:A:697[A]:CYS:SG	2:B:40:GLN:OE1	2.24	0.94
1:A:410:VAL:HG21	3:A:1002:EDO:C1	2.03	0.88
1:A:436[B]:CYS:SG	1:A:439:MET:CB	2.65	0.85
1:A:632[B]:GLN:NE2	2:B:44[B]:ILE:HD12	1.94	0.83
1:A:793:ARG:HG2	7:A:1306:HOH:O	1.78	0.81
1:A:410:VAL:HG21	3:A:1002:EDO:H11	1.62	0.80
1:A:626:GLN:HG3	3:B:2303:EDO:H11	1.64	0.79
1:A:626:GLN:HG3	3:B:2303:EDO:C1	2.13	0.79
1:A:626:GLN:CB	3:B:2303:EDO:H11	2.14	0.77
1:A:410:VAL:HG21	3:A:1002:EDO:H12	1.68	0.74
1:A:632[B]:GLN:HE21	2:B:44[B]:ILE:HD12	1.50	0.73
1:A:638:ASP:HB2	7:A:1379:HOH:O	1.91	0.70
1:A:626:GLN:CG	3:B:2303:EDO:H11	2.23	0.69
1:A:464[B]:SER:OG	1:A:494:LEU:HD11	1.95	0.67
1:A:769[B]:THR:HG21	7:A:1455:HOH:O	1.95	0.67
2:B:66:THR:O	3:B:2303:EDO:H21	1.95	0.67
1:A:433:LEU:O	1:A:436[B]:CYS:SG	2.45	0.63
1:A:424:CYS:SG	1:A:749:HIS:CE1	2.92	0.63
1:A:520:ARG:NH2	7:A:1104:HOH:O	2.32	0.62
1:A:647:LEU:HB3	1:A:716:LEU:HD21	1.81	0.61
1:A:726:PHE:CD2	1:A:729:HIS:HB2	2.37	0.60
1:A:726:PHE:CZ	1:A:728[A]:CYS:SG	2.94	0.59
3:A:1006:EDO:H11	7:A:1210:HOH:O	2.03	0.59
1:A:690[A]:VAL:HG21	1:A:700:LEU:HD21	1.85	0.59
1:A:780:LYS:HD2	1:A:781:PRO:HD2	1.86	0.58
2:B:1:MET:HA	6:B:2304:TRS:H21	1.85	0.56
1:A:543:LYS:HD3	7:A:1434:HOH:O	2.06	0.55
1:A:436[B]:CYS:SG	1:A:436[B]:CYS:O	2.64	0.55
1:A:794:ARG:HH22	3:A:1001:EDO:H21	1.71	0.55
1:A:690[A]:VAL:CG2	1:A:700:LEU:HD21	2.36	0.55
1:A:635:ILE:HD11	1:A:688:ARG:HG2	1.89	0.55
1:A:768[A]:GLN:H	1:A:768[A]:GLN:CD	2.17	0.53
1:A:703[B]:ASN:OD1	1:A:781:PRO:HB3	2.09	0.52
1:A:612:SER:OG	1:A:671:ARG:NE	2.43	0.51
1:A:726:PHE:HE1	1:A:728[A]:CYS:SG	2.22	0.51
1:A:530[A]:PHE:CD2	3:A:1004:EDO:H11	2.45	0.51
1:A:402:ASN:HB2	7:A:1156:HOH:O	2.11	0.50
1:A:732:TYR:HB3	1:A:792:TYR:HB3	1.93	0.50
1:A:766:ASP:O	1:A:769[B]:THR:HG22	2.13	0.49
1:A:793:ARG:CG	7:A:1306:HOH:O	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:LYS:NZ	7:A:1118:HOH:O	2.46	0.48
1:A:794:ARG:HH22	3:A:1001:EDO:C2	2.27	0.48
1:A:641:ARG:CZ	7:A:1133:HOH:O	2.61	0.47
1:A:399:LEU:HG	1:A:445:PHE:CE2	2.50	0.46
1:A:651:VAL:HG11	1:A:716:LEU:HG	1.97	0.46
1:A:771[B]:LYS:NZ	7:A:1123:HOH:O	2.48	0.46
3:A:1007:EDO:H11	7:A:1448:HOH:O	2.15	0.46
1:A:626:GLN:HB3	3:B:2303:EDO:H11	1.98	0.45
1:A:461:MET:HE2	1:A:461:MET:HB3	1.80	0.45
1:A:410:VAL:HG13	7:A:1276:HOH:O	2.16	0.44
2:B:11:LYS:HE2	6:B:2302:TRS:H12	1.99	0.44
1:A:447:PRO:HB2	1:A:449:TYR:CE2	2.53	0.44
1:A:771[B]:LYS:NZ	7:A:1112:HOH:O	2.41	0.43
3:A:1009:EDO:H22	7:A:1112:HOH:O	2.18	0.43
1:A:690[A]:VAL:HG23	1:A:700:LEU:HG	2.00	0.43
1:A:690[B]:VAL:HG13	1:A:698:GLN:HB2	2.00	0.43
1:A:530[A]:PHE:CE2	3:A:1004:EDO:H21	2.54	0.43
2:B:68[B]:HIS:ND1	7:B:2402:HOH:O	2.24	0.42
1:A:464[B]:SER:HG	1:A:494:LEU:HD11	1.85	0.41
2:B:25:ASN:HB3	7:B:2457:HOH:O	2.20	0.41
1:A:620:LYS:NZ	3:A:1012:EDO:H11	2.35	0.40
1:A:776[B]:TYR:OH	1:A:780:LYS:HD3	2.20	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)
7:A:1382:HOH:O	7:A:1457:HOH:O[4_555]	2.18	0.02

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	357/394 (91%)	348 (98%)	9 (2%)	0	100	100
2	B	76/75 (101%)	75 (99%)	1 (1%)	0	100	100
All	All	433/469 (92%)	423 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/352 (93%)	322 (98%)	5 (2%)	57	21
2	B	71/68 (104%)	71 (100%)	0	100	100
All	All	398/420 (95%)	393 (99%)	5 (1%)	65	26

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	CYS
1	A	495	LEU
1	A	716	LEU
1	A	768[A]	GLN
1	A	768[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	533	ASN
1	A	599	GLN
2	B	25	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	EDO	A	1001	-	3,3,3	0.29	0	2,2,2	0.13	0
3	EDO	A	1006	-	3,3,3	0.13	0	2,2,2	0.23	0
3	EDO	A	1009	-	3,3,3	0.56	0	2,2,2	0.74	0
3	EDO	A	1002	-	3,3,3	0.72	0	2,2,2	0.36	0
6	TRS	B	2304	-	7,7,7	0.10	0	9,9,9	0.45	0
5	AYE	B	2301	2,1	3,3,3	0.21	0	1,2,2	1.33	0
4	SO4	A	1013	-	4,4,4	0.25	0	6,6,6	0.15	0
3	EDO	A	1007	-	3,3,3	0.19	0	2,2,2	0.18	0
3	EDO	A	1004	-	3,3,3	0.17	0	2,2,2	0.12	0
3	EDO	A	1008	-	3,3,3	0.65	0	2,2,2	0.28	0
3	EDO	A	1010	-	3,3,3	0.13	0	2,2,2	0.07	0
3	EDO	A	1005	-	3,3,3	0.11	0	2,2,2	0.25	0
6	TRS	B	2302	-	7,7,7	0.13	0	9,9,9	0.32	0
3	EDO	A	1011	-	3,3,3	0.50	0	2,2,2	0.34	0
3	EDO	A	1012	-	3,3,3	0.44	0	2,2,2	0.70	0
3	EDO	B	2303	-	3,3,3	0.52	0	2,2,2	1.13	0
4	SO4	A	1003	-	4,4,4	0.32	0	6,6,6	0.15	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	EDO	A	1001	-	-	1/1/1/1	-
3	EDO	A	1006	-	-	1/1/1/1	-
3	EDO	A	1009	-	-	1/1/1/1	-
3	EDO	A	1002	-	-	1/1/1/1	-
6	TRS	B	2304	-	-	9/9/9/9	-
5	AYE	B	2301	2,1	-	0/1/1/1	-
3	EDO	A	1007	-	-	1/1/1/1	-
3	EDO	A	1004	-	-	1/1/1/1	-
3	EDO	A	1008	-	-	1/1/1/1	-
3	EDO	A	1010	-	-	1/1/1/1	-
3	EDO	A	1005	-	-	1/1/1/1	-
6	TRS	B	2302	-	-	6/9/9/9	-
3	EDO	A	1011	-	-	1/1/1/1	-
3	EDO	A	1012	-	-	0/1/1/1	-
3	EDO	B	2303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2304	TRS	C2-C-C1-O1
6	B	2304	TRS	C3-C-C1-O1
3	A	1001	EDO	O1-C1-C2-O2
3	A	1006	EDO	O1-C1-C2-O2
3	A	1010	EDO	O1-C1-C2-O2
3	A	1011	EDO	O1-C1-C2-O2
6	B	2304	TRS	C1-C-C2-O2
3	A	1007	EDO	O1-C1-C2-O2
3	A	1009	EDO	O1-C1-C2-O2
6	B	2302	TRS	N-C-C2-O2
6	B	2302	TRS	C1-C-C3-O3
6	B	2302	TRS	N-C-C3-O3
6	B	2304	TRS	N-C-C1-O1
6	B	2304	TRS	N-C-C2-O2
6	B	2304	TRS	C1-C-C3-O3
6	B	2304	TRS	N-C-C3-O3
3	A	1008	EDO	O1-C1-C2-O2
3	A	1004	EDO	O1-C1-C2-O2
3	A	1005	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	1002	EDO	O1-C1-C2-O2
3	B	2303	EDO	O1-C1-C2-O2
6	B	2302	TRS	C1-C-C2-O2
6	B	2302	TRS	C3-C-C2-O2
6	B	2302	TRS	C2-C-C3-O3
6	B	2304	TRS	C3-C-C2-O2
6	B	2304	TRS	C2-C-C3-O3

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	EDO	2	0
3	A	1006	EDO	1	0
3	A	1009	EDO	1	0
3	A	1002	EDO	3	0
6	B	2304	TRS	1	0
3	A	1007	EDO	1	0
3	A	1004	EDO	2	0
6	B	2302	TRS	1	0
3	A	1012	EDO	1	0
3	B	2303	EDO	6	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, 95^{th} 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	343/394 (87%)	0.61	53 (15%) 5 5	8, 22, 66, 101	20 (5%)
2	B	75/75 (100%)	0.46	0 100 100	12, 30, 45, 51	3 (4%)
All	All	418/469 (89%)	0.58	53 (12%) 8 9	8, 23, 63, 101	23 (5%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	597	PHE	5.7
1	A	424	CYS	5.4
1	A	495	LEU	5.1
1	A	518	LYS	4.9
1	A	726	PHE	4.9
1	A	479	GLY	4.5
1	A	410	VAL	4.1
1	A	452	VAL	4.1
1	A	530[A]	PHE	4.0
1	A	776[A]	TYR	3.9
1	A	667	VAL	3.8
1	A	496	THR	3.7
1	A	399	LEU	3.7
1	A	547	SER	3.6
1	A	781	PRO	3.6
1	A	449	TYR	3.5
1	A	456	CYS	3.4
1	A	663	THR	3.4
1	A	480	SER	3.3
1	A	392	VAL	3.3
1	A	455	PRO	3.3
1	A	477	GLY	3.3
1	A	394	ILE	3.2
1	A	659	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	662	LYS	2.9
1	A	723	ASN	2.9
1	A	661	THR	2.9
1	A	545	LEU	2.8
1	A	388	SER	2.8
1	A	400	LEU	2.7
1	A	716	LEU	2.7
1	A	546	LEU	2.7
1	A	450	SER	2.6
1	A	517	GLU	2.6
1	A	596	ASP	2.5
1	A	694	THR	2.5
1	A	658	GLY	2.5
1	A	666	GLU	2.5
1	A	693	LYS	2.4
1	A	391	PRO	2.4
1	A	720	GLY	2.4
1	A	453	GLN	2.4
1	A	729	HIS	2.4
1	A	478	SER	2.3
1	A	669	ILE	2.3
1	A	798	LEU	2.2
1	A	520	ARG	2.2
1	A	409	PRO	2.2
1	A	721	VAL	2.1
1	A	780	LYS	2.1
1	A	743[A]	ASN	2.0
1	A	695	GLY	2.0
1	A	402	ASN	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, 95^{th} 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
6	TRS	B	2302	8/8	0.60	0.16	61,80,84,85	0
3	EDO	A	1005	4/4	0.64	0.22	61,77,79,82	0
3	EDO	A	1010	4/4	0.66	0.16	64,71,71,72	0
3	EDO	A	1009	4/4	0.71	0.21	45,48,51,54	0
3	EDO	A	1012	4/4	0.76	0.16	45,56,61,69	0
6	TRS	B	2304	8/8	0.77	0.14	48,57,62,66	0
4	SO4	A	1013	5/5	0.79	0.14	50,62,66,69	0
4	SO4	A	1003	5/5	0.82	0.12	59,64,68,77	0
3	EDO	A	1006	4/4	0.83	0.14	57,59,62,67	0
3	EDO	A	1007	4/4	0.84	0.13	35,48,57,58	0
3	EDO	A	1004	4/4	0.84	0.17	47,56,58,61	0
3	EDO	A	1002	4/4	0.85	0.16	34,40,42,47	0
3	EDO	A	1001	4/4	0.85	0.12	33,41,46,49	0
3	EDO	A	1011	4/4	0.88	0.13	27,44,55,57	0
3	EDO	B	2303	4/4	0.88	0.12	30,35,45,51	0
3	EDO	A	1008	4/4	0.91	0.12	28,35,39,45	0
5	AYE	B	2301	4/4	0.92	0.10	16,18,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.