



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 11:08 AM EDT

PDB ID : 5QKB / pdb_00005qkb
Title : Ground-state model of NUDT5 and corresponding apo datasets for PanDDA analysis
Authors : Dubianok, Y.; Collins, P.; Krojer, T.; Wright, N.; Strain-Damerell, C.; Burgess-Brown, N.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Huber, K.; von Delft, F.
Deposited on : 2018-12-07
Resolution : 1.58 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

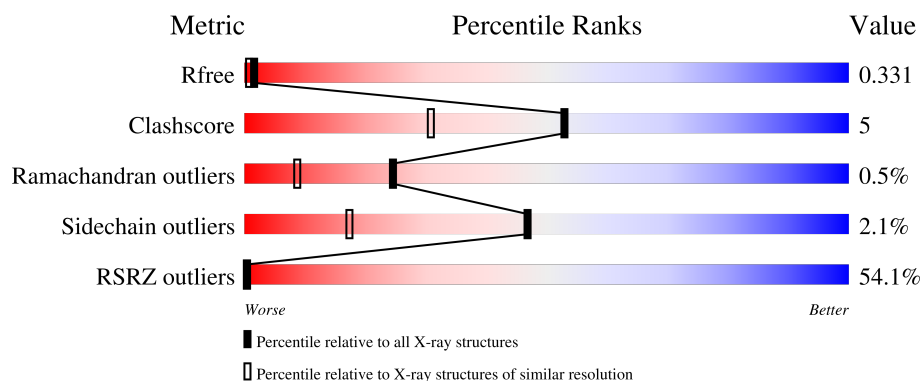
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	209	
1	B	209	
1	C	209	
1	D	209	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5953 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 ADP-sugar pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1450	917	242	283	8			
1	B	194	Total	C	N	O	S	0	0	0
			1464	924	244	288	8			
1	C	192	Total	C	N	O	S	0	0	0
			1402	884	234	277	7			
1	D	189	Total	C	N	O	S	0	1	0
			1395	882	234	271	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UKK9
B	0	SER	-	expression tag	UNP Q9UKK9
C	0	SER	-	expression tag	UNP Q9UKK9
D	0	SER	-	expression tag	UNP Q9UKK9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

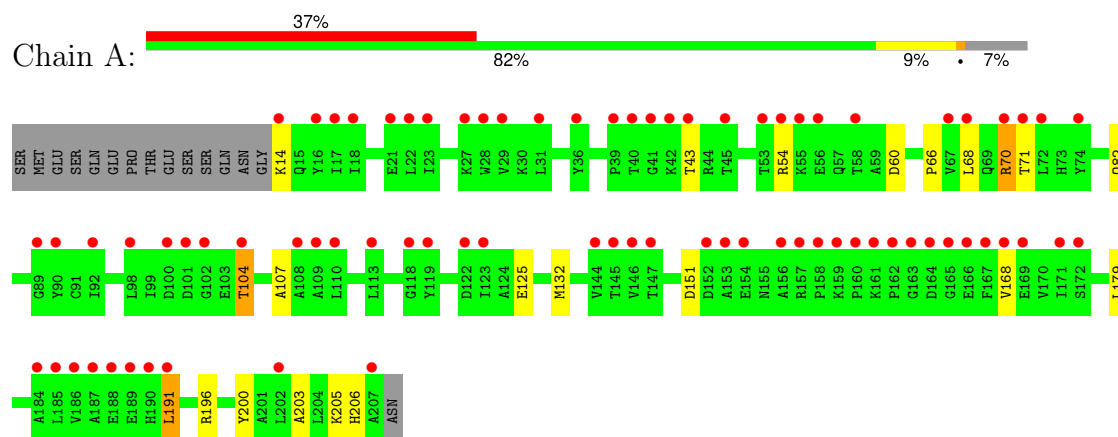
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0
5	B	69	Total O 69 69	0	0
5	C	66	Total O 66 66	0	0
5	D	24	Total O 24 24	0	0

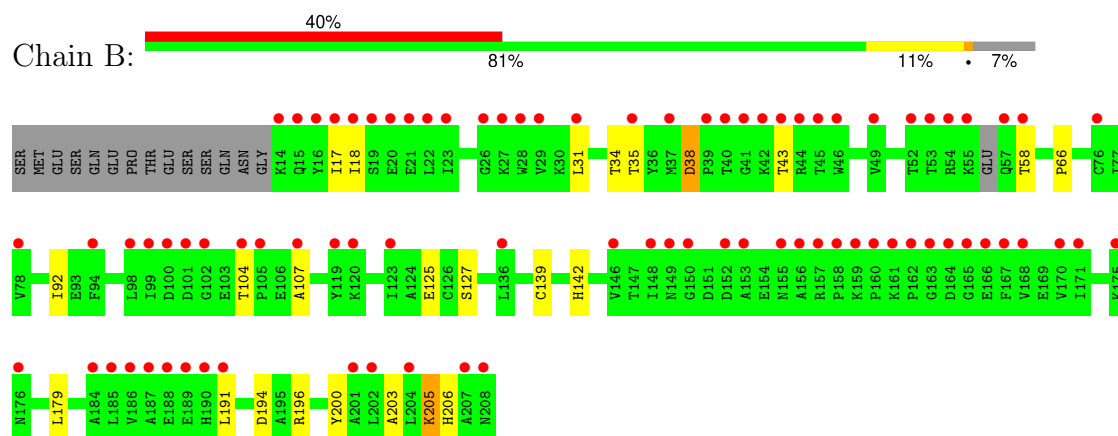
3 Residue-property plots [i](#)

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.

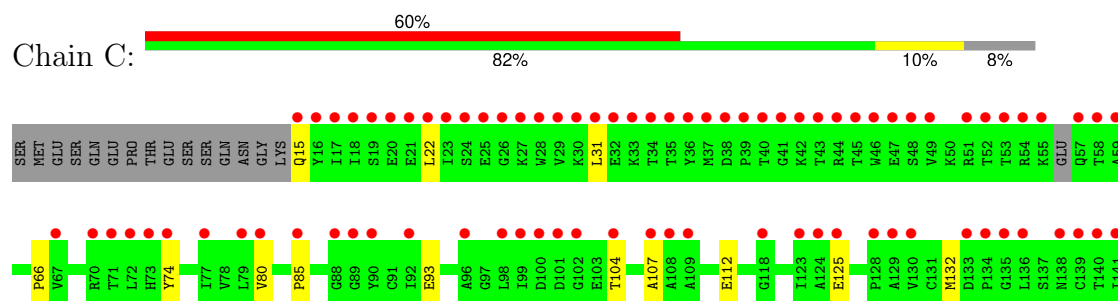
• Molecule 1: ADP-sugar pyrophosphatase

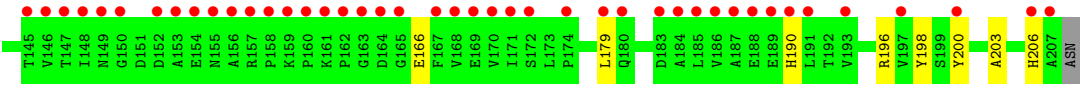


• Molecule 1: ADP-sugar pyrophosphatase

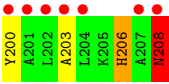
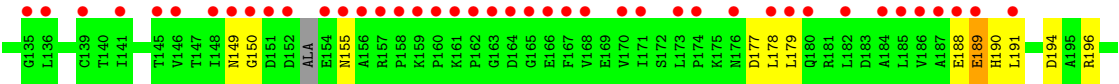
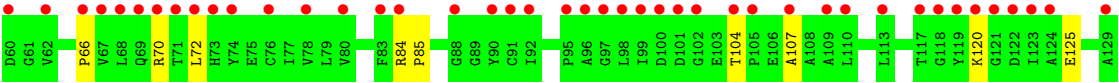
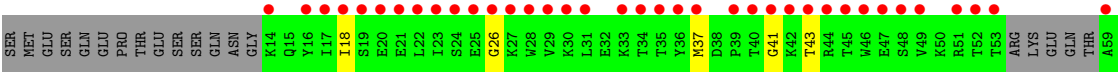
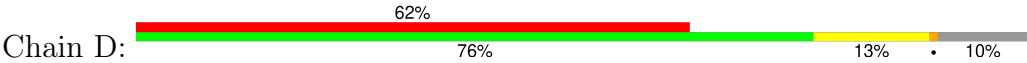


• Molecule 1: ADP-sugar pyrophosphatase





● Molecule 1: ADP-sugar pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.07Å 59.68Å 80.32Å 79.44° 81.82° 75.93°	Depositor
Resolution (Å)	78.54 – 1.58 78.54 – 1.58	Depositor EDS
% Data completeness (in resolution range)	95.5 (78.54-1.58) 100.0 (78.54-1.58)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	262.85 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.219 , 0.250 0.329 , 0.331	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5953	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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: CL, MG, EDO

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	1.31	1/1478 (0.1%)	1.15	0/2019
1	B	1.25	2/1492 (0.1%)	1.16	0/2035
1	C	1.29	2/1429 (0.1%)	1.15	2/1958 (0.1%)
1	D	1.32	4/1420 (0.3%)	1.24	8/1939 (0.4%)
All	All	1.29	9/5819 (0.2%)	1.18	10/7951 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	SER	C-O	-6.61	1.15	1.23
1	D	208	ASN	CG-ND2	6.30	1.46	1.33
1	B	139	CYS	C-O	6.17	1.31	1.23
1	D	179	LEU	N-CA	-5.95	1.39	1.46
1	D	84	ARG	C-O	-5.38	1.19	1.24
1	A	104	THR	CA-C	5.23	1.59	1.52
1	C	80	VAL	CA-C	-5.22	1.46	1.52
1	C	93	GLU	N-CA	5.11	1.52	1.45
1	D	177	ASP	N-CA	-5.01	1.40	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	GLU	N-CA-C	16.57	133.76	110.06
1	C	190	HIS	N-CA-CB	6.59	120.69	110.21
1	D	178	LEU	N-CA-C	6.40	117.91	111.07
1	D	85	PRO	CA-C-N	-6.05	112.77	119.19
1	D	85	PRO	C-N-CA	-6.05	112.77	119.19
1	D	189	GLU	CB-CA-C	-6.01	100.01	111.97
1	D	26	GLY	N-CA-C	-5.61	106.06	112.79
1	C	85	PRO	N-CA-C	5.56	117.48	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	18	ILE	N-CA-C	-5.50	106.34	111.45
1	D	206	HIS	N-CA-C	5.09	117.72	111.82

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	1450	0	1405	17	0
1	B	1464	0	1414	15	0
1	C	1402	0	1298	15	0
1	D	1395	0	1328	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
4	B	4	0	6	2	0
4	C	4	0	6	0	0
5	A	66	0	0	1	0
5	B	69	0	0	2	0
5	C	66	0	0	6	0
5	D	24	0	0	3	0
All	All	5953	0	5457	56	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 (56) 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:D:194:ASP:OD1	1:D:196[A]:ARG:HD3	1.82	0.79
1:C:104:THR:HG23	1:C:107:ALA:H	1.49	0.77
1:A:104:THR:HG23	1:A:107:ALA:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLU:OE1	5:C:401:HOH:O	2.03	0.76
1:D:120:LYS:H	1:D:155:ASN:HD21	1.34	0.73
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.71	0.72
5:C:401:HOH:O	1:D:206:HIS:HE1	1.74	0.69
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:HG3	2.07	0.69
1:D:104:THR:HG23	1:D:107:ALA:H	1.57	0.68
1:C:132:MET:HE1	1:C:196:ARG:CZ	2.28	0.63
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.80	0.63
1:D:189:GLU:O	1:D:190:HIS:C	2.41	0.63
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.82	0.61
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.82	0.60
1:B:104:THR:HG23	1:B:107:ALA:H	1.67	0.60
1:C:112:GLU:OE2	5:C:402:HOH:O	2.16	0.60
4:B:301:EDO:H22	5:B:406:HOH:O	2.01	0.60
1:D:196[B]:ARG:HG3	1:D:196[B]:ARG:HH21	1.67	0.59
4:B:301:EDO:C2	5:B:406:HOH:O	2.51	0.58
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.86	0.58
1:D:188:GLU:HG3	1:D:189:GLU:HG3	1.86	0.56
1:C:206:HIS:HE1	1:D:125:GLU:OE1	1.90	0.54
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.45	0.51
1:A:104:THR:CG2	1:A:107:ALA:H	2.22	0.51
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.46	0.51
1:D:208:ASN:CG	5:D:402:HOH:O	2.54	0.50
1:D:150:GLY:O	5:D:401:HOH:O	2.19	0.49
1:A:71:THR:HG23	1:A:151:ASP:OD2	2.12	0.49
1:A:82:GLN:HG2	1:A:168:VAL:HG22	1.94	0.49
1:A:191:LEU:C	1:A:191:LEU:HD23	2.38	0.49
1:C:166:GLU:OE2	5:C:402:HOH:O	2.19	0.49
1:A:54:ARG:HD3	1:A:60:ASP:OD1	2.13	0.49
1:A:132:MET:O	1:B:196:ARG:NH2	2.46	0.49
1:B:194:ASP:OD2	1:B:196:ARG:NH2	2.41	0.48
1:C:15:GLN:N	5:C:405:HOH:O	2.45	0.48
1:A:200:TYR:OH	1:B:206:HIS:HD2	1.95	0.48
1:D:37:MET:SD	1:D:41:GLY:O	2.72	0.47
1:B:58:THR:CB	1:B:142:HIS:NE2	2.78	0.47
1:D:191:LEU:C	1:D:191:LEU:HD12	2.40	0.46
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.99	0.46
1:B:18:ILE:HD12	1:B:35:THR:HG22	1.96	0.46
1:C:22:LEU:C	1:C:22:LEU:HD13	2.40	0.46
1:D:149:ASN:C	1:D:149:ASN:HD22	2.23	0.45
1:A:179:LEU:HD23	1:A:205:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.52	0.45
1:A:70:ARG:HD3	5:A:419:HOH:O	2.16	0.45
1:A:206:HIS:HE1	1:B:125:GLU:OE1	2.01	0.44
1:A:132:MET:HE1	1:A:196:ARG:CZ	2.48	0.43
1:B:179:LEU:CD2	1:B:205:LYS:HE2	2.48	0.42
1:A:203:ALA:HB2	1:B:200:TYR:CD1	2.55	0.42
1:B:38:ASP:OD1	1:B:38:ASP:C	2.62	0.41
1:C:200:TYR:OH	1:D:206:HIS:HD2	2.03	0.41
1:A:68:LEU:HG	1:A:70:ARG:HD2	2.02	0.41
1:B:17:ILE:HD12	1:B:34:THR:CG2	2.51	0.41
1:C:74:TYR:HB3	5:C:426:HOH:O	2.22	0.40
1:D:70:ARG:HD3	5:D:409:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	192/209 (92%)	184 (96%)	7 (4%)	1 (0%)	24	9
1	B	190/209 (91%)	188 (99%)	1 (0%)	1 (0%)	24	9
1	C	188/209 (90%)	185 (98%)	2 (1%)	1 (0%)	24	9
1	D	184/209 (88%)	180 (98%)	3 (2%)	1 (0%)	24	9
All	All	754/836 (90%)	737 (98%)	13 (2%)	4 (0%)	24	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	B	66	PRO
1	C	66	PRO

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Mol	Chain	Res	Type
1	D	66	PRO

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	151/179 (84%)	147 (97%)	4 (3%)	40	11
1	B	154/179 (86%)	150 (97%)	4 (3%)	40	11
1	C	139/179 (78%)	138 (99%)	1 (1%)	76	61
1	D	142/179 (79%)	139 (98%)	3 (2%)	47	17
All	All	586/716 (82%)	574 (98%)	12 (2%)	47	20

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	43	THR
1	A	70	ARG
1	A	191	LEU
1	B	31	LEU
1	B	38	ASP
1	B	43	THR
1	B	205	LYS
1	C	31	LEU
1	D	43	THR
1	D	72	LEU
1	D	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	73	HIS
1	A	206	HIS

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Mol	Chain	Res	Type
1	B	73	HIS
1	B	82	GLN
1	B	206	HIS
1	C	15	GLN
1	C	206	HIS
1	D	15	GLN
1	D	149	ASN
1	D	155	ASN
1	D	190	HIS
1	D	206	HIS

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](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	$\# Z > 2$
4	EDO	B	301	-	3,3,3	0.84	0	2,2,2	0.29	0
4	EDO	C	301	-	3,3,3	0.60	0	2,2,2	0.41	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
4	EDO	B	301	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	EDO	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	194/209 (92%)	2.01	78 (40%) 0 1	16, 26, 54, 70	0
1	B	194/209 (92%)	2.22	84 (43%) 0 1	18, 30, 61, 74	0
1	C	192/209 (91%)	2.73	125 (65%) 0 0	18, 30, 54, 63	0
1	D	189/209 (90%)	2.97	129 (68%) 0 0	11, 32, 55, 68	1 (0%)
All	All	769/836 (91%)	2.48	416 (54%) 0 0	11, 30, 55, 74	1 (0%)

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	ASN	8.8
1	D	16	TYR	8.3
1	D	74	TYR	8.2
1	C	16	TYR	8.1
1	B	28	TRP	8.0
1	D	53	THR	8.0
1	C	43	THR	7.9
1	D	18	ILE	7.9
1	C	23	ILE	7.7
1	B	58	THR	7.7
1	C	18	ILE	7.5
1	B	35	THR	7.5
1	C	145	THR	7.2
1	A	67	VAL	7.1
1	B	165	GLY	7.1
1	A	28	TRP	7.0
1	C	28	TRP	6.9
1	D	23	ILE	6.9
1	D	156	ALA	6.9
1	D	167	PHE	6.7
1	C	22	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	74	TYR	6.6
1	C	40	THR	6.5
1	C	58	THR	6.5
1	C	39	PRO	6.5
1	D	174	PRO	6.4
1	D	202	LEU	6.3
1	B	14	LYS	6.2
1	A	167	PHE	6.2
1	A	56	GLU	6.1
1	B	207	ALA	6.1
1	C	136	LEU	6.1
1	B	17	ILE	6.1
1	C	67	VAL	6.1
1	C	146	VAL	6.0
1	B	16	TYR	6.0
1	A	22	LEU	5.9
1	C	55	LYS	5.9
1	B	191	LEU	5.8
1	C	184	ALA	5.8
1	C	17	ILE	5.7
1	A	165	GLY	5.7
1	D	43	THR	5.7
1	D	31	LEU	5.6
1	A	146	VAL	5.6
1	A	191	LEU	5.6
1	D	22	LEU	5.6
1	A	122	ASP	5.5
1	C	53	THR	5.5
1	B	159	LYS	5.5
1	D	152	ASP	5.5
1	C	150	GLY	5.5
1	D	207	ALA	5.5
1	D	14	LYS	5.5
1	D	27	LYS	5.5
1	D	99	ILE	5.5
1	A	162	PRO	5.4
1	C	168	VAL	5.4
1	D	28	TRP	5.4
1	D	100	ASP	5.3
1	C	191	LEU	5.2
1	B	101	ASP	5.2
1	C	29	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	160	PRO	5.2
1	D	162	PRO	5.2
1	D	40	THR	5.1
1	A	190	HIS	5.1
1	D	29	VAL	5.1
1	B	176	ASN	5.1
1	B	163	GLY	5.0
1	D	160	PRO	5.0
1	D	113	LEU	5.0
1	B	158	PRO	4.9
1	B	19	SER	4.9
1	D	78	VAL	4.9
1	A	158	PRO	4.9
1	B	55	LYS	4.9
1	C	187	ALA	4.9
1	A	160	PRO	4.8
1	B	100	ASP	4.8
1	D	159	LYS	4.8
1	D	157	ARG	4.8
1	B	45	THR	4.8
1	B	18	ILE	4.8
1	B	208	ASN	4.8
1	C	27	LYS	4.8
1	D	73	HIS	4.7
1	C	167	PHE	4.7
1	C	190	HIS	4.7
1	A	157	ARG	4.7
1	A	109	ALA	4.7
1	B	162	PRO	4.6
1	D	70	ARG	4.6
1	A	189	GLU	4.6
1	C	207	ALA	4.6
1	D	201	ALA	4.6
1	C	52	THR	4.5
1	D	17	ILE	4.5
1	A	58	THR	4.5
1	A	72	LEU	4.5
1	D	90	TYR	4.4
1	D	52	THR	4.4
1	A	23	ILE	4.4
1	D	88	GLY	4.4
1	D	98	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	46	TRP	4.4
1	D	119	TYR	4.3
1	C	15	GLN	4.3
1	B	156	ALA	4.3
1	B	22	LEU	4.2
1	A	147	THR	4.2
1	A	159	LYS	4.2
1	B	43	THR	4.2
1	D	164	ASP	4.2
1	C	31	LEU	4.2
1	B	104	THR	4.2
1	B	102	GLY	4.2
1	A	113	LEU	4.1
1	D	165	GLY	4.1
1	D	161	LYS	4.1
1	A	41	GLY	4.1
1	A	102	GLY	4.1
1	B	167	PHE	4.1
1	C	162	PRO	4.1
1	A	153	ALA	4.1
1	C	36	TYR	4.1
1	A	101	ASP	4.0
1	B	190	HIS	4.0
1	C	161	LYS	4.0
1	D	68	LEU	4.0
1	C	30	LYS	4.0
1	D	123	ILE	4.0
1	C	57	GLN	4.0
1	C	153	ALA	4.0
1	B	157	ARG	3.9
1	D	104	THR	3.9
1	D	37	MET	3.9
1	D	49	VAL	3.9
1	D	158	PRO	3.9
1	C	104	THR	3.9
1	C	135	GLY	3.8
1	C	165	GLY	3.8
1	B	40	THR	3.8
1	A	207	ALA	3.8
1	A	40	THR	3.8
1	D	171	ILE	3.8
1	A	100	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	29	VAL	3.7
1	B	123	ILE	3.7
1	D	168	VAL	3.7
1	C	41	GLY	3.7
1	D	139	CYS	3.7
1	C	37	MET	3.7
1	D	151	ASP	3.7
1	A	92	ILE	3.7
1	B	23	ILE	3.7
1	C	46	TRP	3.7
1	B	175	LYS	3.7
1	B	168	VAL	3.7
1	C	21	GLU	3.7
1	D	166	GLU	3.7
1	D	51	ARG	3.7
1	D	59	ALA	3.7
1	D	154	GLU	3.6
1	B	202	LEU	3.6
1	C	35	THR	3.6
1	C	98	LEU	3.6
1	A	17	ILE	3.6
1	A	161	LYS	3.6
1	B	20	GLU	3.6
1	C	189	GLU	3.6
1	B	164	ASP	3.6
1	D	72	LEU	3.6
1	D	184	ALA	3.6
1	C	54	ARG	3.6
1	A	172	SER	3.6
1	C	164	ASP	3.6
1	D	20	GLU	3.5
1	C	48	SER	3.5
1	C	99	ILE	3.5
1	B	201	ALA	3.5
1	A	45	THR	3.5
1	A	104	THR	3.5
1	A	164	ASP	3.5
1	A	31	LEU	3.5
1	D	136	LEU	3.5
1	D	122	ASP	3.5
1	B	57	GLN	3.5
1	B	54	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	19	SER	3.5
1	C	172	SER	3.5
1	A	14	LYS	3.5
1	D	96	ALA	3.5
1	D	178	LEU	3.4
1	B	171	ILE	3.4
1	D	148	ILE	3.4
1	C	102	GLY	3.4
1	C	197	VAL	3.4
1	A	188	GLU	3.4
1	D	42	LYS	3.3
1	B	99	ILE	3.3
1	C	171	ILE	3.3
1	C	49	VAL	3.3
1	A	163	GLY	3.3
1	A	39	PRO	3.3
1	B	39	PRO	3.3
1	B	31	LEU	3.3
1	C	72	LEU	3.3
1	C	156	ALA	3.3
1	D	25	GLU	3.3
1	D	39	PRO	3.3
1	A	187	ALA	3.3
1	D	173	LEU	3.3
1	A	54	ARG	3.3
1	C	179	LEU	3.2
1	D	149	ASN	3.2
1	C	34	THR	3.2
1	D	186	VAL	3.2
1	A	156	ALA	3.2
1	D	150	GLY	3.2
1	D	34	THR	3.2
1	D	45	THR	3.2
1	C	92	ILE	3.2
1	C	24	SER	3.2
1	D	97	GLY	3.2
1	D	204	LEU	3.2
1	C	160	PRO	3.2
1	D	62	VAL	3.2
1	D	121	GLY	3.2
1	A	185	LEU	3.1
1	B	136	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	170	VAL	3.1
1	B	153	ALA	3.1
1	C	25	GLU	3.1
1	D	21	GLU	3.1
1	D	36	TYR	3.1
1	B	152	ASP	3.1
1	B	161	LYS	3.1
1	B	49	VAL	3.1
1	B	185	LEU	3.1
1	C	125	GLU	3.1
1	C	163	GLY	3.1
1	D	33	LYS	3.1
1	C	100	ASP	3.1
1	D	101	ASP	3.1
1	C	186	VAL	3.0
1	D	146	VAL	3.0
1	A	16	TYR	3.0
1	B	41	GLY	3.0
1	A	18	ILE	3.0
1	D	124	ALA	3.0
1	D	170	VAL	3.0
1	C	124	ALA	3.0
1	A	152	ASP	3.0
1	C	101	ASP	3.0
1	C	42	LYS	3.0
1	C	141	ILE	2.9
1	D	47	GLU	2.9
1	B	15	GLN	2.9
1	D	66	PRO	2.9
1	C	118	GLY	2.9
1	D	163	GLY	2.9
1	D	129	ALA	2.9
1	C	134	PRO	2.9
1	D	44	ARG	2.9
1	A	43	THR	2.9
1	B	52	THR	2.9
1	B	21	GLU	2.9
1	C	73	HIS	2.8
1	C	26	GLY	2.8
1	B	107	ALA	2.8
1	D	69	GLN	2.8
1	C	140	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	117	THR	2.8
1	C	129	ALA	2.8
1	D	107	ALA	2.8
1	C	70	ARG	2.8
1	D	19	SER	2.8
1	A	53	THR	2.8
1	D	110	LEU	2.8
1	D	179	LEU	2.8
1	D	67	VAL	2.7
1	D	71	THR	2.7
1	D	109	ALA	2.7
1	B	29	VAL	2.7
1	B	146	VAL	2.7
1	A	154	GLU	2.7
1	D	26	GLY	2.7
1	A	55	LYS	2.7
1	C	51	ARG	2.7
1	B	186	VAL	2.7
1	D	155	ASN	2.7
1	A	123	ILE	2.7
1	A	184	ALA	2.6
1	D	102	GLY	2.6
1	D	118	GLY	2.6
1	C	138	ASN	2.6
1	A	71	THR	2.6
1	C	154	GLU	2.6
1	C	157	ARG	2.6
1	B	120	LYS	2.6
1	D	203	ALA	2.6
1	B	189	GLU	2.6
1	D	180	GLN	2.6
1	B	98	LEU	2.6
1	D	191	LEU	2.6
1	B	44	ARG	2.6
1	B	150	GLY	2.6
1	A	108	ALA	2.6
1	C	147	THR	2.6
1	C	185	LEU	2.6
1	D	182	LEU	2.6
1	C	152	ASP	2.6
1	D	41	GLY	2.6
1	C	139	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	91	CYS	2.5
1	C	20	GLU	2.5
1	C	149	ASN	2.5
1	C	109	ALA	2.5
1	C	155	ASN	2.5
1	D	141	ILE	2.5
1	C	158	PRO	2.5
1	B	184	ALA	2.5
1	C	107	ALA	2.5
1	C	148	ILE	2.5
1	C	85	PRO	2.5
1	C	183	ASP	2.5
1	C	32	GLU	2.4
1	A	110	LEU	2.4
1	C	128	PRO	2.4
1	D	83	PHE	2.4
1	A	169	GLU	2.4
1	B	26	GLY	2.4
1	D	105	PRO	2.4
1	D	185	LEU	2.4
1	B	46	TRP	2.4
1	A	89	GLY	2.4
1	C	80	VAL	2.4
1	D	76	CYS	2.4
1	C	188	GLU	2.4
1	D	189	GLU	2.4
1	C	174	PRO	2.4
1	C	77	ILE	2.4
1	C	45	THR	2.4
1	A	36	TYR	2.4
1	A	90	TYR	2.4
1	A	119	TYR	2.4
1	D	48	SER	2.4
1	B	155	ASN	2.4
1	A	166	GLU	2.4
1	C	38	ASP	2.3
1	A	168	VAL	2.3
1	D	35	THR	2.3
1	C	123	ILE	2.3
1	B	187	ALA	2.3
1	C	59	ALA	2.3
1	A	70	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	42	LYS	2.3
1	C	170	VAL	2.3
1	A	21	GLU	2.3
1	B	105	PRO	2.3
1	B	42	LYS	2.3
1	C	44	ARG	2.2
1	C	71	THR	2.2
1	B	166	GLU	2.2
1	B	188	GLU	2.2
1	B	204	LEU	2.2
1	C	79	LEU	2.2
1	A	171	ILE	2.2
1	B	148	ILE	2.2
1	C	90	TYR	2.2
1	C	180	GLN	2.2
1	C	47	GLU	2.2
1	C	159	LYS	2.2
1	D	176	ASN	2.2
1	A	202	LEU	2.2
1	B	37	MET	2.2
1	C	200	TYR	2.2
1	A	118	GLY	2.2
1	D	135	GLY	2.2
1	B	94	PHE	2.2
1	C	133	ASP	2.2
1	A	144	VAL	2.2
1	C	130	VAL	2.2
1	D	80	VAL	2.2
1	B	27	LYS	2.2
1	D	30	LYS	2.2
1	A	98	LEU	2.1
1	C	96	ALA	2.1
1	A	74	TYR	2.1
1	C	169	GLU	2.1
1	C	206	HIS	2.1
1	A	186	VAL	2.1
1	D	24	SER	2.1
1	D	145	THR	2.1
1	D	188	GLU	2.1
1	B	119	TYR	2.1
1	D	200	TYR	2.1
1	D	120	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	88	GLY	2.1
1	C	89	GLY	2.1
1	D	60	ASP	2.1
1	C	33	LYS	2.1
1	D	95	PRO	2.1
1	D	187	ALA	2.0
1	B	76	CYS	2.0
1	D	92	ILE	2.0
1	B	149	ASN	2.0
1	A	27	LYS	2.0
1	A	145	THR	2.0
1	B	53	THR	2.0
1	D	84	ARG	2.0
1	C	108	ALA	2.0
1	B	78	VAL	2.0
1	C	193	VAL	2.0
1	A	68	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	303	1/1	0.74	0.11	68,68,68,68	0
4	EDO	B	301	4/4	0.74	0.14	34,36,38,40	0
4	EDO	C	301	4/4	0.75	0.19	39,56,59,67	0
2	MG	C	302	1/1	0.80	0.10	39,39,39,39	0
2	MG	D	301	1/1	0.81	0.09	26,26,26,26	0
3	CL	A	303	1/1	0.84	0.27	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	302	1/1	0.88	0.09	50,50,50,50	0
2	MG	D	302	1/1	0.89	0.18	35,35,35,35	0
2	MG	C	303	1/1	0.94	0.05	27,27,27,27	0
2	MG	B	302	1/1	0.97	0.04	26,26,26,26	0
2	MG	A	301	1/1	0.98	0.06	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.