



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:57 AM UTC

PDB ID : 5QTL / pdb_00005qtl
Title : PanDDA analysis group deposition – Crystal Structure of NUDT5 in complex with GB-0804
Authors : Dubianok, Y.; Krojer, T.; Kovacs, H.; Moriaud, F.; Wright, N.; Strain-Damerell, C.; Burgess-Brown, N.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; von Delft, F.
Deposited on : 2019-10-31
Resolution : 1.73 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

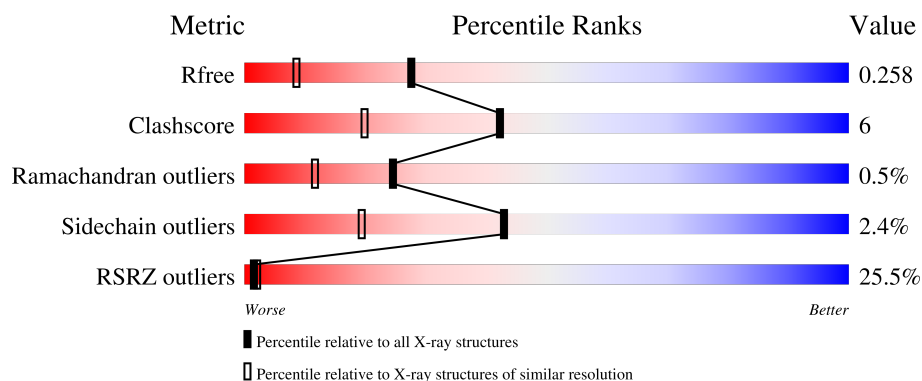
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	15% 84% 9% 7%
1	B	209	20% 79% 14% 7%
1	C	209	28% 76% 15% 8%
1	D	209	32% 78% 14% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6223 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 NUDT5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1466	927	245	286	8			
1	B	195	Total	C	N	O	S	0	0	0
			1477	931	247	291	8			
1	C	193	Total	C	N	O	S	0	0	0
			1445	911	242	284	8			
1	D	194	Total	C	N	O	S	0	1	0
			1470	928	248	286	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

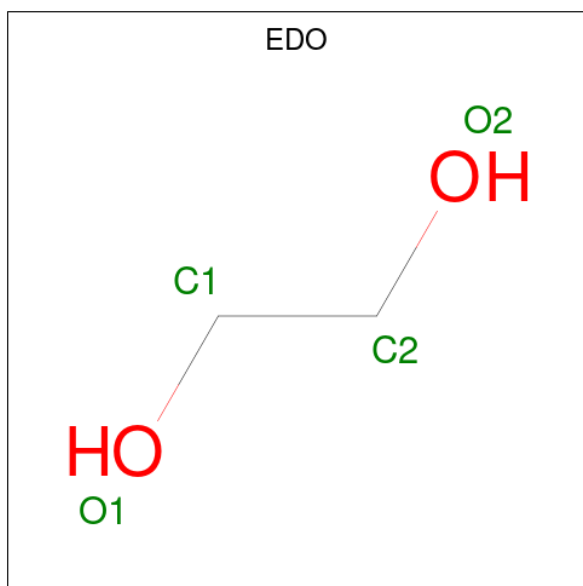
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

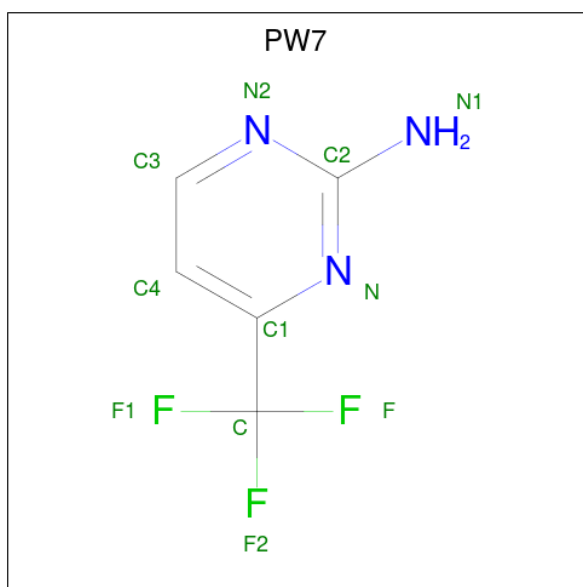
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

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



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

- Molecule 5 is 4-(trifluoromethyl)pyrimidin-2-amine (CCD ID: PW7) (formula: $C_5H_4F_3N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	F	N	0	0
			11	5	3	3		
5	B	1	Total	C	F	N	0	0
			11	5	3	3		
5	C	1	Total	C	F	N	0	0
			11	5	3	3		
5	D	1	Total	C	F	N	0	0
			11	5	3	3		

- Molecule 6 is water.

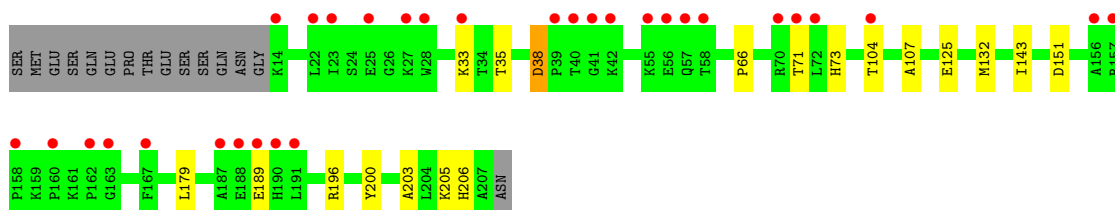
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total	O	0	0
			88	88		
6	B	75	Total	O	0	0
			75	75		
6	C	78	Total	O	0	0
			78	78		
6	D	47	Total	O	0	0
			47	47		

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.

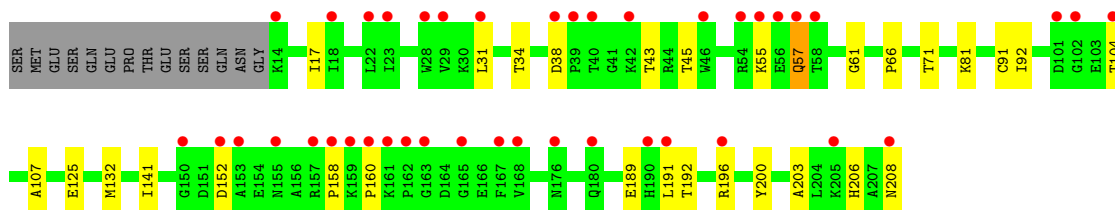
• Molecule 1: NUDT5

Chain A: 



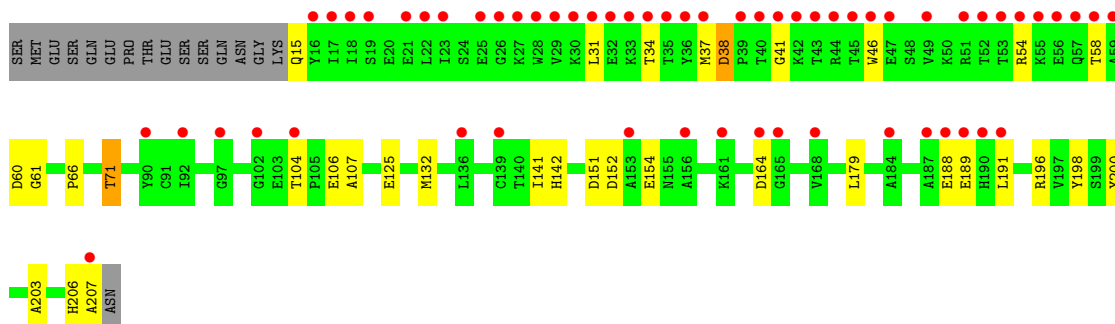
• Molecule 1: NUDT5

Chain B: 



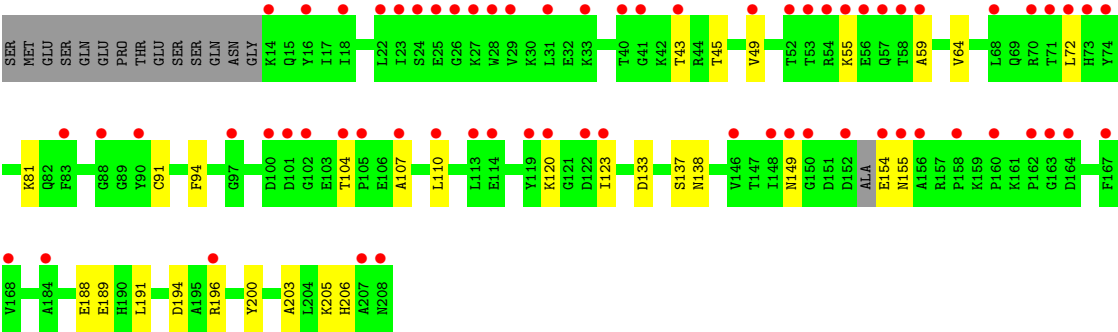
• Molecule 1: NUDT5

Chain C: 



• Molecule 1: NUDT5

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.33Å 59.82Å 80.18Å 79.34° 81.47° 75.65°	Depositor
Resolution (Å)	78.34 – 1.73 78.34 – 1.73	Depositor EDS
% Data completeness (in resolution range)	96.5 (78.34-1.73) 96.5 (78.34-1.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.221 , 0.253 0.233 , 0.258	Depositor DCC
R_{free} test set	4566 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6223	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% 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: EDO, CL, MG, PW7

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	1.09	2/1494 (0.1%)	1.21	0/2037
1	B	1.05	0/1506	1.22	1/2055 (0.0%)
1	C	1.08	0/1473	1.32	1/2012 (0.0%)
1	D	1.07	0/1498	1.35	1/2043 (0.0%)
All	All	1.07	2/5971 (0.0%)	1.28	3/8147 (0.0%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	ILE	C-O	5.67	1.30	1.23
1	A	35	THR	C-O	5.19	1.30	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	THR	CA-CB-OG1	-6.37	100.05	109.60
1	C	207	ALA	CA-C-O	-5.28	111.83	120.80
1	D	138	ASN	N-CA-C	-5.07	106.68	112.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	38	ASP	Sidechain

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	1466	0	1437	14	0
1	B	1477	0	1429	21	0
1	C	1445	0	1380	25	0
1	D	1470	0	1422	24	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	A	4	0	6	0	0
4	B	8	0	12	2	0
4	C	12	0	18	1	0
5	B	22	0	0	0	0
5	C	11	0	0	0	0
5	D	11	0	0	0	0
6	A	88	0	0	0	0
6	B	75	0	0	2	0
6	C	78	0	0	3	0
6	D	47	0	0	2	0
All	All	6223	0	5704	73	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 6.

All (73) 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:154:GLU:OE1	6:D:601:HOH:O	1.67	1.11
1:A:104:THR:HG23	1:A:107:ALA:H	1.39	0.87
1:B:104:THR:HG23	1:B:107:ALA:H	1.41	0.85
1:C:104:THR:HG23	1:C:107:ALA:H	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.63	0.80
1:B:55:LYS:H	1:B:57:GLN:NE2	1.80	0.79
1:A:71:THR:HG23	1:A:151:ASP:OD2	1.83	0.77
1:C:125:GLU:OE1	6:C:401:HOH:O	2.02	0.76
4:B:502:EDO:C2	6:B:603:HOH:O	2.40	0.70
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.74	0.69
4:B:502:EDO:H22	6:B:603:HOH:O	1.92	0.68
1:D:120:LYS:H	1:D:155:ASN:HD21	1.42	0.66
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.78	0.65
6:C:401:HOH:O	1:D:206:HIS:HE1	1.81	0.64
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.80	0.62
1:A:104:THR:CG2	1:A:107:ALA:H	2.11	0.60
1:D:104:THR:HG23	1:D:107:ALA:H	1.67	0.59
1:D:194:ASP:OD1	1:D:196[A]:ARG:HD3	2.04	0.58
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.87	0.57
1:C:132:MET:HE1	1:C:196:ARG:CZ	2.35	0.56
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.41	0.55
1:D:188:GLU:HG3	1:D:189:GLU:HG3	1.87	0.55
1:C:191:LEU:HD12	1:C:191:LEU:O	2.07	0.54
1:C:132:MET:O	1:D:196[B]:ARG:NH1	2.41	0.53
1:D:194:ASP:OD1	1:D:196[B]:ARG:HB2	2.08	0.53
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.92	0.52
1:B:158:PRO:O	1:B:160:PRO:HD3	2.09	0.52
1:C:152:ASP:OD1	1:C:154:GLU:N	2.38	0.52
1:A:132:MET:HE1	1:A:196:ARG:CZ	2.42	0.50
1:A:206:HIS:HE1	1:B:125:GLU:OE1	1.94	0.50
1:C:37:MET:HE1	1:C:41:GLY:O	2.12	0.50
1:B:189:GLU:OE2	1:B:191:LEU:HD11	2.11	0.50
1:D:149:ASN:C	1:D:149:ASN:HD22	2.20	0.49
1:C:38:ASP:OD1	1:C:38:ASP:C	2.55	0.49
1:B:55:LYS:H	1:B:57:GLN:HE21	1.58	0.48
1:B:55:LYS:N	1:B:57:GLN:NE2	2.56	0.48
1:B:38:ASP:OD1	1:B:38:ASP:C	2.57	0.48
1:A:200:TYR:OH	1:B:206:HIS:HD2	1.96	0.48
1:C:54:ARG:HD3	1:C:60:ASP:OD1	2.14	0.47
1:C:191:LEU:HD12	1:C:191:LEU:C	2.39	0.47
1:D:81:LYS:HA	1:D:91:CYS:O	2.15	0.47
1:D:188:GLU:CG	1:D:189:GLU:HG3	2.44	0.47
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.50	0.47
1:B:132:MET:HE1	1:B:196:ARG:CZ	2.45	0.46
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:HIS:CD2	1:D:200:TYR:OH	2.64	0.46
1:D:191:LEU:C	1:D:191:LEU:HD12	2.41	0.46
1:C:37:MET:HE1	1:C:41:GLY:C	2.39	0.46
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.50	0.46
1:B:34:THR:O	1:B:45:THR:HA	2.16	0.46
1:A:179:LEU:HD23	1:A:205:LYS:HD2	1.97	0.45
1:C:34:THR:OG1	1:C:46:TRP:HB3	2.16	0.45
1:C:58:THR:CB	1:C:142:HIS:NE2	2.80	0.45
1:C:71:THR:OG1	1:C:151:ASP:OD2	2.32	0.45
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.51	0.45
1:D:64:VAL:O	1:D:94:PHE:HB3	2.16	0.44
1:B:55:LYS:N	1:B:57:GLN:HE22	2.16	0.43
1:D:149:ASN:C	1:D:149:ASN:ND2	2.76	0.43
1:B:91:CYS:HA	1:B:192:THR:O	2.19	0.43
1:B:61:GLY:O	1:B:141:ILE:HA	2.19	0.43
1:C:188:GLU:C	1:C:189:GLU:HG3	2.42	0.43
1:A:38:ASP:C	1:A:38:ASP:OD1	2.62	0.42
1:C:104:THR:OG1	1:C:106:GLU:OE2	2.38	0.42
4:C:304:EDO:O1	1:D:133:ASP:OD2	2.37	0.42
1:B:81:LYS:NZ	1:B:189:GLU:OE2	2.52	0.41
1:B:17:ILE:HD12	1:B:34:THR:CG2	2.50	0.41
1:C:15:GLN:N	6:C:408:HOH:O	2.52	0.41
1:A:104:THR:HG22	1:A:107:ALA:CB	2.50	0.41
1:A:71:THR:O	1:A:73:HIS:HD2	2.04	0.40
1:D:110:LEU:HG	1:D:123:ILE:HD11	2.03	0.40
1:D:205:LYS:O	6:D:602:HOH:O	2.21	0.40
1:C:61:GLY:O	1:C:141:ILE:HA	2.21	0.40
1:D:49:VAL:O	1:D:137:SER:HA	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%)	187 (97%)	4 (2%)	1 (0%)	24	12
1	B	193/209 (92%)	189 (98%)	3 (2%)	1 (0%)	24	12
1	C	191/209 (91%)	186 (97%)	4 (2%)	1 (0%)	24	12
1	D	191/209 (91%)	180 (94%)	10 (5%)	1 (0%)	24	12
All	All	767/836 (92%)	742 (97%)	21 (3%)	4 (0%)	24	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	59	ALA
1	A	66	PRO
1	B	66	PRO
1	C	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	155/179 (87%)	152 (98%)	3 (2%)	50	28
1	B	156/179 (87%)	151 (97%)	5 (3%)	34	11
1	C	149/179 (83%)	146 (98%)	3 (2%)	48	26
1	D	154/179 (86%)	150 (97%)	4 (3%)	40	17
All	All	614/716 (86%)	599 (98%)	15 (2%)	43	19

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	38	ASP
1	A	189	GLU
1	B	31	LEU
1	B	43	THR
1	B	57	GLN
1	B	152	ASP

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Mol	Chain	Res	Type
1	B	208	ASN
1	C	31	LEU
1	C	71	THR
1	C	164	ASP
1	D	43	THR
1	D	45	THR
1	D	55	LYS
1	D	72	LEU

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	73	HIS
1	A	206	HIS
1	B	15	GLN
1	B	57	GLN
1	B	82	GLN
1	B	206	HIS
1	C	57	GLN
1	C	190	HIS
1	C	206	HIS
1	D	15	GLN
1	D	149	ASN
1	D	155	ASN
1	D	206	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	C	304	-	3,3,3	0.08	0	2,2,2	0.05	0
4	EDO	B	506	-	3,3,3	0.10	0	2,2,2	0.20	0
4	EDO	B	502	-	3,3,3	0.31	0	2,2,2	0.16	0
4	EDO	C	306	-	3,3,3	0.07	0	2,2,2	0.06	0
4	EDO	C	301	-	3,3,3	0.23	0	2,2,2	0.34	0
4	EDO	A	304	-	3,3,3	0.09	0	2,2,2	0.18	0
5	PW7	B	505	-	11,11,11	1.43	2 (18%)	16,16,16	1.46	2 (12%)
5	PW7	B	501	-	11,11,11	1.53	1 (9%)	16,16,16	1.50	3 (18%)
5	PW7	D	501	-	11,11,11	1.88	3 (27%)	16,16,16	1.22	2 (12%)
5	PW7	C	305	-	11,11,11	1.64	3 (27%)	16,16,16	1.21	2 (12%)

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	C	304	-	-	0/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	B	502	-	-	0/1/1/1	-
4	EDO	C	306	-	-	0/1/1/1	-
4	EDO	C	301	-	-	1/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
5	PW7	B	505	-	-	0/6/6/6	0/1/1/1
5	PW7	B	501	-	-	0/6/6/6	0/1/1/1
5	PW7	D	501	-	-	0/6/6/6	0/1/1/1
5	PW7	C	305	-	-	0/6/6/6	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	PW7	C2-N2	3.95	1.41	1.35
5	D	501	PW7	C2-N2	3.66	1.40	1.35
5	B	505	PW7	C2-N2	3.50	1.40	1.35
5	D	501	PW7	C2-N	3.23	1.41	1.35
5	C	305	PW7	C2-N	3.14	1.40	1.35
5	C	305	PW7	C2-N2	2.89	1.39	1.35
5	B	505	PW7	C2-N	2.37	1.39	1.35
5	D	501	PW7	C2-N1	2.30	1.38	1.33
5	C	305	PW7	C-C1	2.20	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	PW7	C2-N-C1	-4.20	113.54	117.08
5	B	505	PW7	C2-N-C1	-3.86	113.82	117.08
5	C	305	PW7	C2-N-C1	-3.26	114.33	117.08
5	D	501	PW7	C2-N-C1	-3.09	114.47	117.08
5	B	505	PW7	C4-C1-N	2.98	126.30	122.29
5	B	501	PW7	C4-C1-N	2.86	126.14	122.29
5	D	501	PW7	C4-C1-N	2.62	125.82	122.29
5	B	501	PW7	C4-C1-C	-2.19	117.90	120.98
5	C	305	PW7	C4-C1-N	2.02	125.01	122.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	304	EDO	1	0
4	B	502	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.96	31 (15%) 5 6	15, 30, 53, 63	14 (7%)
1	B	195/209 (93%)	1.14	41 (21%) 2 3	14, 34, 59, 71	17 (8%)
1	C	193/209 (92%)	1.51	59 (30%) 1 1	23, 35, 58, 70	25 (12%)
1	D	194/209 (92%)	1.92	67 (34%) 1 1	12, 38, 64, 74	25 (12%)
All	All	776/836 (92%)	1.38	198 (25%) 1 2	12, 34, 59, 74	81 (10%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	ALA	10.9
1	A	14	LYS	10.1
1	D	72	LEU	10.1
1	A	191	LEU	9.7
1	D	71	THR	8.5
1	B	152	ASP	7.6
1	C	164	ASP	7.5
1	A	56	GLU	7.4
1	A	42	LYS	7.1
1	C	58	THR	7.1
1	C	43	THR	6.9
1	D	70	ARG	6.7
1	A	33	LYS	6.7
1	A	188	GLU	6.4
1	B	180	GLN	6.4
1	A	70	ARG	6.2
1	A	58	THR	6.2
1	D	58	THR	6.2
1	D	154	GLU	6.1
1	C	26	GLY	6.0
1	D	29	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	28	TRP	5.8
1	B	58	THR	5.8
1	C	31	LEU	5.8
1	C	29	VAL	5.8
1	D	120	LYS	5.8
1	C	16	TYR	5.8
1	B	205	LYS	5.7
1	D	74	TYR	5.6
1	B	46	TRP	5.6
1	D	208	ASN	5.6
1	C	55	LYS	5.6
1	A	190	HIS	5.5
1	C	23	ILE	5.4
1	D	56	GLU	5.3
1	C	57	GLN	5.2
1	B	54	ARG	5.1
1	B	56	GLU	5.1
1	B	208	ASN	5.1
1	A	28	TRP	5.0
1	C	136	LEU	5.0
1	C	56	GLU	5.0
1	B	55	LYS	4.9
1	C	17	ILE	4.8
1	B	39	PRO	4.8
1	B	31	LEU	4.7
1	D	57	GLN	4.7
1	A	189	GLU	4.7
1	A	72	LEU	4.6
1	B	40	THR	4.6
1	C	18	ILE	4.6
1	D	59	ALA	4.4
1	D	122	ASP	4.4
1	D	31	LEU	4.4
1	D	28	TRP	4.3
1	D	158	PRO	4.2
1	D	114	GLU	4.2
1	C	34	THR	4.2
1	D	55	LYS	4.1
1	B	57	GLN	4.1
1	D	167	PHE	4.1
1	D	156	ALA	4.0
1	D	53	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	16	TYR	4.0
1	A	41	GLY	3.7
1	C	207	ALA	3.7
1	D	97	GLY	3.7
1	C	37	MET	3.7
1	D	148	ILE	3.6
1	B	38	ASP	3.6
1	C	184	ALA	3.6
1	C	22	LEU	3.6
1	A	157	ARG	3.6
1	D	52	THR	3.6
1	D	23	ILE	3.5
1	B	163	GLY	3.5
1	D	100	ASP	3.5
1	B	102	GLY	3.4
1	C	45	THR	3.4
1	B	28	TRP	3.4
1	B	160	PRO	3.4
1	B	153	ALA	3.4
1	D	54	ARG	3.4
1	C	168	VAL	3.3
1	B	162	PRO	3.3
1	B	196	ARG	3.3
1	C	30	LYS	3.3
1	B	176	ASN	3.2
1	C	104	THR	3.2
1	B	191	LEU	3.2
1	D	155	ASN	3.2
1	C	187	ALA	3.2
1	D	101	ASP	3.2
1	C	39	PRO	3.1
1	A	167	PHE	3.1
1	D	152	ASP	3.1
1	C	59	ALA	3.1
1	C	41	GLY	3.0
1	D	196[A]	ARG	3.0
1	C	21	GLU	3.0
1	C	161	LYS	3.0
1	B	157	ARG	3.0
1	B	158	PRO	3.0
1	D	160	PRO	3.0
1	C	19	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	44	ARG	2.9
1	C	51	ARG	2.9
1	C	40	THR	2.9
1	D	149	ASN	2.9
1	C	97	GLY	2.9
1	C	165	GLY	2.9
1	B	104	THR	2.8
1	D	25	GLU	2.8
1	D	14	LYS	2.8
1	A	57	GLN	2.8
1	C	35	THR	2.8
1	C	53	THR	2.8
1	B	167	PHE	2.8
1	D	73	HIS	2.8
1	B	14	LYS	2.8
1	D	102	GLY	2.8
1	C	27	LYS	2.8
1	B	101	ASP	2.8
1	D	163	GLY	2.8
1	C	188	GLU	2.7
1	D	168	VAL	2.7
1	A	23	ILE	2.7
1	A	22	LEU	2.7
1	A	40	THR	2.7
1	D	113	LEU	2.7
1	B	159	LYS	2.6
1	D	88	GLY	2.6
1	D	164	ASP	2.6
1	C	25	GLU	2.6
1	A	158	PRO	2.6
1	A	163	GLY	2.6
1	D	22	LEU	2.6
1	A	160	PRO	2.6
1	A	104	THR	2.5
1	A	27	LYS	2.5
1	C	49	VAL	2.5
1	C	92	ILE	2.5
1	B	42	LYS	2.5
1	D	119	TYR	2.5
1	D	104	THR	2.5
1	C	102	GLY	2.5
1	D	27	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	162	PRO	2.4
1	D	184	ALA	2.4
1	C	42	LYS	2.4
1	B	190	HIS	2.4
1	C	153	ALA	2.4
1	C	36	TYR	2.4
1	D	18	ILE	2.4
1	C	52	THR	2.4
1	C	46	TRP	2.4
1	A	25	GLU	2.4
1	A	39	PRO	2.3
1	D	43	THR	2.3
1	C	33	LYS	2.3
1	D	107	ALA	2.3
1	B	161	LYS	2.3
1	D	68	LEU	2.3
1	B	155	ASN	2.3
1	C	54	ARG	2.3
1	D	83	PHE	2.3
1	B	165	GLY	2.3
1	D	26	GLY	2.3
1	D	41	GLY	2.3
1	B	168	VAL	2.3
1	D	49	VAL	2.3
1	B	22	LEU	2.2
1	A	162	PRO	2.2
1	D	40	THR	2.2
1	C	139	CYS	2.2
1	B	18	ILE	2.2
1	A	71	THR	2.2
1	D	105	PRO	2.2
1	D	24	SER	2.2
1	B	150	GLY	2.2
1	C	32	GLU	2.1
1	C	156	ALA	2.1
1	D	110	LEU	2.1
1	A	55	LYS	2.1
1	C	47	GLU	2.1
1	C	189	GLU	2.1
1	B	23	ILE	2.1
1	A	187	ALA	2.1
1	D	146	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	190	HIS	2.1
1	C	90	TYR	2.1
1	D	90	TYR	2.1
1	D	150	GLY	2.0
1	C	191	LEU	2.0
1	D	123	ILE	2.0
1	A	156	ALA	2.0
1	B	29	VAL	2.0
1	D	33	LYS	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(Å ²)	Q<0.9
2	MG	B	504	1/1	0.64	0.17	70,70,70,70	0
5	PW7	D	501	11/11	0.80	0.18	40,48,65,66	11
4	EDO	C	301	4/4	0.83	0.14	36,47,49,60	0
4	EDO	C	304	4/4	0.86	0.14	37,37,38,39	4
5	PW7	C	305	11/11	0.86	0.14	36,42,55,58	11
4	EDO	B	506	4/4	0.86	0.15	26,29,29,30	4
5	PW7	B	501	11/11	0.87	0.14	35,39,51,51	11
4	EDO	A	304	4/4	0.87	0.12	30,33,34,34	0
4	EDO	C	306	4/4	0.87	0.12	33,36,36,38	4
5	PW7	B	505	11/11	0.88	0.15	28,31,38,41	11
2	MG	A	302	1/1	0.89	0.08	52,52,52,52	0
4	EDO	B	502	4/4	0.89	0.12	45,45,48,48	0
3	CL	A	303	1/1	0.90	0.20	67,67,67,67	0
2	MG	C	302	1/1	0.95	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	503	1/1	0.96	0.06	45,45,45,45	0
2	MG	A	301	1/1	0.97	0.08	33,33,33,33	0
2	MG	B	503	1/1	0.97	0.04	34,34,34,34	0
2	MG	C	303	1/1	0.98	0.06	34,34,34,34	0
2	MG	D	502	1/1	0.99	0.06	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.