



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:57 PM UTC

PDB ID : 5QJ7 / pdb_00005qj7
Title : PanDDA analysis group deposition of models with modelled events (e.g. bound ligands) – Crystal Structure of NUDT5 in complex with Z32327641
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 : 2018-10-31
Resolution : 1.56 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

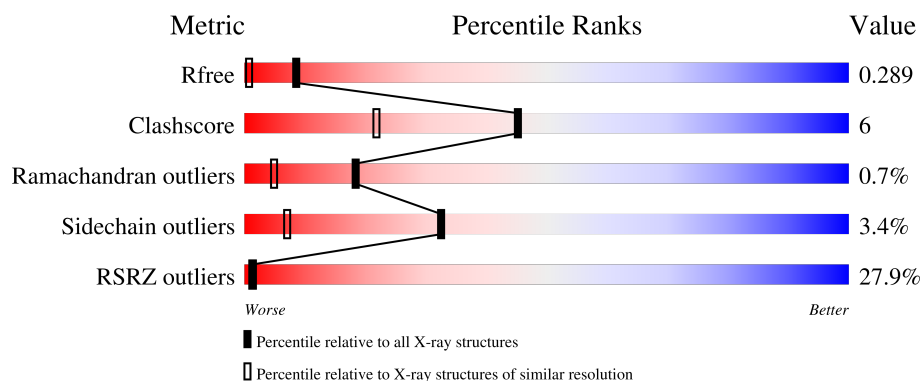
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	13% 82% 10% 7%
1	B	209	17% 78% 14% 7%
1	C	209	29% 78% 11% 8%
1	D	209	44% 70% 20% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6140 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
			1466	927	245	286	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
			1412	890	238	277	7			
1	D	190	Total	C	N	O	S	0	1	0
			1415	897	236	274	8			

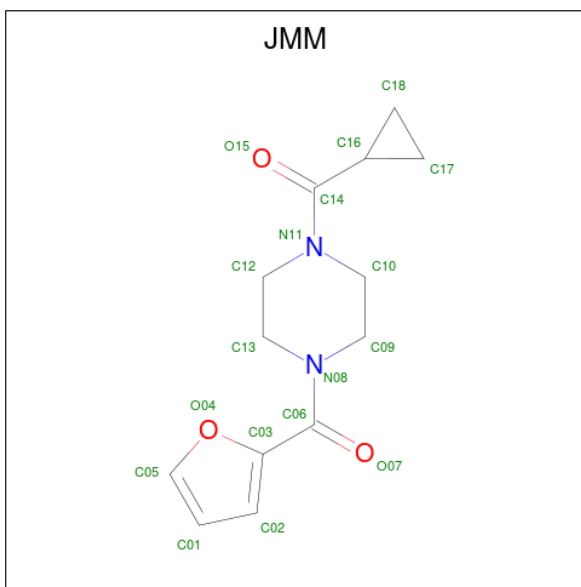
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UUKK9
B	0	SER	-	expression tag	UNP Q9UUKK9
C	0	SER	-	expression tag	UNP Q9UUKK9
D	0	SER	-	expression tag	UNP Q9UUKK9

- 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 [4-(cyclopropanecarbonyl)piperazin-1-yl](furan-2-yl)methanone (CCD ID: JMM) (formula: C₁₃H₁₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	13	2	3		
3	A	1	Total	C	N	O	0	0
			18	13	2	3		
3	C	1	Total	C	N	O	0	0
			18	13	2	3		
3	D	1	Total	C	N	O	0	0
			18	13	2	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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	D	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

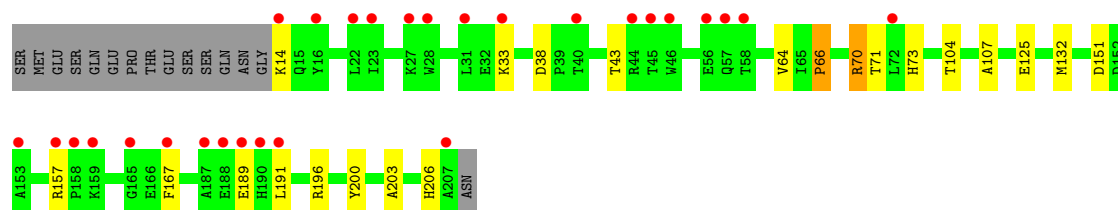
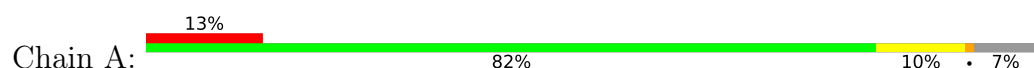
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	77	Total O 77 77	0	0
6	B	74	Total O 74 74	0	0
6	C	83	Total O 83 83	0	0
6	D	44	Total O 44 44	0	0

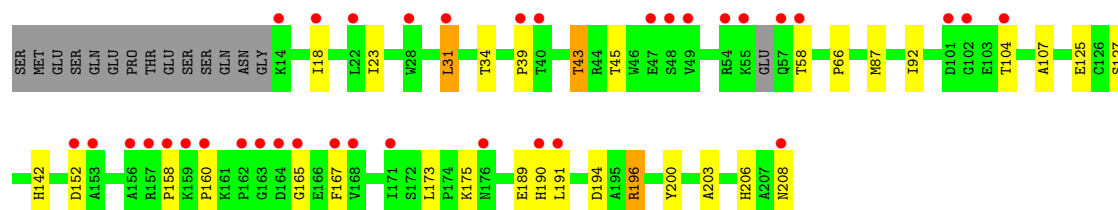
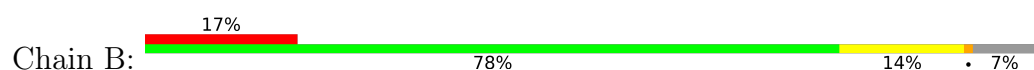
3 Residue-property plots [i](#)

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.

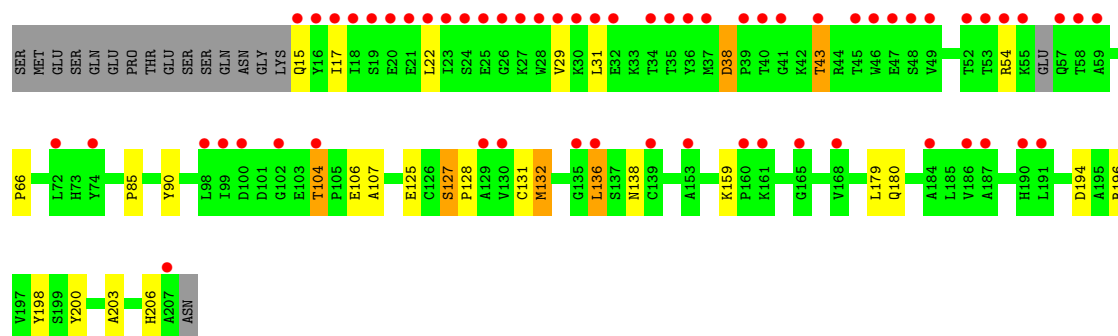
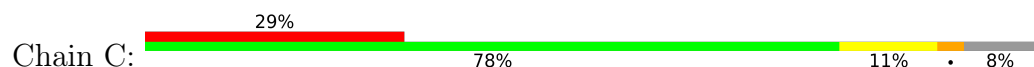
- Molecule 1: ADP-sugar pyrophosphatase



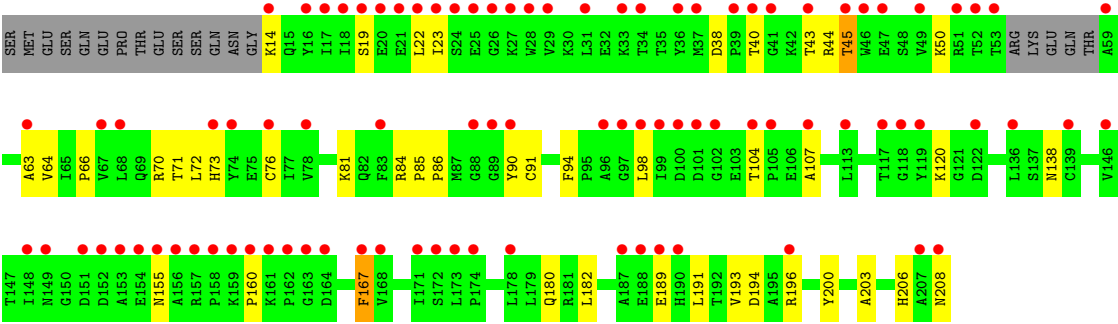
- Molecule 1: ADP-sugar pyrophosphatase



- 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	49.34Å 59.79Å 79.91Å 79.38° 81.48° 75.77°	Depositor
Resolution (Å)	78.08 – 1.56 78.08 – 1.56	Depositor EDS
% Data completeness (in resolution range)	94.9 (78.08-1.56) 94.9 (78.08-1.56)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.237 , 0.274 0.255 , 0.289	Depositor DCC
R_{free} test set	6244 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6140	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, JMM, 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	1.27	0/1494	1.17	2/2037 (0.1%)
1	B	1.23	3/1492 (0.2%)	1.18	2/2035 (0.1%)
1	C	1.32	4/1439 (0.3%)	1.25	10/1969 (0.5%)
1	D	1.33	3/1443 (0.2%)	1.22	7/1973 (0.4%)
All	All	1.29	10/5868 (0.2%)	1.21	21/8014 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	ARG	C-O	-6.71	1.18	1.24
1	D	182	LEU	CA-C	-6.49	1.44	1.52
1	C	104	THR	CA-C	6.01	1.59	1.53
1	C	180	GLN	C-O	-5.99	1.17	1.24
1	D	138	ASN	CA-C	-5.18	1.45	1.52
1	B	196	ARG	NE-CZ	5.18	1.38	1.33
1	C	159	LYS	C-O	-5.12	1.20	1.25
1	B	127	SER	C-O	-5.10	1.17	1.23
1	B	173	LEU	CA-C	-5.09	1.48	1.52
1	C	29	VAL	N-CA	5.08	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	GLU	N-CA-C	7.50	120.48	109.07
1	A	157	ARG	CA-C-N	7.41	127.84	119.83
1	A	157	ARG	C-N-CA	7.41	127.84	119.83
1	C	85	PRO	N-CA-C	7.26	119.56	110.70
1	D	85	PRO	N-CA-C	7.23	119.52	110.70
1	C	127	SER	CA-C-N	-7.19	113.31	120.21
1	C	127	SER	C-N-CA	-7.19	113.31	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	ILE	CB-CA-C	-6.45	102.76	111.15
1	C	159	LYS	CA-C-N	-6.39	113.18	119.76
1	C	159	LYS	C-N-CA	-6.39	113.18	119.76
1	D	19	SER	N-CA-C	6.17	118.23	108.79
1	C	38	ASP	CA-C-N	6.12	125.52	118.85
1	C	38	ASP	C-N-CA	6.12	125.52	118.85
1	B	18	ILE	N-CA-C	-6.08	105.90	111.67
1	C	22	LEU	N-CA-C	5.69	117.35	109.15
1	D	138	ASN	N-CA-C	-5.45	106.21	112.92
1	D	193	VAL	N-CA-C	-5.37	100.65	108.97
1	D	45	THR	N-CA-C	5.32	116.36	108.86
1	B	43	THR	CB-CA-C	5.26	118.43	109.80
1	C	132	MET	N-CA-C	5.04	117.55	111.40
1	D	63	ALA	N-CA-C	-5.03	100.84	109.24

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	1466	0	1437	15	0
1	B	1464	0	1414	19	0
1	C	1412	0	1320	22	0
1	D	1415	0	1353	27	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	36	0	0	0	0
3	C	18	0	0	0	0
3	D	18	0	0	0	0
4	A	4	0	6	0	0
4	B	8	0	12	1	0
4	C	8	0	12	0	0
4	D	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	77	0	0	1	0
6	B	74	0	0	1	0
6	C	83	0	0	4	0
6	D	44	0	0	5	0
All	All	6140	0	5560	67	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 (67) 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:B:92:ILE:HD11	1:B:191:LEU:HD13	1.51	0.92
1:C:104:THR:HG23	1:C:107:ALA:H	1.37	0.90
1:A:70:ARG:NH1	6:A:401:HOH:O	2.07	0.87
1:D:120:LYS:H	1:D:155:ASN:HD21	1.26	0.83
1:C:125:GLU:OE1	6:C:401:HOH:O	1.97	0.82
1:B:23:ILE:HD12	1:B:31:LEU:HD22	1.69	0.75
1:B:104:THR:HG23	1:B:107:ALA:H	1.52	0.72
1:D:76:CYS:SG	6:D:418:HOH:O	2.48	0.72
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.73	0.69
1:A:104:THR:HG23	1:A:107:ALA:H	1.63	0.64
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.78	0.64
1:A:71:THR:HG23	1:A:151:ASP:OD2	1.99	0.63
1:D:104:THR:HG23	1:D:107:ALA:H	1.64	0.62
1:D:71:THR:O	1:D:73:HIS:ND1	2.37	0.56
1:C:132:MET:HE1	1:C:196:ARG:CZ	2.36	0.56
1:D:180:GLN:CB	6:D:435:HOH:O	2.54	0.54
1:A:132:MET:HE1	1:A:196:ARG:CZ	2.38	0.54
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.42	0.54
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.39	0.53
1:C:136:LEU:HD13	1:C:136:LEU:O	2.08	0.53
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.92	0.52
6:C:401:HOH:O	1:D:206:HIS:HE1	1.93	0.52
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.94	0.51
1:B:58:THR:CB	1:B:142:HIS:NE2	2.74	0.51
1:C:132:MET:O	1:D:196[B]:ARG:NH1	2.44	0.51
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.94	0.51
1:A:206:HIS:O	1:B:175:LYS:NZ	2.43	0.51
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:THR:OG1	1:C:106:GLU:OE2	2.30	0.50
1:B:189:GLU:HB3	1:B:191:LEU:HD12	1.94	0.50
1:C:136:LEU:HD13	1:C:136:LEU:C	2.39	0.48
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.97	0.48
1:C:43:THR:OG1	6:C:402:HOH:O	2.20	0.47
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.49	0.46
4:B:302:EDO:C2	6:B:401:HOH:O	2.63	0.46
1:C:127:SER:HB2	1:C:128:PRO:HD2	1.98	0.46
1:D:38:ASP:C	1:D:38:ASP:OD1	2.58	0.46
1:C:90:TYR:OH	1:D:14:LYS:HB3	2.15	0.46
1:B:158:PRO:O	1:B:160:PRO:HD3	2.16	0.45
1:D:38:ASP:OD1	1:D:40:THR:OG1	2.27	0.45
1:A:64:VAL:O	1:A:66:PRO:HD3	2.16	0.45
1:B:190:HIS:O	1:B:190:HIS:CG	2.69	0.45
1:C:138:ASN:HB3	1:D:86:PRO:O	2.17	0.45
1:A:206:HIS:HE1	1:B:125:GLU:OE1	1.99	0.45
1:D:44:ARG:NH1	6:D:404:HOH:O	2.42	0.45
1:C:104:THR:HG23	1:C:107:ALA:N	2.19	0.45
1:B:194:ASP:CG	1:B:196:ARG:HH21	2.24	0.45
1:C:131:CYS:SG	1:D:194:ASP:HA	2.57	0.44
1:A:104:THR:CG2	1:A:107:ALA:H	2.27	0.44
1:C:38:ASP:HB2	1:D:167:PHE:CE2	2.53	0.43
1:A:71:THR:O	1:A:73:HIS:HD2	2.02	0.43
1:D:208:ASN:ND2	6:D:407:HOH:O	2.51	0.43
1:B:165:GLY:O	1:B:167:PHE:CE1	2.72	0.42
1:D:194:ASP:OD1	1:D:196[A]:ARG:HD3	2.20	0.42
1:C:15:GLN:N	6:C:407:HOH:O	2.51	0.42
1:D:22:LEU:HD23	1:D:23:ILE:N	2.35	0.42
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.55	0.42
1:B:87:MET:HE3	1:B:87:MET:HB3	1.86	0.41
1:B:92:ILE:HG13	1:B:191:LEU:HD22	2.02	0.41
1:D:64:VAL:O	1:D:94:PHE:HB3	2.19	0.41
1:B:34:THR:O	1:B:45:THR:HA	2.21	0.41
1:A:38:ASP:OD1	1:A:38:ASP:C	2.62	0.41
1:D:98:LEU:HD21	4:D:304:EDO:H11	2.03	0.41
1:A:167:PHE:CZ	1:B:39:PRO:HD2	2.56	0.41
1:D:90:TYR:O	6:D:401:HOH:O	2.22	0.41
1:D:81:LYS:HA	1:D:91:CYS:O	2.20	0.40
1:D:191:LEU:HD12	1:D:191:LEU:C	2.47	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	192/209 (92%)	186 (97%)	5 (3%)	1 (0%)	24	8
1	B	190/209 (91%)	185 (97%)	4 (2%)	1 (0%)	24	8
1	C	188/209 (90%)	183 (97%)	4 (2%)	1 (0%)	24	8
1	D	187/209 (90%)	181 (97%)	4 (2%)	2 (1%)	11	2
All	All	757/836 (91%)	735 (97%)	17 (2%)	5 (1%)	18	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	160	PRO
1	C	66	PRO
1	A	66	PRO
1	B	66	PRO
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	155/179 (87%)	149 (96%)	6 (4%)	28	5
1	B	154/179 (86%)	150 (97%)	4 (3%)	40	13
1	C	141/179 (79%)	137 (97%)	4 (3%)	38	11
1	D	145/179 (81%)	139 (96%)	6 (4%)	27	4
All	All	595/716 (83%)	575 (97%)	20 (3%)	32	7

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	33	LYS
1	A	43	THR
1	A	70	ARG
1	A	189	GLU
1	A	191	LEU
1	B	31	LEU
1	B	43	THR
1	B	152	ASP
1	B	208	ASN
1	C	31	LEU
1	C	43	THR
1	C	54	ARG
1	C	136	LEU
1	D	43	THR
1	D	45	THR
1	D	50	LYS
1	D	70	ARG
1	D	72	LEU
1	D	167	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	180	GLN
1	A	206	HIS
1	B	15	GLN
1	B	69	GLN
1	B	206	HIS
1	C	206	HIS
1	D	149	ASN
1	D	155	ASN
1	D	206	HIS
1	D	208	ASN

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	301	-	3,3,3	0.46	0	2,2,2	0.70	0
4	EDO	B	302	-	3,3,3	0.80	0	2,2,2	0.36	0
4	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.36	0
4	EDO	D	304	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	A	305	-	3,3,3	0.64	0	2,2,2	0.38	0
3	JMM	A	304	-	20,20,20	2.36	4 (20%)	27,28,28	0.91	1 (3%)
3	JMM	D	303	-	20,20,20	2.44	2 (10%)	27,28,28	1.27	4 (14%)
3	JMM	C	304	-	20,20,20	1.61	2 (10%)	27,28,28	1.49	3 (11%)
4	EDO	C	305	-	3,3,3	0.54	0	2,2,2	0.54	0
3	JMM	A	303	-	20,20,20	1.97	3 (15%)	27,28,28	1.49	6 (22%)

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	301	-	-	0/1/1/1	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	D	304	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	305	-	-	0/1/1/1	-
3	JMM	A	304	-	-	5/16/28/28	0/3/3/3
3	JMM	D	303	-	-	2/16/28/28	0/3/3/3
3	JMM	C	304	-	-	8/16/28/28	0/3/3/3
4	EDO	C	305	-	-	0/1/1/1	-
3	JMM	A	303	-	-	2/16/28/28	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	303	JMM	C14-N11	8.72	1.47	1.35
3	A	304	JMM	C14-N11	6.73	1.44	1.35
3	A	303	JMM	C14-N11	6.67	1.44	1.35
3	A	304	JMM	C06-N08	5.89	1.45	1.34
3	D	303	JMM	C06-N08	5.12	1.43	1.34
3	C	304	JMM	C06-N08	4.19	1.42	1.34
3	C	304	JMM	C14-N11	3.89	1.40	1.35
3	A	303	JMM	C06-N08	3.63	1.41	1.34
3	A	304	JMM	C16-C14	-3.09	1.47	1.51
3	A	303	JMM	C13-N08	2.70	1.51	1.47
3	A	304	JMM	C13-N08	2.43	1.51	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	JMM	C09-N08-C13	3.94	120.73	112.68
3	C	304	JMM	C16-C14-N11	-3.87	115.16	118.80
3	A	303	JMM	C12-N11-C10	-3.18	106.19	112.68
3	C	304	JMM	C09-C10-N11	-3.01	104.43	110.42
3	D	303	JMM	C16-C14-N11	2.99	121.62	118.80
3	C	304	JMM	O15-C14-C16	2.90	125.13	120.86
3	D	303	JMM	C10-C09-N08	2.83	116.05	110.42
3	A	303	JMM	O07-C06-N08	-2.56	118.62	122.67
3	A	303	JMM	C12-C13-N08	2.38	115.15	110.42
3	A	304	JMM	C12-C13-N08	2.31	115.00	110.42
3	D	303	JMM	O15-C14-N11	-2.29	118.88	121.61
3	A	303	JMM	C10-N11-C14	-2.07	115.53	123.30
3	D	303	JMM	C09-C10-N11	2.05	114.50	110.42
3	A	303	JMM	C10-C09-N08	2.03	114.45	110.42

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	304	JMM	O15-C14-N11-C12
3	C	304	JMM	C16-C14-N11-C12
3	C	304	JMM	N11-C14-C16-C18
3	C	304	JMM	O15-C14-C16-C18
3	D	303	JMM	O15-C14-N11-C12
3	D	303	JMM	C16-C14-N11-C12
3	C	304	JMM	O15-C14-N11-C10
3	C	304	JMM	C16-C14-N11-C10
3	A	303	JMM	C16-C14-N11-C12
3	A	303	JMM	O15-C14-N11-C12
3	A	304	JMM	O15-C14-N11-C10
4	D	304	EDO	O1-C1-C2-O2
3	A	304	JMM	O15-C14-C16-C18
3	A	304	JMM	N11-C14-C16-C18
3	A	304	JMM	C16-C14-N11-C10
3	C	304	JMM	O07-C06-N08-C09
3	A	304	JMM	O07-C06-N08-C13
3	C	304	JMM	C03-C06-N08-C09

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	EDO	1	0
4	D	304	EDO	1	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%)	0.87	28 (14%) 6 7	16, 27, 50, 59	13 (6%)
1	B	194/209 (92%)	1.04	35 (18%) 3 4	18, 31, 53, 71	6 (3%)
1	C	192/209 (91%)	1.45	61 (31%) 1 1	18, 33, 56, 64	8 (4%)
1	D	190/209 (90%)	2.38	91 (47%) 0 0	11, 36, 56, 75	19 (10%)
All	All	770/836 (92%)	1.43	215 (27%) 1 1	11, 32, 55, 75	46 (5%)

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	PRO	11.7
1	D	207	ALA	11.3
1	D	160	PRO	10.8
1	D	157	ARG	8.9
1	A	190	HIS	8.4
1	B	28	TRP	8.1
1	D	161	LYS	8.0
1	D	16	TYR	7.9
1	D	208	ASN	7.7
1	B	208	ASN	7.6
1	B	152	ASP	7.5
1	A	58	THR	7.5
1	C	28	TRP	7.2
1	C	23	ILE	7.0
1	D	37	MET	6.8
1	D	97	GLY	6.5
1	D	159	LYS	6.4
1	D	29	VAL	6.3
1	A	28	TRP	6.2
1	A	57	GLN	6.2
1	A	188	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	190	HIS	5.9
1	B	49	VAL	5.8
1	C	18	ILE	5.5
1	C	16	TYR	5.5
1	C	54	ARG	5.4
1	A	56	GLU	5.3
1	C	22	LEU	5.2
1	D	188	GLU	5.2
1	D	23	ILE	5.0
1	A	189	GLU	5.0
1	D	28	TRP	5.0
1	C	40	THR	4.9
1	D	74	TYR	4.8
1	C	58	THR	4.8
1	D	189	GLU	4.7
1	D	18	ILE	4.6
1	D	153	ALA	4.6
1	A	27	LYS	4.5
1	D	90	TYR	4.4
1	D	154	GLU	4.3
1	A	167	PHE	4.3
1	B	48	SER	4.2
1	D	88	GLY	4.2
1	C	25	GLU	4.2
1	D	168	VAL	4.2
1	D	26	GLY	4.1
1	D	167	PHE	4.0
1	D	196[A]	ARG	4.0
1	C	26	GLY	3.9
1	C	31	LEU	3.9
1	D	22	LEU	3.9
1	B	47	GLU	3.9
1	C	160	PRO	3.9
1	C	35	THR	3.9
1	D	152	ASP	3.9
1	D	173	LEU	3.8
1	C	46	TRP	3.8
1	B	163	GLY	3.8
1	A	72	LEU	3.7
1	D	96	ALA	3.7
1	D	151	ASP	3.7
1	D	27	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	58	THR	3.5
1	D	40	THR	3.5
1	A	46	TRP	3.5
1	D	31	LEU	3.5
1	B	176	ASN	3.5
1	A	157	ARG	3.4
1	D	155	ASN	3.4
1	D	46	TRP	3.4
1	D	101	ASP	3.4
1	C	43	THR	3.4
1	D	68	LEU	3.4
1	D	171	ILE	3.3
1	D	149	ASN	3.3
1	C	139	CYS	3.3
1	D	104	THR	3.3
1	D	21	GLU	3.3
1	A	207	ALA	3.3
1	C	207	ALA	3.3
1	D	164	ASP	3.3
1	D	14	LYS	3.3
1	C	190	HIS	3.2
1	B	101	ASP	3.2
1	D	49	VAL	3.2
1	C	74	TYR	3.2
1	D	156	ALA	3.2
1	B	22	LEU	3.2
1	C	104	THR	3.1
1	B	190	HIS	3.1
1	D	119	TYR	3.1
1	B	40	THR	3.1
1	A	31	LEU	3.1
1	D	148	ILE	3.1
1	B	165	GLY	3.0
1	C	53	THR	3.0
1	A	33	LYS	3.0
1	C	29	VAL	3.0
1	C	47	GLU	3.0
1	D	83	PHE	3.0
1	C	48	SER	3.0
1	B	18	ILE	3.0
1	D	43	THR	3.0
1	C	27	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	53	THR	2.9
1	D	17	ILE	2.9
1	D	33	LYS	2.9
1	A	45	THR	2.9
1	D	139	CYS	2.9
1	C	59	ALA	2.9
1	B	191	LEU	2.9
1	D	76	CYS	2.9
1	B	156	ALA	2.8
1	D	47	GLU	2.8
1	C	34	THR	2.8
1	C	98	LEU	2.8
1	D	98	LEU	2.8
1	C	129	ALA	2.8
1	C	17	ILE	2.8
1	D	41	GLY	2.8
1	D	122	ASP	2.8
1	C	136	LEU	2.8
1	C	187	ALA	2.8
1	A	14	LYS	2.8
1	D	34	THR	2.8
1	A	16	TYR	2.8
1	C	36	TYR	2.8
1	C	39	PRO	2.8
1	C	168	VAL	2.7
1	D	99	ILE	2.7
1	B	14	LYS	2.7
1	C	161	LYS	2.7
1	D	73	HIS	2.7
1	C	186	VAL	2.7
1	C	102	GLY	2.7
1	C	24	SER	2.7
1	D	36	TYR	2.7
1	C	49	VAL	2.7
1	C	57	GLN	2.7
1	A	40	THR	2.6
1	D	102	GLY	2.6
1	B	167	PHE	2.6
1	B	31	LEU	2.6
1	C	19	SER	2.6
1	B	157	ARG	2.6
1	A	191	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	159	LYS	2.6
1	B	39	PRO	2.6
1	D	118	GLY	2.6
1	C	184	ALA	2.5
1	D	52	THR	2.5
1	C	99	ILE	2.5
1	B	102	GLY	2.5
1	C	130	VAL	2.5
1	D	146	VAL	2.5
1	C	55	LYS	2.5
1	D	59	ALA	2.5
1	D	107	ALA	2.5
1	C	165	GLY	2.5
1	B	162	PRO	2.5
1	D	162	PRO	2.5
1	D	174	PRO	2.5
1	C	45	THR	2.5
1	B	153	ALA	2.4
1	C	21	GLU	2.4
1	C	135	GLY	2.4
1	D	39	PRO	2.4
1	C	100	ASP	2.4
1	B	104	THR	2.4
1	D	45	THR	2.4
1	C	191	LEU	2.4
1	A	153	ALA	2.4
1	C	41	GLY	2.4
1	D	187	ALA	2.3
1	D	67	VAL	2.3
1	B	160	PRO	2.3
1	C	52	THR	2.3
1	D	117	THR	2.3
1	D	136	LEU	2.3
1	B	164	ASP	2.3
1	A	158	PRO	2.3
1	D	24	SER	2.3
1	C	153	ALA	2.3
1	D	19	SER	2.3
1	D	51	ARG	2.3
1	D	20	GLU	2.3
1	D	100	ASP	2.2
1	D	89	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	159	LYS	2.2
1	B	171	ILE	2.2
1	D	78	VAL	2.2
1	C	72	LEU	2.2
1	B	54	ARG	2.2
1	A	23	ILE	2.1
1	A	165	GLY	2.1
1	A	44	ARG	2.1
1	D	172	SER	2.1
1	C	32	GLU	2.1
1	B	55	LYS	2.1
1	D	63	ALA	2.1
1	D	178	LEU	2.1
1	D	25	GLU	2.1
1	C	37	MET	2.1
1	B	57	GLN	2.1
1	D	163	GLY	2.1
1	B	158	PRO	2.1
1	A	187	ALA	2.1
1	C	20	GLU	2.1
1	D	105	PRO	2.1
1	B	168	VAL	2.0
1	C	30	LYS	2.0
1	C	15	GLN	2.0
1	A	22	LEU	2.0
1	D	113	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
4	EDO	D	304	4/4	0.76	0.19	36,39,39,42	4
3	JMM	C	304	18/18	0.77	0.19	39,44,54,55	18
4	EDO	B	302	4/4	0.81	0.13	40,43,46,47	0
3	JMM	D	303	18/18	0.84	0.22	37,43,58,61	18
4	EDO	C	301	4/4	0.86	0.12	35,46,50,52	0
2	MG	B	304	1/1	0.86	0.25	80,80,80,80	0
2	MG	C	302	1/1	0.88	0.13	46,46,46,46	0
5	CL	B	301	1/1	0.88	0.17	65,65,65,65	0
3	JMM	A	303	18/18	0.90	0.17	24,30,36,39	18
2	MG	D	301	1/1	0.92	0.05	30,30,30,30	0
3	JMM	A	304	18/18	0.92	0.12	28,38,51,54	18
4	EDO	C	305	4/4	0.93	0.11	35,35,35,36	0
4	EDO	A	305	4/4	0.95	0.08	23,26,27,28	0
2	MG	A	302	1/1	0.95	0.11	45,45,45,45	0
4	EDO	B	305	4/4	0.96	0.10	25,26,26,26	4
2	MG	D	302	1/1	0.97	0.12	37,37,37,37	0
2	MG	C	303	1/1	0.97	0.06	36,36,36,36	0
2	MG	B	303	1/1	0.98	0.04	29,29,29,29	0
2	MG	A	301	1/1	0.99	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.