



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:13 AM EDT

PDB ID : 5QJB / pdb_00005qjb
Title : PanDDA analysis group deposition of models with modelled events (e.g. bound ligands) – Crystal Structure of NUDT5 in complex with Z1787627869
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 : 1.66 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

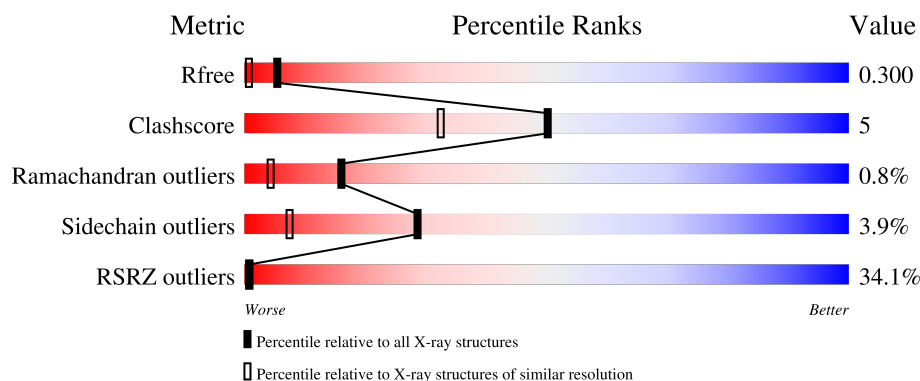
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	18% 86% 7% 7%
1	B	209	11% 86% 6% 7%
1	C	209	35% 79% 11% 8%
1	D	209	61% 76% 14% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6070 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	1	0
			1469	931	244	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
			1416	893	239	277	7			
1	D	189	Total	C	N	O	S	0	1	0
			1399	885	235	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

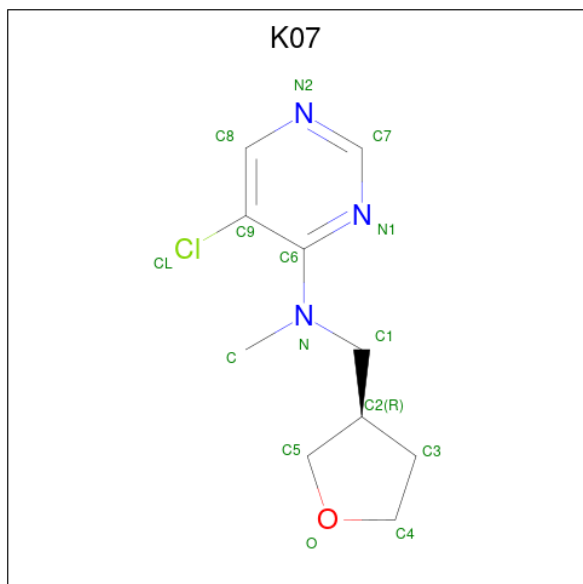
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 5-chloro-N-methyl-N-{[(3R)-oxolan-3-yl]methyl}pyrimidin-4-amine (CCD ID: K07) (formula: C₁₀H₁₄ClN₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			15	10	1	3	1		
4	A	1	Total	C	Cl	N	O	0	0
			15	10	1	3	1		
4	C	1	Total	C	Cl	N	O	0	0
			15	10	1	3	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

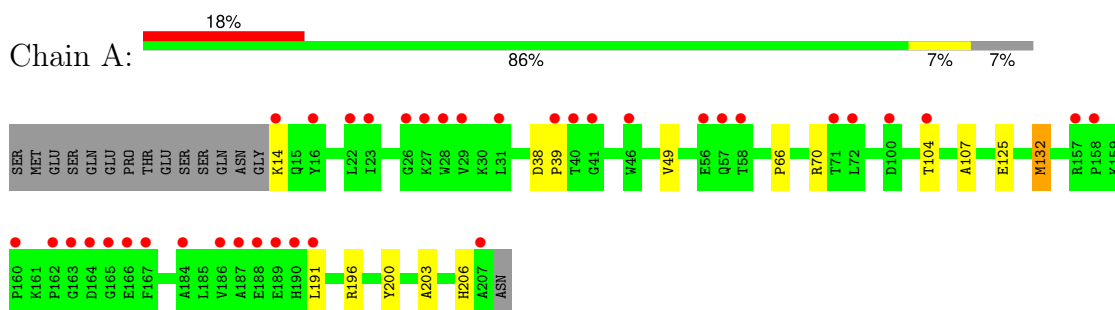
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	0
			80	80		
6	B	75	Total	O	0	0
			75	75		
6	C	74	Total	O	0	0
			74	74		
6	D	27	Total	O	0	0
			27	27		

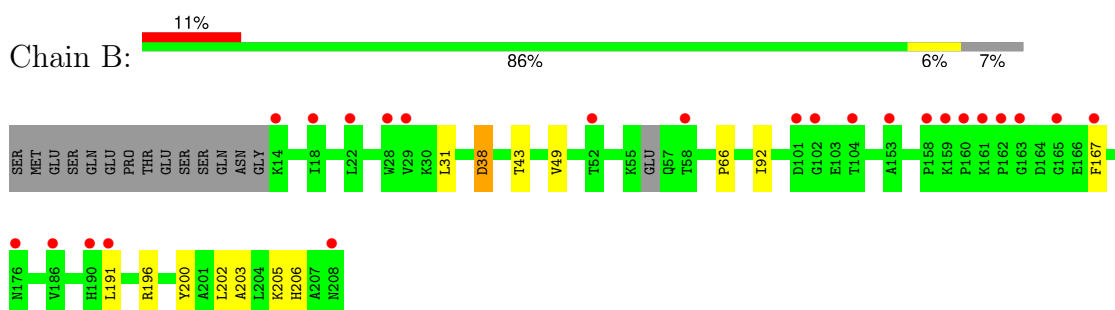
3 Residue-property plots [i](#)

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.

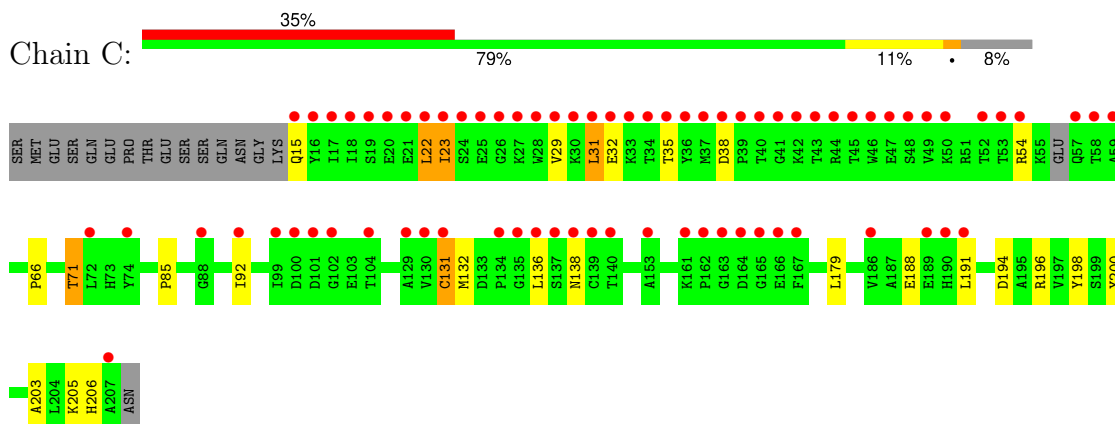
- Molecule 1: ADP-sugar pyrophosphatase



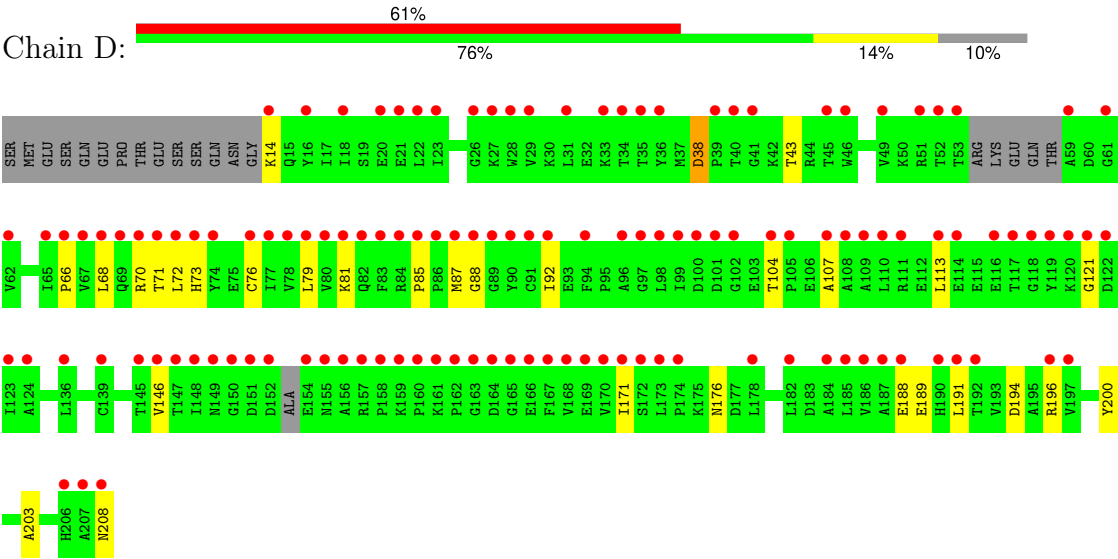
- Molecule 1: ADP-sugar pyrophosphatase



- 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	49.60Å 60.13Å 79.86Å 79.31° 80.90° 75.37°	Depositor
Resolution (Å)	77.93 – 1.66 77.93 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.8 (77.93-1.66) 95.9 (77.93-1.66)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.250 , 0.291 0.265 , 0.300	Depositor DCC
R_{free} test set	5199 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.6	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	0.94	EDS
Total number of atoms	6070	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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, EDO, MG, K07

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	1.06	0/1498	1.02	1/2044 (0.0%)
1	B	0.94	0/1492	1.01	1/2035 (0.0%)
1	C	1.06	1/1443 (0.1%)	1.12	5/1973 (0.3%)
1	D	1.03	0/1424	1.18	4/1943 (0.2%)
All	All	1.03	1/5857 (0.0%)	1.09	11/7995 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	CYS	CA-CB	5.27	1.61	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	GLU	N-CA-C	16.29	129.63	110.41
1	D	85	PRO	N-CA-C	9.70	122.54	110.70
1	C	38	ASP	CA-C-N	5.48	125.14	119.05
1	C	38	ASP	C-N-CA	5.48	125.14	119.05
1	C	71	THR	CB-CA-C	-5.47	101.71	110.79
1	D	176	ASN	N-CA-C	5.39	119.35	112.34
1	A	132	MET	N-CA-C	5.37	116.94	111.14
1	D	188	GLU	N-CA-C	5.31	119.72	112.88
1	C	85	PRO	N-CA-C	5.23	117.08	110.70
1	C	188	GLU	N-CA-C	5.16	118.72	112.23
1	B	202	LEU	N-CA-C	5.11	116.53	111.07

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	1469	0	1428	14	0
1	B	1464	0	1414	13	0
1	C	1416	0	1331	25	0
1	D	1399	0	1339	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	1	0	0	0	0
4	A	30	0	0	0	0
4	C	15	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
6	A	80	0	0	0	0
6	B	75	0	0	0	1
6	C	74	0	0	1	0
6	D	27	0	0	0	1
All	All	6070	0	5530	60	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 5.

All (60) 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:C:22:LEU:HD13	1:C:23:ILE:N	1.50	1.24
1:D:196[B]:ARG:HH21	1:D:196[B]:ARG:CG	1.49	1.22
1:C:22:LEU:HD13	1:C:22:LEU:C	1.75	1.11
1:D:196[B]:ARG:HG3	1:D:196[B]:ARG:NH2	1.56	1.00
1:D:196[B]:ARG:HH21	1:D:196[B]:ARG:HG3	0.72	0.89
1:C:22:LEU:C	1:C:22:LEU:CD1	2.48	0.84
1:C:31:LEU:HD23	1:C:32:GLU:H	1.47	0.80
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.63	0.78
1:C:22:LEU:CD1	1:C:23:ILE:N	2.43	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:N	2.36	0.73
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.71	0.72
1:C:22:LEU:HD13	1:C:23:ILE:CA	2.20	0.72
1:C:131:CYS:SG	1:D:194:ASP:HA	2.31	0.69
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:CB	2.57	0.67
1:D:196[B]:ARG:CG	1:D:196[B]:ARG:NH2	2.20	0.66
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.81	0.63
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.34	0.62
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:CA	2.63	0.62
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.81	0.62
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.86	0.59
1:C:31:LEU:O	1:C:32:GLU:HG3	2.05	0.57
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.40	0.55
1:A:104:THR:HG23	1:A:107:ALA:H	1.73	0.54
1:A:132:MET:O	1:B:196:ARG:NH2	2.41	0.54
1:D:196[B]:ARG:HH21	1:D:196[B]:ARG:CB	2.15	0.54
1:A:132:MET:HE1	1:A:196:ARG:CZ	2.39	0.52
1:D:92:ILE:HD11	1:D:191:LEU:HD22	1.92	0.52
1:C:15:GLN:N	6:C:402:HOH:O	2.43	0.52
1:A:39:PRO:HG2	1:B:167:PHE:CD2	2.47	0.50
1:A:206:HIS:CD2	1:B:200:TYR:OH	2.60	0.50
1:C:22:LEU:HA	1:C:32:GLU:HG2	1.95	0.49
1:A:39:PRO:CG	1:B:167:PHE:CG	2.98	0.47
1:C:92:ILE:HD11	1:C:191:LEU:HD22	1.97	0.47
1:D:81:LYS:CB	1:D:171:ILE:HD12	2.46	0.45
1:C:31:LEU:HD23	1:C:32:GLU:N	2.23	0.45
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.52	0.45
1:A:39:PRO:HD2	1:B:167:PHE:CE1	2.52	0.44
1:C:179:LEU:HD23	1:C:205:LYS:HD2	2.00	0.44
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.50	0.44
1:D:79:LEU:HB2	1:D:171:ILE:O	2.19	0.43
1:D:92:ILE:HD11	1:D:191:LEU:CD2	2.49	0.43
1:A:39:PRO:HG2	1:B:167:PHE:CG	2.54	0.43
1:C:22:LEU:HD22	1:C:23:ILE:H	1.84	0.42
1:D:71:THR:O	1:D:73:HIS:ND1	2.51	0.42
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.54	0.42
1:C:131:CYS:SG	1:D:194:ASP:CA	3.06	0.42
1:A:104:THR:CG2	1:A:107:ALA:H	2.33	0.42
1:D:196[B]:ARG:CB	1:D:196[B]:ARG:CZ	2.98	0.41
1:A:49:VAL:HG11	1:B:49:VAL:HG21	2.02	0.41
1:D:38:ASP:C	1:D:38:ASP:OD1	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASP:OD1	1:B:38:ASP:C	2.64	0.41
1:C:206:HIS:HD2	1:D:200:TYR:OH	2.04	0.41
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:H	2.15	0.41
1:C:132:MET:O	1:D:196[B]:ARG:NH1	2.53	0.41
1:D:121:GLY:HA3	1:D:146:VAL:CG1	2.51	0.41
1:D:113:LEU:CD2	1:D:146:VAL:HG11	2.51	0.40
1:C:132:MET:HE1	1:C:196:ARG:CZ	2.50	0.40
1:D:104:THR:HG23	1:D:107:ALA:H	1.87	0.40
1:C:31:LEU:O	1:C:32:GLU:CG	2.70	0.40
1:C:138:ASN:HA	1:D:87:MET:SD	2.62	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)
6:B:403:HOH:O	6:D:403:HOH:O[1_655]	2.16	0.04

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	193/209 (92%)	187 (97%)	5 (3%)	1 (0%)	24	10
1	B	190/209 (91%)	187 (98%)	2 (1%)	1 (0%)	24	10
1	C	188/209 (90%)	181 (96%)	5 (3%)	2 (1%)	11	2
1	D	184/209 (88%)	169 (92%)	13 (7%)	2 (1%)	11	2
All	All	755/836 (90%)	724 (96%)	25 (3%)	6 (1%)	16	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	GLY
1	A	66	PRO
1	B	66	PRO
1	D	66	PRO
1	C	66	PRO
1	C	23	ILE

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	154/179 (86%)	150 (97%)	4 (3%)	40	17
1	B	154/179 (86%)	150 (97%)	4 (3%)	40	17
1	C	142/179 (79%)	135 (95%)	7 (5%)	22	5
1	D	143/179 (80%)	135 (94%)	8 (6%)	19	3
All	All	593/716 (83%)	570 (96%)	23 (4%)	28	7

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	38	ASP
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	22	LEU
1	C	29	VAL
1	C	31	LEU
1	C	35	THR
1	C	54	ARG
1	C	71	THR
1	C	136	LEU
1	D	14	LYS

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Mol	Chain	Res	Type
1	D	38	ASP
1	D	43	THR
1	D	68	LEU
1	D	70	ARG
1	D	72	LEU
1	D	76	CYS
1	D	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	206	HIS
1	B	69	GLN
1	B	206	HIS
1	C	206	HIS
1	D	138	ASN
1	D	155	ASN
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 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
5	EDO	C	301	-	3,3,3	0.56	0	2,2,2	0.18	0
4	K07	A	305	-	15,16,16	2.05	3 (20%)	17,21,21	2.53	4 (23%)
4	K07	C	304	-	15,16,16	2.67	4 (26%)	17,21,21	2.96	6 (35%)
5	EDO	A	306	-	3,3,3	0.60	0	2,2,2	0.43	0
4	K07	A	304	-	15,16,16	2.16	3 (20%)	17,21,21	2.76	6 (35%)
5	EDO	B	301	-	3,3,3	0.63	0	2,2,2	0.19	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
5	EDO	C	301	-	-	0/1/1/1	-
4	K07	A	305	-	-	3/8/15/15	0/2/2/2
4	K07	C	304	-	-	2/8/15/15	0/2/2/2
5	EDO	A	306	-	-	0/1/1/1	-
4	K07	A	304	-	-	2/8/15/15	0/2/2/2
5	EDO	B	301	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	K07	C1-N	6.44	1.52	1.46
4	A	305	K07	C1-N	5.63	1.52	1.46
4	C	304	K07	C9-C6	5.54	1.46	1.39
4	A	304	K07	C1-N	4.98	1.51	1.46
4	A	304	K07	C9-C6	4.26	1.44	1.39
4	C	304	K07	C6-N1	3.99	1.41	1.34
4	A	304	K07	C6-N1	3.96	1.41	1.34
4	A	305	K07	C9-C6	3.62	1.44	1.39
4	A	305	K07	C6-N1	3.47	1.40	1.34
4	C	304	K07	C7-N2	2.31	1.38	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	K07	C6-C9-CL	8.94	129.92	121.50
4	A	304	K07	C6-C9-CL	8.26	129.28	121.50
4	A	305	K07	C6-C9-CL	7.93	128.97	121.50
4	C	304	K07	C8-C9-CL	-5.02	111.33	118.57
4	A	305	K07	C8-C9-CL	-3.97	112.85	118.57
4	C	304	K07	C9-C6-N1	-3.87	116.96	123.00
4	A	304	K07	C8-C9-CL	-3.86	113.00	118.57
4	A	304	K07	C9-C6-N1	-3.55	117.46	123.00
4	A	305	K07	C9-C6-N1	-3.42	117.67	123.00
4	C	304	K07	N1-C6-N	-3.13	113.09	116.86
4	A	304	K07	C7-N1-C6	2.84	118.78	111.83
4	A	304	K07	N1-C6-N	-2.79	113.50	116.86
4	C	304	K07	C7-N1-C6	2.56	118.10	111.83
4	A	305	K07	C7-N1-C6	2.53	118.00	111.83
4	C	304	K07	C1-N-C6	-2.15	117.63	120.71
4	A	304	K07	C9-C8-N2	2.02	124.60	122.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	K07	C2-C1-N-C
4	A	305	K07	C2-C1-N-C6
4	A	305	K07	N-C1-C2-C5
4	A	305	K07	N-C1-C2-C3
4	C	304	K07	C2-C1-N-C6
4	C	304	K07	C2-C1-N-C
4	A	304	K07	C2-C1-N-C6
5	B	301	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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%)	1.15	37 (19%) 3 3	11, 30, 52, 66	16 (8%)
1	B	194/209 (92%)	1.09	24 (12%) 8 9	23, 36, 61, 78	3 (1%)
1	C	192/209 (91%)	1.84	74 (38%) 1 0	20, 37, 67, 78	5 (2%)
1	D	189/209 (90%)	3.09	127 (67%) 0 0	9, 47, 69, 88	17 (8%)
All	All	769/836 (91%)	1.78	262 (34%) 1 1	9, 37, 65, 88	41 (5%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167[A]	PHE	17.2
1	D	207	ALA	14.0
1	A	186	VAL	11.3
1	D	196[A]	ARG	10.9
1	D	158	PRO	10.8
1	A	187	ALA	10.6
1	D	89	GLY	10.5
1	C	191	LEU	10.3
1	A	191	LEU	10.0
1	D	156	ALA	10.0
1	C	21	GLU	9.9
1	D	84	ARG	9.7
1	D	208	ASN	9.5
1	D	90	TYR	9.3
1	D	152	ASP	8.9
1	D	88	GLY	8.4
1	B	208	ASN	8.1
1	D	149	ASN	8.0
1	B	14	LYS	7.7
1	D	157	ARG	7.7
1	C	189	GLU	7.6

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Mol	Chain	Res	Type	RSRZ
1	D	154	GLU	7.6
1	D	28	TRP	7.5
1	A	190	HIS	7.4
1	D	206	HIS	7.4
1	C	23	ILE	7.3
1	A	166	GLU	7.1
1	C	18	ILE	6.3
1	C	190	HIS	6.3
1	A	188	GLU	6.2
1	A	189	GLU	6.0
1	D	160	PRO	6.0
1	D	151	ASP	5.9
1	C	31	LEU	5.9
1	C	49	VAL	5.9
1	C	22	LEU	5.9
1	C	39	PRO	5.9
1	D	167	PHE	5.8
1	B	28	TRP	5.8
1	C	43	THR	5.7
1	C	54	ARG	5.7
1	B	165	GLY	5.6
1	D	22	LEU	5.5
1	D	155	ASN	5.5
1	D	168	VAL	5.4
1	C	16	TYR	5.4
1	D	87	MET	5.3
1	D	78	VAL	5.3
1	C	165	GLY	5.1
1	D	23	ILE	5.0
1	C	34	THR	4.9
1	C	35	THR	4.9
1	A	41	GLY	4.9
1	D	97	GLY	4.9
1	D	119	TYR	4.9
1	C	29	VAL	4.9
1	D	96	ALA	4.8
1	D	29	VAL	4.8
1	D	74	TYR	4.7
1	C	40	THR	4.6
1	D	120	LYS	4.6
1	D	118	GLY	4.6
1	D	31	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	40	THR	4.5
1	C	36	TYR	4.5
1	C	26	GLY	4.3
1	D	68	LEU	4.3
1	C	17	ILE	4.2
1	C	163	GLY	4.2
1	C	46	TRP	4.1
1	D	121	GLY	4.1
1	D	122	ASP	4.0
1	D	117	THR	4.0
1	C	167	PHE	4.0
1	D	110	LEU	4.0
1	A	72	LEU	4.0
1	D	98	LEU	4.0
1	C	99	ILE	3.9
1	D	86	PRO	3.9
1	D	53	THR	3.9
1	A	164	ASP	3.9
1	C	48	SER	3.9
1	B	167	PHE	3.9
1	C	136	LEU	3.8
1	C	104	THR	3.8
1	C	30	LYS	3.7
1	D	67	VAL	3.7
1	D	170	VAL	3.7
1	D	184	ALA	3.7
1	C	139	CYS	3.7
1	C	162	PRO	3.7
1	D	162	PRO	3.7
1	C	53	THR	3.7
1	C	58	THR	3.7
1	C	207	ALA	3.6
1	D	187	ALA	3.6
1	C	32	GLU	3.6
1	D	101	ASP	3.6
1	A	56	GLU	3.6
1	C	24	SER	3.6
1	C	137	SER	3.6
1	B	159	LYS	3.5
1	D	185	LEU	3.5
1	D	148	ILE	3.5
1	D	26	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	123	ILE	3.4
1	D	79	LEU	3.4
1	C	45	THR	3.4
1	A	31	LEU	3.4
1	D	159	LYS	3.4
1	C	25	GLU	3.4
1	D	107	ALA	3.4
1	C	15	GLN	3.4
1	D	34	THR	3.4
1	D	76	CYS	3.3
1	C	138	ASN	3.3
1	B	58	THR	3.3
1	D	192	THR	3.3
1	D	83	PHE	3.3
1	B	101	ASP	3.3
1	C	37	MET	3.3
1	D	92	ILE	3.3
1	C	161	LYS	3.2
1	D	70	ARG	3.2
1	D	150	GLY	3.2
1	B	190	HIS	3.2
1	C	131	CYS	3.2
1	D	59	ALA	3.2
1	D	80	VAL	3.2
1	C	134	PRO	3.2
1	D	27	LYS	3.2
1	D	182	LEU	3.2
1	A	28	TRP	3.2
1	A	58	THR	3.2
1	D	69	GLN	3.1
1	D	109	ALA	3.1
1	C	19	SER	3.1
1	D	161	LYS	3.1
1	D	186	VAL	3.1
1	A	39	PRO	3.1
1	D	35	THR	3.1
1	D	82	GLN	3.0
1	D	171	ILE	3.0
1	D	146	VAL	3.0
1	D	99	ILE	3.0
1	D	191	LEU	3.0
1	D	45	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	113	LEU	3.0
1	B	158	PRO	3.0
1	D	174	PRO	3.0
1	A	40	THR	2.9
1	C	28	TRP	2.9
1	A	23	ILE	2.9
1	C	101	ASP	2.9
1	B	104	THR	2.9
1	A	163	GLY	2.9
1	D	71	THR	2.9
1	D	18	ILE	2.9
1	D	73	HIS	2.9
1	B	153	ALA	2.8
1	D	49	VAL	2.8
1	A	165	GLY	2.8
1	D	188	GLU	2.8
1	D	77	ILE	2.8
1	D	114	GLU	2.8
1	D	166	GLU	2.8
1	D	36	TYR	2.8
1	A	57	GLN	2.8
1	D	94	PHE	2.8
1	C	47	GLU	2.8
1	D	14	LYS	2.8
1	A	26	GLY	2.8
1	D	124	ALA	2.7
1	D	173	LEU	2.7
1	C	100	ASP	2.7
1	D	147	THR	2.7
1	C	27	LYS	2.7
1	C	42	LYS	2.7
1	B	162	PRO	2.7
1	A	100	ASP	2.7
1	B	191	LEU	2.7
1	D	136	LEU	2.7
1	C	135	GLY	2.7
1	A	184	ALA	2.7
1	D	164	ASP	2.7
1	D	39	PRO	2.7
1	A	22	LEU	2.7
1	C	186	VAL	2.7
1	D	16	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	163	GLY	2.7
1	D	61	GLY	2.7
1	A	29	VAL	2.6
1	D	111	ARG	2.6
1	C	140	THR	2.6
1	B	18	ILE	2.6
1	D	105	PRO	2.6
1	D	145	THR	2.6
1	D	197	VAL	2.6
1	B	176	ASN	2.6
1	A	46	TRP	2.6
1	C	166	GLU	2.6
1	D	21	GLU	2.6
1	D	104	THR	2.5
1	D	91	CYS	2.5
1	D	172	SER	2.5
1	D	62	VAL	2.5
1	B	160	PRO	2.5
1	C	88	GLY	2.5
1	D	102	GLY	2.5
1	C	20	GLU	2.5
1	D	178	LEU	2.5
1	C	59	ALA	2.5
1	D	108	ALA	2.5
1	D	81	LYS	2.5
1	D	46	TRP	2.5
1	C	57	GLN	2.4
1	D	85	PRO	2.4
1	A	16	TYR	2.4
1	B	29	VAL	2.4
1	B	102	GLY	2.4
1	D	100	ASP	2.4
1	D	20	GLU	2.4
1	C	41	GLY	2.3
1	C	129	ALA	2.3
1	D	190	HIS	2.3
1	C	33	LYS	2.3
1	A	160	PRO	2.3
1	A	157	ARG	2.3
1	A	14	LYS	2.3
1	C	102	GLY	2.3
1	D	41	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	50	LYS	2.2
1	D	163	GLY	2.2
1	C	74	TYR	2.2
1	D	65	ILE	2.2
1	C	130	VAL	2.2
1	A	158	PRO	2.2
1	D	33	LYS	2.2
1	B	22	LEU	2.2
1	A	104	THR	2.2
1	D	66	PRO	2.2
1	C	72	LEU	2.1
1	D	52	THR	2.1
1	D	165	GLY	2.1
1	B	161	LYS	2.1
1	D	116	GLU	2.1
1	A	71	THR	2.1
1	B	52	THR	2.1
1	C	52	THR	2.1
1	A	27	LYS	2.1
1	A	207	ALA	2.1
1	B	186	VAL	2.1
1	D	139	CYS	2.1
1	D	169	GLU	2.1
1	C	38	ASP	2.1
1	C	92	ILE	2.1
1	C	164	ASP	2.0
1	C	44	ARG	2.0
1	D	51	ARG	2.0
1	D	72	LEU	2.0
1	A	162	PRO	2.0
1	C	153	ALA	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	C	302	1/1	0.58	0.15	80,80,80,80	0
4	K07	A	305	15/15	0.80	0.20	38,40,45,47	15
4	K07	C	304	15/15	0.81	0.20	53,64,70,70	0
5	EDO	C	301	4/4	0.82	0.14	39,49,51,58	0
5	EDO	B	301	4/4	0.84	0.13	39,41,41,44	0
4	K07	A	304	15/15	0.85	0.15	48,49,51,53	15
3	CL	A	303	1/1	0.86	0.17	67,67,67,67	0
2	MG	A	302	1/1	0.86	0.10	77,77,77,77	0
5	EDO	A	306	4/4	0.90	0.10	26,28,28,28	0
2	MG	D	301	1/1	0.92	0.08	40,40,40,40	0
2	MG	B	303	1/1	0.92	0.12	78,78,78,78	0
2	MG	D	302	1/1	0.95	0.09	48,48,48,48	0
2	MG	C	303	1/1	0.98	0.05	32,32,32,32	0
2	MG	B	302	1/1	0.98	0.03	33,33,33,33	0
2	MG	A	301	1/1	0.99	0.04	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.