



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 12:07 PM EDT

PDB ID : 5QKA / pdb_00005qka
Title : PanDDA analysis group deposition of models with modelled events (e.g. bound ligands) – Crystal Structure of NUDT5 in complex with Z2377835233
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 : 1.55 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

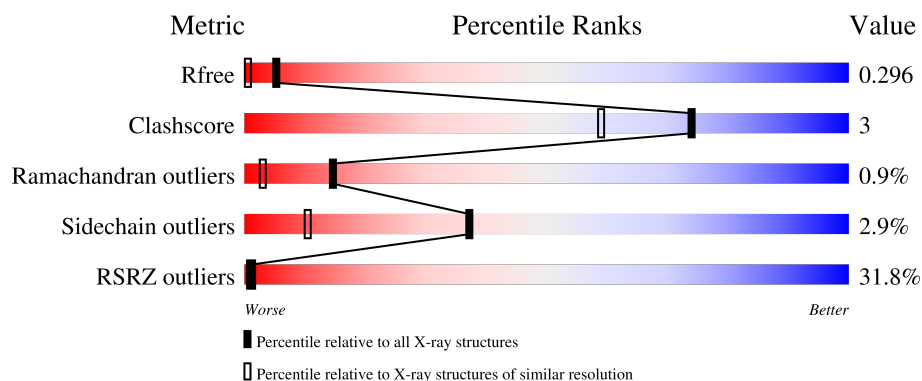
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



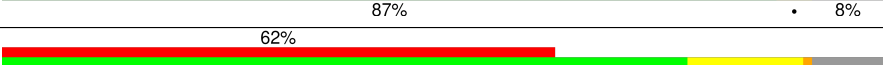

The reported resolution of this entry is 1.55 Å.

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}	164625	1935 (1.56-1.56)
Clashscore	180529	2073 (1.56-1.56)
Ramachandran outliers	177936	2037 (1.56-1.56)
Sidechain outliers	177891	2034 (1.56-1.56)
RSRZ outliers	164620	1935 (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	
1	B	209	
1	C	209	
1	D	209	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5986 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	190	Total	C	N	O	S	0	1	0
			1400	885	235	272	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

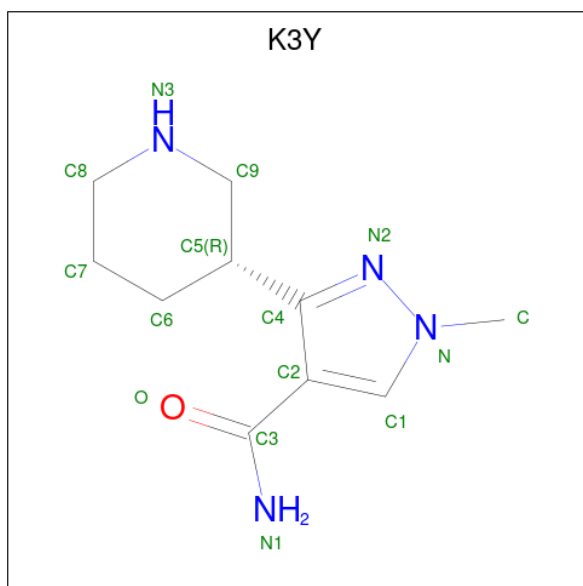
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

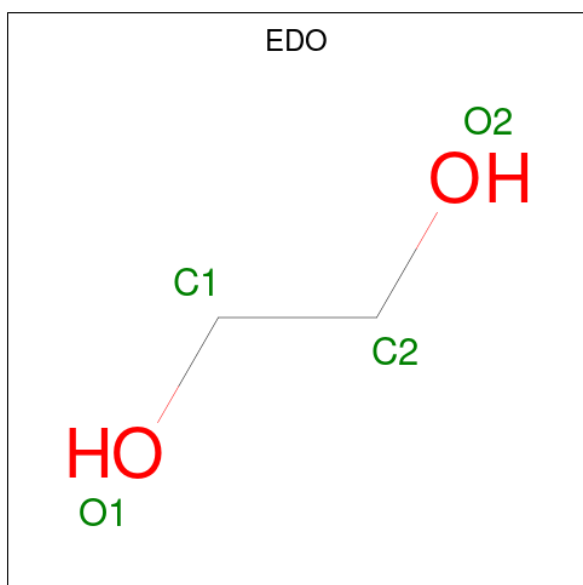
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Cl		0	0
			1	1			

- Molecule 4 is 1-methyl-3-[(3R)-piperidin-3-yl]-1H-pyrazole-4-carboxamide (CCD ID: K3Y) (formula: C₁₀H₁₆N₄O).



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

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



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

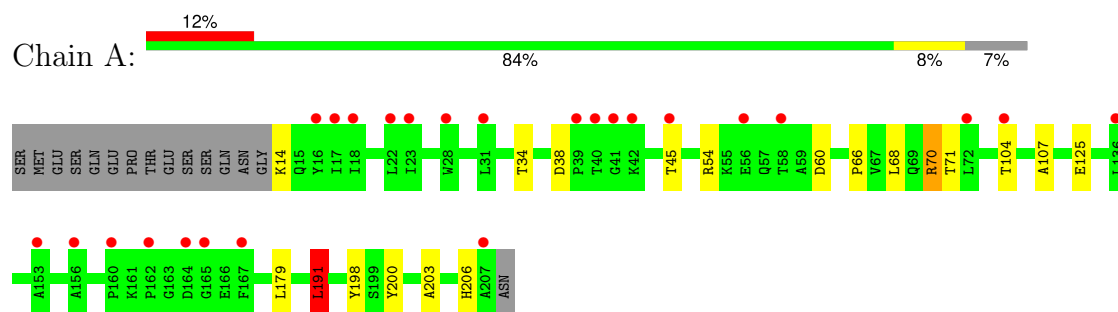
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	72	Total O 72 72	0	0
6	B	65	Total O 65 65	0	0
6	C	65	Total O 65 65	0	0
6	D	28	Total O 28 28	0	0

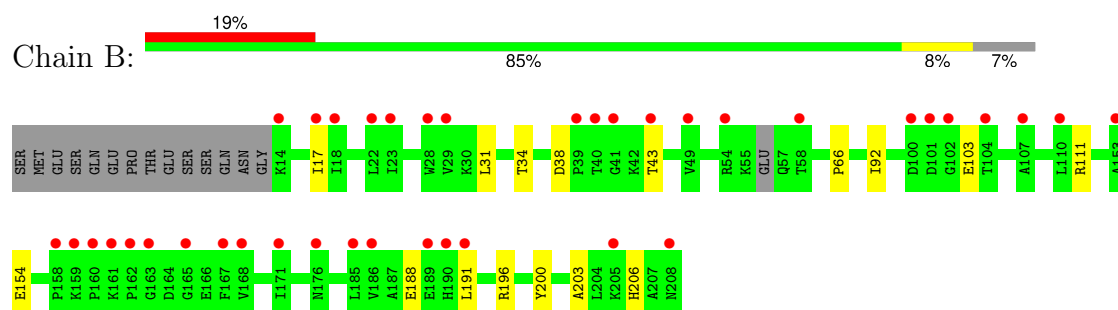
3 Residue-property plots [i](#)

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.

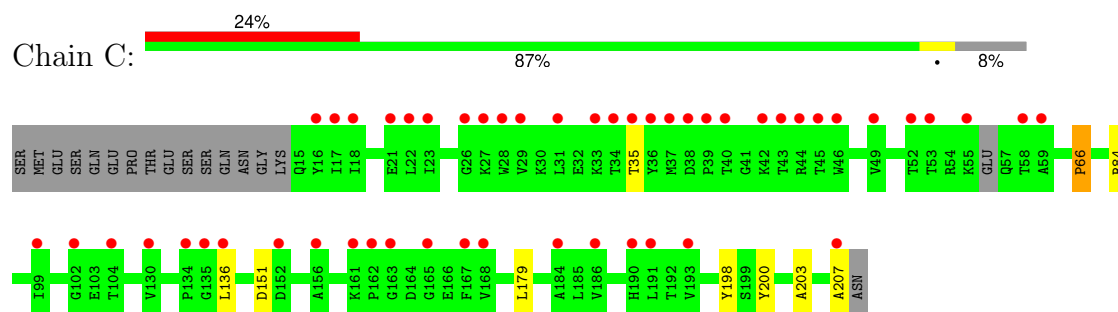
- Molecule 1: ADP-sugar pyrophosphatase



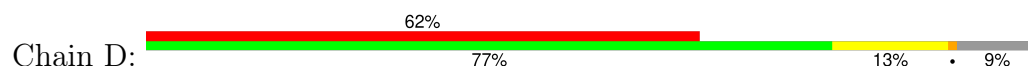
- Molecule 1: ADP-sugar pyrophosphatase

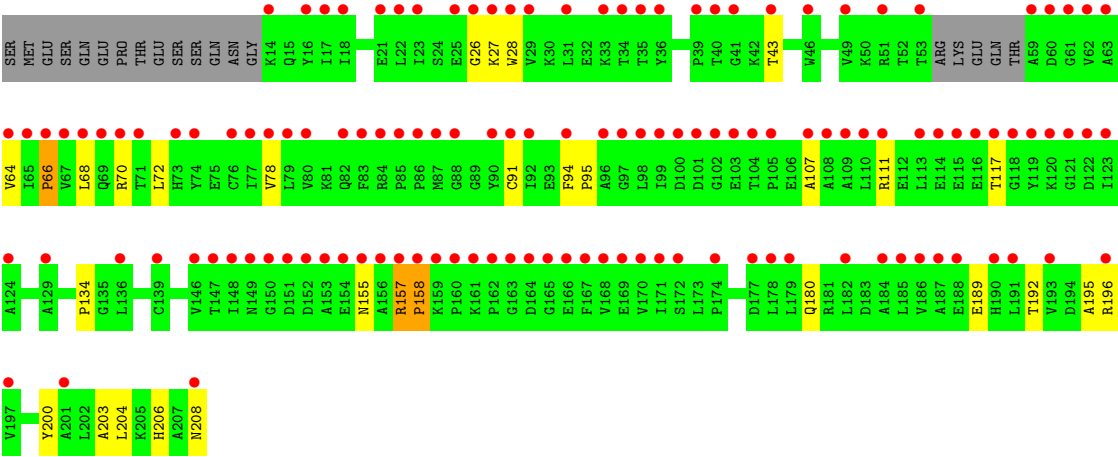


- Molecule 1: ADP-sugar pyrophosphatase



- 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	49.75Å 60.12Å 79.52Å 79.24° 81.03° 75.23°	Depositor
Resolution (Å)	77.61 – 1.55 77.61 – 1.55	Depositor EDS
% Data completeness (in resolution range)	92.9 (77.61-1.55) 92.9 (77.61-1.55)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.245 , 0.286 0.256 , 0.296	Depositor DCC
R_{free} test set	6405 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.3	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	5986	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: K3Y, MG, CL, 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	0.85	0/1478	0.92	2/2019 (0.1%)
1	B	0.75	0/1492	0.89	1/2035 (0.0%)
1	C	0.82	0/1429	0.89	1/1958 (0.1%)
1	D	0.79	0/1426	0.93	1/1949 (0.1%)
All	All	0.80	0/5825	0.91	5/7961 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	196	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	D	189	GLU	N-CA-C	5.75	126.52	111.00
1	C	151	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	191	LEU	CA-CB-CG	5.05	126.91	115.30

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	11	0
1	B	1464	0	1414	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1402	0	1298	7	0
1	D	1400	0	1334	18	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	15	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	8	0	12	0	0
6	A	72	0	0	0	0
6	B	65	0	0	1	0
6	C	65	0	0	1	0
6	D	28	0	0	1	0
All	All	5986	0	5475	34	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 3.

All (34) 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:26:GLY:O	1:D:28:TRP:N	2.17	0.72
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.73	0.71
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.78	0.64
1:A:104:THR:HG23	1:A:107:ALA:H	1.63	0.64
1:D:107:ALA:O	1:D:111:ARG:HB3	2.03	0.58
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.85	0.57
6:C:403:HOH:O	1:D:206:HIS:HE1	1.87	0.57
1:B:154:GLU:OE1	6:B:401:HOH:O	2.18	0.56
1:D:157:ARG:N	1:D:158:PRO:CD	2.68	0.56
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.41	0.55
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.42	0.54
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.91	0.53
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.44	0.52
1:D:64:VAL:O	1:D:95:PRO:HD2	2.10	0.52
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.94	0.50
1:A:191:LEU:C	1:A:191:LEU:HD23	2.33	0.49
1:D:66:PRO:HG2	1:D:78:VAL:HB	1.95	0.49
1:A:179:LEU:HD11	1:A:198:TYR:CZ	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.49	0.48
1:A:200:TYR:OH	1:B:206:HIS:HD2	1.97	0.47
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.99	0.46
1:B:103:GLU:OE2	1:B:111:ARG:NE	2.30	0.46
1:A:34:THR:O	1:A:45:THR:HA	2.16	0.46
1:B:17:ILE:HD12	1:B:34:THR:CG2	2.46	0.46
1:D:180:GLN:CB	6:D:408:HOH:O	2.64	0.45
1:D:155:ASN:O	1:D:158:PRO:HD2	2.17	0.44
1:D:195:ALA:HB3	1:D:196[B]:ARG:NH1	2.32	0.44
1:A:68:LEU:HG	1:A:70:ARG:HD2	2.00	0.44
1:C:84:ARG:HG3	1:D:134:PRO:HB2	2.02	0.41
1:C:207:ALA:HB2	1:D:204:LEU:HD23	2.02	0.41
1:A:54:ARG:HD3	1:A:60:ASP:OD1	2.21	0.41
1:D:64:VAL:O	1:D:94:PHE:HB3	2.20	0.41
1:D:107:ALA:O	1:D:111:ARG:CB	2.69	0.40
1:D:91:CYS:HA	1:D:192:THR:O	2.22	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%)	25	8
1	B	190/209 (91%)	185 (97%)	4 (2%)	1 (0%)	25	8
1	C	188/209 (90%)	184 (98%)	3 (2%)	1 (0%)	25	8
1	D	187/209 (90%)	168 (90%)	15 (8%)	4 (2%)	5	0
All	All	757/836 (91%)	723 (96%)	27 (4%)	7 (1%)	14	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	27	LYS
1	D	158	PRO
1	D	66	PRO
1	A	66	PRO
1	B	66	PRO
1	D	157	ARG
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	151/179 (84%)	147 (97%)	4 (3%)	41	13
1	B	154/179 (86%)	150 (97%)	4 (3%)	41	13
1	C	139/179 (78%)	136 (98%)	3 (2%)	47	19
1	D	142/179 (79%)	136 (96%)	6 (4%)	25	4
All	All	586/716 (82%)	569 (97%)	17 (3%)	37	10

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	38	ASP
1	A	71	THR
1	A	191	LEU
1	B	31	LEU
1	B	38	ASP
1	B	43	THR
1	B	188	GLU
1	C	35	THR
1	C	66	PRO
1	C	136	LEU
1	D	43	THR
1	D	68	LEU
1	D	70	ARG
1	D	72	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	117	THR
1	D	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	206	HIS
1	B	73	HIS
1	B	206	HIS
1	C	206	HIS
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 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	K3Y	A	304	-	13,16,16	2.66	4 (30%)	12,22,22	1.71	4 (33%)
5	EDO	C	304	-	3,3,3	0.44	0	2,2,2	0.38	0
5	EDO	B	301	-	3,3,3	0.62	0	2,2,2	0.21	0
5	EDO	A	305	-	3,3,3	0.55	0	2,2,2	0.53	0
5	EDO	C	301	-	3,3,3	0.68	0	2,2,2	0.34	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	K3Y	A	304	-	-	1/1/16/16	0/2/2/2
5	EDO	C	304	-	-	1/1/1/1	-
5	EDO	B	301	-	-	1/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	C	301	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	K3Y	C2-C4	6.55	1.46	1.38
4	A	304	K3Y	C-N	-3.87	1.44	1.47
4	A	304	K3Y	C3-N1	3.83	1.40	1.33
4	A	304	K3Y	C2-C3	-3.73	1.45	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	K3Y	C6-C5-C4	2.80	115.45	111.43
4	A	304	K3Y	C2-C1-N	-2.52	106.11	109.47
4	A	304	K3Y	C6-C5-C9	-2.49	105.46	109.98
4	A	304	K3Y	C1-C2-C3	-2.34	122.23	128.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	K3Y	C1-C2-C3-O
5	B	301	EDO	O1-C1-C2-O2
5	C	304	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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%)	0.93	25 (12%) 9 10	23, 33, 55, 71	0
1	B	194/209 (92%)	1.25	39 (20%) 3 3	19, 39, 69, 81	1 (0%)
1	C	192/209 (91%)	1.46	51 (26%) 2 2	22, 38, 74, 93	0
1	D	190/209 (90%)	3.00	130 (68%) 0 0	9, 47, 72, 111	11 (5%)
All	All	770/836 (92%)	1.65	245 (31%) 1 1	9, 39, 69, 111	12 (1%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28	TRP	13.0
1	D	26	GLY	11.7
1	D	158	PRO	11.1
1	D	160	PRO	11.1
1	D	196[A]	ARG	9.9
1	D	156	ALA	9.6
1	D	25	GLU	8.8
1	D	27	LYS	7.8
1	B	28	TRP	7.7
1	D	29	VAL	7.2
1	D	159	LYS	7.0
1	D	155	ASN	6.8
1	D	68	LEU	6.6
1	B	205	LYS	6.6
1	D	157	ARG	6.3
1	D	168	VAL	6.2
1	C	34	THR	6.1
1	D	110	LEU	6.1
1	D	167	PHE	6.0
1	C	35	THR	5.9
1	C	39	PRO	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	23	ILE	5.8
1	C	43	THR	5.6
1	D	31	LEU	5.6
1	C	22	LEU	5.4
1	D	59	ALA	5.2
1	D	83	PHE	5.2
1	D	67	VAL	5.0
1	D	171	ILE	4.9
1	D	117	THR	4.8
1	D	23	ILE	4.8
1	D	170	VAL	4.7
1	D	152	ASP	4.7
1	C	36	TYR	4.6
1	B	162	PRO	4.6
1	D	74	TYR	4.5
1	A	23	ILE	4.5
1	C	46	TRP	4.5
1	D	40	THR	4.4
1	A	41	GLY	4.4
1	D	165	GLY	4.4
1	D	119	TYR	4.3
1	C	135	GLY	4.3
1	D	90	TYR	4.3
1	D	121	GLY	4.3
1	D	86	PRO	4.3
1	D	78	VAL	4.3
1	C	16	TYR	4.3
1	C	165	GLY	4.3
1	D	162	PRO	4.2
1	B	101	ASP	4.2
1	B	58	THR	4.1
1	C	37	MET	4.1
1	C	40	THR	4.0
1	B	167	PHE	4.0
1	D	22	LEU	4.0
1	D	62	VAL	4.0
1	C	28	TRP	4.0
1	D	136	LEU	4.0
1	D	191	LEU	4.0
1	D	114	GLU	3.9
1	D	92	ILE	3.9
1	D	122	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	THR	3.9
1	C	29	VAL	3.9
1	D	99	ILE	3.9
1	C	31	LEU	3.9
1	C	136	LEU	3.9
1	D	108	ALA	3.9
1	D	100	ASP	3.8
1	D	208	ASN	3.8
1	B	14	LYS	3.8
1	D	98	LEU	3.8
1	D	77	ILE	3.7
1	D	82	GLN	3.7
1	D	41	GLY	3.7
1	D	153	ALA	3.7
1	A	39	PRO	3.7
1	D	39	PRO	3.7
1	D	148	ILE	3.7
1	C	21	GLU	3.6
1	C	17	ILE	3.6
1	D	80	VAL	3.6
1	D	101	ASP	3.5
1	D	166	GLU	3.5
1	D	79	LEU	3.5
1	A	16	TYR	3.5
1	B	165	GLY	3.5
1	D	104	THR	3.5
1	D	151	ASP	3.5
1	B	153	ALA	3.4
1	B	29	VAL	3.4
1	C	44	ARG	3.4
1	D	116	GLU	3.4
1	A	17	ILE	3.4
1	B	18	ILE	3.4
1	D	97	GLY	3.3
1	C	42	LYS	3.3
1	B	40	THR	3.3
1	D	107	ALA	3.3
1	D	184	ALA	3.3
1	D	73	HIS	3.3
1	C	58	THR	3.2
1	D	164	ASP	3.2
1	D	109	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	176	ASN	3.2
1	D	185	LEU	3.2
1	D	51	ARG	3.2
1	D	123	ILE	3.2
1	B	158	PRO	3.1
1	B	160	PRO	3.1
1	B	168	VAL	3.1
1	C	130	VAL	3.1
1	D	96	ALA	3.1
1	A	58	THR	3.1
1	C	134	PRO	3.1
1	C	168	VAL	3.1
1	D	193	VAL	3.1
1	D	102	GLY	3.0
1	D	120	LYS	3.0
1	C	26	GLY	3.0
1	D	61	GLY	3.0
1	D	118	GLY	3.0
1	D	111	ARG	3.0
1	C	49	VAL	2.9
1	D	169	GLU	2.9
1	D	201	ALA	2.9
1	B	104	THR	2.9
1	C	33	LYS	2.9
1	A	18	ILE	2.9
1	A	104	THR	2.9
1	D	33	LYS	2.9
1	A	28	TRP	2.9
1	C	104	THR	2.9
1	D	76	CYS	2.8
1	D	113	LEU	2.8
1	D	65	ILE	2.8
1	D	70	ARG	2.8
1	B	186	VAL	2.8
1	D	186	VAL	2.8
1	D	91	CYS	2.8
1	A	153	ALA	2.8
1	A	136	LEU	2.8
1	B	191	LEU	2.8
1	D	60	ASP	2.7
1	C	190	HIS	2.7
1	C	99	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	17	ILE	2.7
1	D	16	TYR	2.7
1	C	191	LEU	2.7
1	D	178	LEU	2.7
1	D	146	VAL	2.7
1	A	207	ALA	2.7
1	B	190	HIS	2.7
1	A	160	PRO	2.7
1	D	53	THR	2.7
1	B	107	ALA	2.7
1	A	167	PHE	2.7
1	A	31	LEU	2.6
1	D	88	GLY	2.6
1	A	156	ALA	2.6
1	D	187	ALA	2.6
1	A	40	THR	2.6
1	B	208	ASN	2.6
1	D	18	ILE	2.6
1	C	167	PHE	2.5
1	D	154	GLU	2.5
1	A	56	GLU	2.5
1	B	100	ASP	2.5
1	A	162	PRO	2.5
1	B	39	PRO	2.5
1	D	174	PRO	2.5
1	B	23	ILE	2.5
1	C	18	ILE	2.5
1	D	188	GLU	2.5
1	A	72	LEU	2.4
1	D	190	HIS	2.4
1	A	165	GLY	2.4
1	C	102	GLY	2.4
1	D	147	THR	2.4
1	B	161	LYS	2.4
1	D	149	ASN	2.4
1	C	27	LYS	2.4
1	B	41	GLY	2.4
1	B	49	VAL	2.4
1	C	207	ALA	2.4
1	D	139	CYS	2.4
1	C	161	LYS	2.4
1	A	164	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	22	LEU	2.3
1	B	22	LEU	2.3
1	D	182	LEU	2.3
1	D	34	THR	2.3
1	D	71	THR	2.3
1	C	59	ALA	2.3
1	C	38	ASP	2.3
1	D	49	VAL	2.3
1	B	110	LEU	2.3
1	D	46	TRP	2.3
1	B	102	GLY	2.3
1	C	163	GLY	2.3
1	D	35	THR	2.3
1	B	17	ILE	2.3
1	B	185	LEU	2.3
1	C	162	PRO	2.3
1	D	172	SER	2.3
1	D	87	MET	2.3
1	B	159	LYS	2.3
1	D	150	GLY	2.3
1	D	161	LYS	2.3
1	C	152	ASP	2.3
1	D	177	ASP	2.3
1	D	94	PHE	2.2
1	D	84	ARG	2.2
1	D	85	PRO	2.2
1	D	124	ALA	2.2
1	B	163	GLY	2.2
1	D	64	VAL	2.2
1	D	115	GLU	2.2
1	C	53	THR	2.2
1	D	43	THR	2.2
1	D	105	PRO	2.2
1	D	129	ALA	2.2
1	B	171	ILE	2.2
1	B	189	GLU	2.2
1	D	69	GLN	2.2
1	D	66	PRO	2.2
1	D	63	ALA	2.2
1	D	179	LEU	2.2
1	A	45	THR	2.1
1	D	163	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	55	LYS	2.1
1	D	103	GLU	2.1
1	C	186	VAL	2.1
1	A	42	LYS	2.1
1	D	14	LYS	2.1
1	D	21	GLU	2.1
1	D	36	TYR	2.1
1	B	54	ARG	2.0
1	C	156	ALA	2.0
1	B	43	THR	2.0
1	C	52	THR	2.0
1	C	184	ALA	2.0
1	C	193	VAL	2.0
1	D	197	VAL	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 monosaccharides 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
4	K3Y	A	304	15/15	0.66	0.25	50,52,61,68	15
5	EDO	C	304	4/4	0.77	0.18	45,47,48,48	0
5	EDO	C	301	4/4	0.80	0.16	38,46,47,49	0
2	MG	A	302	1/1	0.84	0.13	71,71,71,71	0
2	MG	C	302	1/1	0.86	0.13	85,85,85,85	0
5	EDO	A	305	4/4	0.88	0.12	30,31,31,31	0
5	EDO	B	301	4/4	0.89	0.10	43,48,49,50	0
3	CL	A	303	1/1	0.90	0.19	70,70,70,70	0
2	MG	B	303	1/1	0.91	0.09	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	D	301	1/1	0.92	0.09	45,45,45,45	0
2	MG	D	302	1/1	0.96	0.10	50,50,50,50	0
2	MG	C	303	1/1	0.99	0.03	36,36,36,36	0
2	MG	A	301	1/1	0.99	0.02	32,32,32,32	0
2	MG	B	302	1/1	0.99	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.