



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:55 AM UTC

PDB ID : 5QK0 / pdb_00005qk0
Title : PanDDA analysis group deposition of models with modelled events (e.g. bound ligands) – Crystal Structure of NUDT5 in complex with Z1270312110
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 : 1.44 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

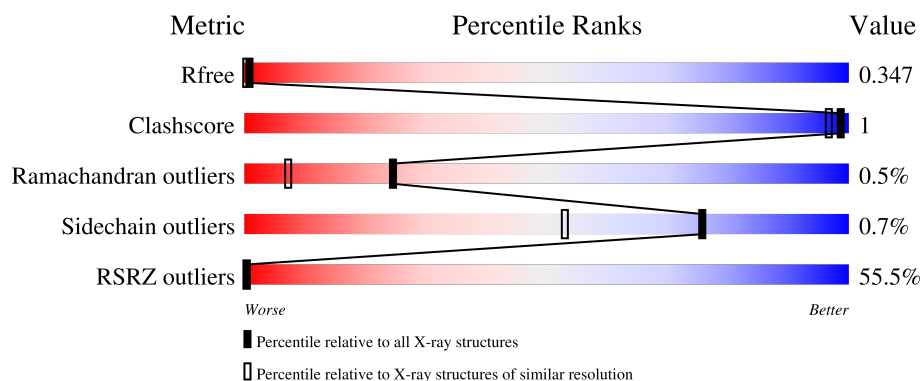
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	32% 89% 7%
1	B	209	46% 90% 7%
1	C	209	53% 90% 8%
1	D	209	74% 89% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5990 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			

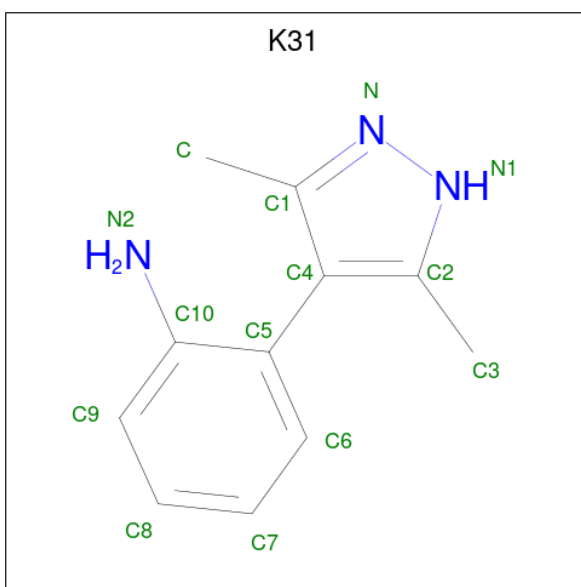
There are 4 discrepancies between the modelled and reference sequences:

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).

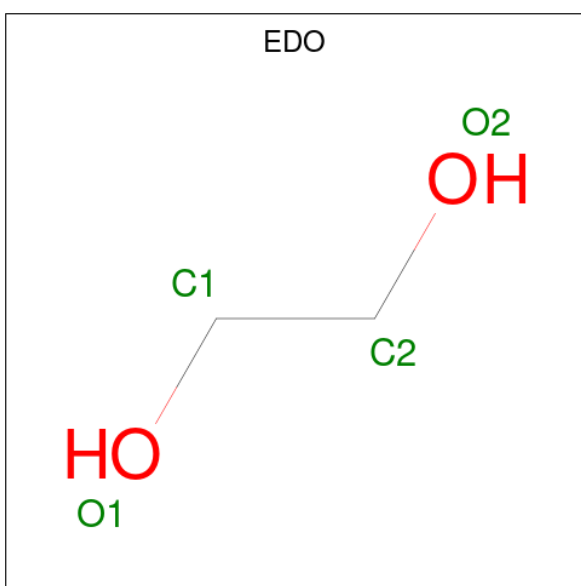
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 2-(3,5-dimethyl-1H-pyrazol-4-yl)aniline (CCD ID: K31) (formula: C₁₁H₁₃N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	11	3		
3	B	1	Total	C	N	0	0
			14	11	3		

- 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	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

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

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

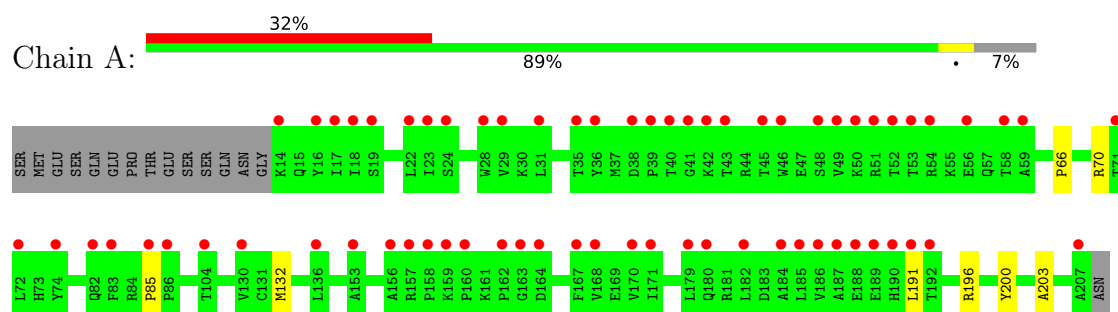
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	63	Total	O	0	0
			63	63		
6	C	64	Total	O	0	0
			64	64		
6	D	28	Total	O	0	0
			28	28		

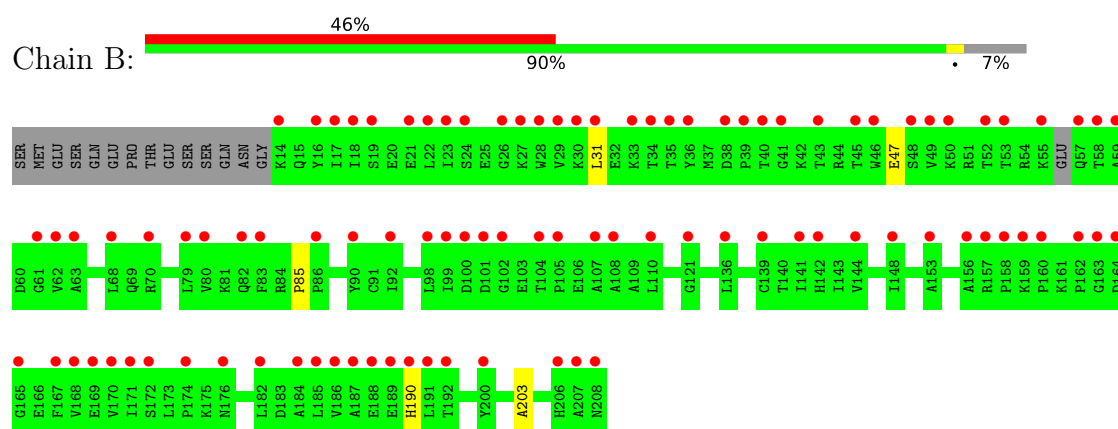
3 Residue-property plots [i](#)

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.

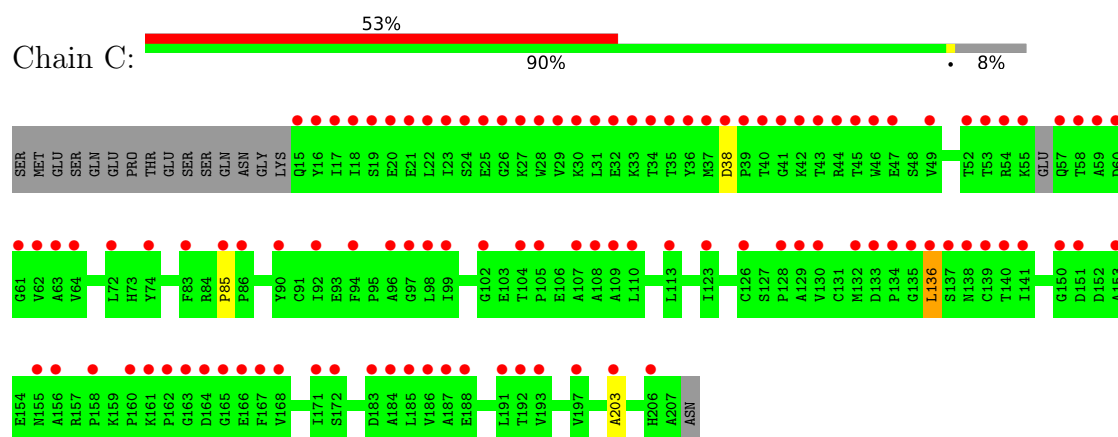
- Molecule 1: ADP-sugar pyrophosphatase



- Molecule 1: ADP-sugar pyrophosphatase

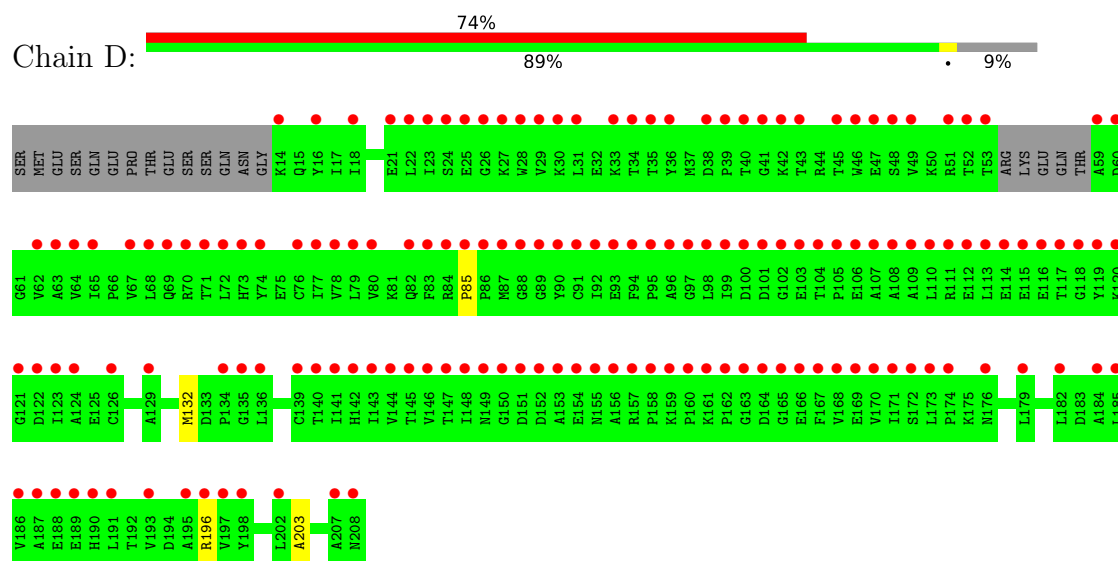


- Molecule 1: ADP-sugar pyrophosphatase



● Molecule 1: ADP-sugar pyrophosphatase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.67Å 60.15Å 79.78Å 79.37° 80.65° 75.23°	Depositor
Resolution (Å)	77.83 – 1.44 77.83 – 1.44	Depositor EDS
% Data completeness (in resolution range)	82.3 (77.83-1.44) 82.3 (77.83-1.44)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.306 , 0.338 0.322 , 0.347	Depositor DCC
R_{free} test set	7947 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.2	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	0.93	EDS
Total number of atoms	5990	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 6.45% 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, K31, EDO, CL

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	0.49	0/1478	0.68	1/2019 (0.0%)
1	B	0.51	0/1492	0.70	1/2035 (0.0%)
1	C	0.51	0/1429	0.78	3/1958 (0.2%)
1	D	0.53	0/1426	0.72	1/1949 (0.1%)
All	All	0.51	0/5825	0.72	6/7961 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ASP	CA-C-N	10.37	130.03	119.24
1	C	38	ASP	C-N-CA	10.37	130.03	119.24
1	B	85	PRO	N-CA-C	5.59	117.52	110.70
1	D	85	PRO	N-CA-C	5.58	117.51	110.70
1	C	85	PRO	N-CA-C	5.41	117.31	110.70
1	A	85	PRO	N-CA-C	5.28	117.14	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1464	0	1414	2	0
1	C	1402	0	1298	1	0
1	D	1400	0	1334	3	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	14	0	0	0	0
3	B	14	0	0	0	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
5	B	1	0	0	0	0
6	A	66	0	0	0	0
6	B	63	0	0	0	0
6	C	64	0	0	0	0
6	D	28	0	0	0	0
All	All	5990	0	5475	6	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 1.

All (6) 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:A:203:ALA:HB3	1:B:203:ALA:HB3	1.71	0.72
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.75	0.69
1:D:132:MET:HE1	1:D:196[A]:ARG:NH1	2.27	0.50
1:A:132:MET:HE1	1:A:196:ARG:CZ	2.44	0.48
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.49	0.48
1:D:132:MET:HE1	1:D:196[A]:ARG:CZ	2.48	0.44

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%)	187 (97%)	4 (2%)	1 (0%)	24	7
1	B	190/209 (91%)	185 (97%)	3 (2%)	2 (1%)	11	2
1	C	188/209 (90%)	181 (96%)	6 (3%)	1 (0%)	24	7
1	D	187/209 (90%)	178 (95%)	9 (5%)	0	100	100
All	All	757/836 (91%)	731 (97%)	22 (3%)	4 (0%)	24	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	GLU
1	C	136	LEU
1	B	190	HIS
1	A	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%)	149 (99%)	2 (1%)	61	29
1	B	154/179 (86%)	153 (99%)	1 (1%)	78	57
1	C	139/179 (78%)	138 (99%)	1 (1%)	76	53
1	D	142/179 (79%)	142 (100%)	0	100	100
All	All	586/716 (82%)	582 (99%)	4 (1%)	76	53

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	191	LEU
1	B	31	LEU
1	C	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	C	15	GLN
1	D	149	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 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	$\# Z > 2$
4	EDO	A	304	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	C	301	-	3,3,3	0.44	0	2,2,2	0.28	0
3	K31	A	303	-	15,15,15	1.30	2 (13%)	20,21,21	1.10	1 (5%)
3	K31	B	305	-	15,15,15	1.32	2 (13%)	20,21,21	1.25	2 (10%)
4	EDO	B	302	-	3,3,3	0.44	0	2,2,2	0.33	0
4	EDO	B	306	-	3,3,3	0.42	0	2,2,2	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
3	K31	A	303	-	-	0/4/4/4	0/2/2/2
3	K31	B	305	-	-	0/4/4/4	0/2/2/2
4	EDO	B	302	-	-	1/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	305	K31	C5-C4	-3.22	1.44	1.50
3	A	303	K31	C5-C4	-2.94	1.44	1.50
3	A	303	K31	C2-N1	2.40	1.39	1.34
3	B	305	K31	C2-N1	2.38	1.39	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	K31	C2-C4-C1	2.60	106.22	104.91
3	A	303	K31	C2-C4-C1	2.15	105.99	104.91
3	B	305	K31	C3-C2-N1	2.07	125.08	121.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	EDO	O1-C1-C2-O2
4	B	306	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%)	1.93	67 (34%) 1 1	20, 32, 50, 55	7 (3%)
1	B	194/209 (92%)	2.31	96 (49%) 0 0	18, 37, 58, 66	4 (2%)
1	C	192/209 (91%)	2.69	110 (57%) 0 0	22, 37, 76, 88	1 (0%)
1	D	190/209 (90%)	3.54	154 (81%) 0 0	8, 47, 76, 83	6 (3%)
All	All	770/836 (92%)	2.61	427 (55%) 0 0	8, 38, 72, 88	18 (2%)

All (427) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	PRO	11.1
1	A	191	LEU	10.7
1	C	136	LEU	10.4
1	D	196[A]	ARG	10.4
1	C	16	TYR	10.0
1	D	159	LYS	9.3
1	C	36	TYR	8.9
1	D	190	HIS	8.6
1	C	18	ILE	8.4
1	D	110	LEU	8.0
1	D	119	TYR	7.8
1	A	189	GLU	7.8
1	C	43	THR	7.8
1	D	29	VAL	7.7
1	A	190	HIS	7.5
1	D	189	GLU	7.4
1	D	167	PHE	7.3
1	C	22	LEU	7.3
1	B	23	ILE	7.2
1	D	136	LEU	7.0
1	B	58	THR	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	35	THR	6.8
1	B	165	GLY	6.8
1	C	39	PRO	6.7
1	C	135	GLY	6.7
1	C	23	ILE	6.6
1	A	187	ALA	6.6
1	B	189	GLU	6.5
1	D	188	GLU	6.5
1	D	74	TYR	6.5
1	B	190	HIS	6.5
1	C	17	ILE	6.5
1	B	206	HIS	6.4
1	C	42	LYS	6.2
1	A	39	PRO	6.2
1	D	120	LYS	6.2
1	D	101	ASP	6.2
1	D	124	ALA	6.1
1	D	165	GLY	6.1
1	B	208	ASN	6.1
1	C	59	ALA	6.0
1	D	23	ILE	6.0
1	D	28	TRP	6.0
1	D	168	VAL	6.0
1	D	114	GLU	5.9
1	D	148	ILE	5.9
1	C	52	THR	5.9
1	D	99	ILE	5.9
1	C	28	TRP	5.8
1	A	31	LEU	5.8
1	D	153	ALA	5.8
1	B	18	ILE	5.7
1	D	105	PRO	5.7
1	D	73	HIS	5.7
1	D	152	ASP	5.6
1	C	31	LEU	5.6
1	C	26	GLY	5.5
1	C	46	TRP	5.5
1	D	16	TYR	5.5
1	B	28	TRP	5.5
1	D	46	TRP	5.5
1	D	22	LEU	5.4
1	D	113	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	41	GLY	5.4
1	B	40	THR	5.4
1	C	53	THR	5.4
1	D	121	GLY	5.3
1	C	29	VAL	5.3
1	A	104	THR	5.3
1	D	123	ILE	5.3
1	B	31	LEU	5.3
1	D	96	ALA	5.3
1	D	98	LEU	5.2
1	A	22	LEU	5.1
1	A	185	LEU	5.1
1	B	191	LEU	5.1
1	C	49	VAL	5.1
1	B	43	THR	5.1
1	B	102	GLY	5.1
1	D	107	ALA	5.1
1	C	162	PRO	5.1
1	C	37	MET	5.1
1	D	49	VAL	5.1
1	C	45	THR	5.0
1	C	15	GLN	5.0
1	C	58	THR	5.0
1	D	170	VAL	5.0
1	D	118	GLY	5.0
1	A	167	PHE	4.9
1	C	19	SER	4.9
1	D	26	GLY	4.9
1	D	80	VAL	4.9
1	C	34	THR	4.9
1	B	167	PHE	4.8
1	C	167	PHE	4.8
1	A	41	GLY	4.8
1	D	162	PRO	4.8
1	B	49	VAL	4.8
1	A	29	VAL	4.7
1	B	101	ASP	4.7
1	D	109	ALA	4.7
1	C	21	GLU	4.7
1	B	53	THR	4.7
1	D	155	ASN	4.7
1	B	186	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	4.7
1	D	83	PHE	4.7
1	D	117	THR	4.5
1	B	170	VAL	4.5
1	D	90	TYR	4.5
1	D	71	THR	4.5
1	C	98	LEU	4.5
1	B	52	THR	4.5
1	B	185	LEU	4.5
1	D	108	ALA	4.4
1	D	111	ARG	4.4
1	C	104	THR	4.4
1	C	40	THR	4.4
1	D	31	LEU	4.3
1	D	62	VAL	4.3
1	C	55	LYS	4.3
1	C	161	LYS	4.3
1	D	34	THR	4.2
1	A	46	TRP	4.2
1	D	169	GLU	4.2
1	D	163	GLY	4.2
1	A	160	PRO	4.2
1	D	160	PRO	4.2
1	A	188	GLU	4.1
1	D	51	ARG	4.1
1	B	22	LEU	4.1
1	D	100	ASP	4.1
1	B	48	SER	4.1
1	C	54	ARG	4.1
1	B	55	LYS	4.1
1	D	72	LEU	4.1
1	D	104	THR	4.0
1	B	187	ALA	4.0
1	D	184	ALA	4.0
1	D	164	ASP	4.0
1	C	163	GLY	4.0
1	D	97	GLY	4.0
1	D	116	GLU	4.0
1	A	162	PRO	4.0
1	D	78	VAL	4.0
1	D	146	VAL	4.0
1	D	166	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	144	VAL	3.9
1	C	107	ALA	3.9
1	C	20	GLU	3.9
1	D	112	GLU	3.9
1	C	38	ASP	3.9
1	B	158	PRO	3.9
1	D	193	VAL	3.9
1	B	153	ALA	3.9
1	D	191	LEU	3.9
1	B	162	PRO	3.9
1	C	134	PRO	3.8
1	C	168	VAL	3.8
1	D	67	VAL	3.8
1	A	72	LEU	3.8
1	D	208	ASN	3.8
1	A	184	ALA	3.8
1	C	24	SER	3.8
1	A	163	GLY	3.8
1	C	102	GLY	3.8
1	C	187	ALA	3.8
1	B	160	PRO	3.7
1	D	79	LEU	3.7
1	B	46	TRP	3.7
1	A	157	ARG	3.7
1	C	165	GLY	3.7
1	D	115	GLU	3.6
1	D	39	PRO	3.6
1	D	185	LEU	3.6
1	B	157	ARG	3.6
1	D	102	GLY	3.6
1	A	56	GLU	3.6
1	D	151	ASP	3.6
1	B	39	PRO	3.6
1	C	158	PRO	3.6
1	A	164	ASP	3.6
1	D	18	ILE	3.6
1	C	33	LYS	3.6
1	C	44	ARG	3.6
1	C	160	PRO	3.5
1	C	41	GLY	3.5
1	A	28	TRP	3.5
1	D	82	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	36	TYR	3.5
1	C	27	LYS	3.5
1	A	43	THR	3.5
1	D	150	GLY	3.5
1	D	182	LEU	3.5
1	B	14	LYS	3.4
1	C	137	SER	3.4
1	D	36	TYR	3.4
1	B	99	ILE	3.4
1	A	40	THR	3.4
1	A	50	LYS	3.3
1	D	64	VAL	3.3
1	A	83	PHE	3.3
1	D	122	ASP	3.3
1	B	27	LYS	3.3
1	B	163	GLY	3.3
1	C	133	ASP	3.3
1	A	16	TYR	3.3
1	A	58	THR	3.3
1	D	69	GLN	3.3
1	C	150	GLY	3.3
1	B	34	THR	3.3
1	D	154	GLU	3.3
1	D	70	ARG	3.2
1	D	171	ILE	3.2
1	B	104	THR	3.2
1	C	140	THR	3.2
1	D	197	VAL	3.2
1	A	52	THR	3.2
1	D	35	THR	3.2
1	D	95	PRO	3.2
1	B	29	VAL	3.2
1	D	129	ALA	3.2
1	C	110	LEU	3.2
1	D	85	PRO	3.2
1	C	99	ILE	3.2
1	D	59	ALA	3.2
1	D	156	ALA	3.2
1	A	53	THR	3.1
1	B	188	GLU	3.1
1	A	23	ILE	3.1
1	B	30	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	153	ALA	3.1
1	A	186	VAL	3.1
1	A	45	THR	3.1
1	C	185	LEU	3.1
1	D	172	SER	3.1
1	D	87	MET	3.1
1	A	59	ALA	3.1
1	C	193	VAL	3.0
1	A	86	PRO	3.0
1	C	30	LYS	3.0
1	B	169	GLU	3.0
1	B	108	ALA	3.0
1	A	42	LYS	3.0
1	D	65	ILE	2.9
1	C	206	HIS	2.9
1	A	168	VAL	2.9
1	B	80	VAL	2.9
1	C	171	ILE	2.9
1	D	92	ILE	2.9
1	A	49	VAL	2.9
1	A	51	ARG	2.9
1	C	72	LEU	2.9
1	A	158	PRO	2.9
1	B	19	SER	2.9
1	B	159	LYS	2.9
1	D	86	PRO	2.9
1	C	74	TYR	2.9
1	C	130	VAL	2.9
1	D	53	THR	2.9
1	D	147	THR	2.9
1	B	136	LEU	2.9
1	C	83	PHE	2.8
1	B	184	ALA	2.8
1	D	63	ALA	2.8
1	C	25	GLU	2.8
1	D	94	PHE	2.8
1	B	50	LYS	2.8
1	D	157	ARG	2.8
1	B	61	GLY	2.8
1	D	38	ASP	2.8
1	A	180	GLN	2.8
1	B	62	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	168	VAL	2.8
1	D	40	THR	2.8
1	D	45	THR	2.8
1	B	176	ASN	2.8
1	D	139	CYS	2.8
1	D	174	PRO	2.8
1	D	179	LEU	2.8
1	C	62	VAL	2.7
1	B	24	SER	2.7
1	D	106	GLU	2.7
1	B	70	ARG	2.7
1	D	149	ASN	2.7
1	D	33	LYS	2.7
1	B	105	PRO	2.7
1	B	107	ALA	2.7
1	C	109	ALA	2.7
1	D	187	ALA	2.7
1	B	192	THR	2.7
1	C	32	GLU	2.7
1	C	184	ALA	2.7
1	B	148	ILE	2.7
1	D	143	ILE	2.7
1	B	83	PHE	2.7
1	A	71	THR	2.6
1	D	186	VAL	2.6
1	C	86	PRO	2.6
1	B	41	GLY	2.6
1	C	203	ALA	2.6
1	D	43	THR	2.6
1	A	18	ILE	2.6
1	B	17	ILE	2.6
1	B	33	LYS	2.6
1	C	64	VAL	2.6
1	A	14	LYS	2.5
1	D	60	ASP	2.5
1	D	134	PRO	2.5
1	A	24	SER	2.5
1	B	59	ALA	2.5
1	C	139	CYS	2.5
1	B	200	TYR	2.5
1	D	48	SER	2.5
1	D	84	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	63	ALA	2.5
1	C	96	ALA	2.5
1	D	91	CYS	2.5
1	A	171	ILE	2.5
1	C	141	ILE	2.5
1	D	89	GLY	2.5
1	D	173	LEU	2.5
1	A	130	VAL	2.5
1	C	197	VAL	2.5
1	B	139	CYS	2.4
1	D	207	ALA	2.4
1	B	171	ILE	2.4
1	A	38	ASP	2.4
1	B	38	ASP	2.4
1	D	145	THR	2.4
1	D	25	GLU	2.4
1	D	27	LYS	2.4
1	D	161	LYS	2.4
1	A	17	ILE	2.4
1	D	77	ILE	2.4
1	B	79	LEU	2.4
1	B	98	LEU	2.4
1	B	110	LEU	2.4
1	C	188	GLU	2.4
1	A	36	TYR	2.4
1	C	61	GLY	2.4
1	D	88	GLY	2.4
1	D	195	ALA	2.4
1	B	16	TYR	2.4
1	B	172	SER	2.4
1	C	172	SER	2.4
1	D	52	THR	2.4
1	A	54	ARG	2.3
1	D	141	ILE	2.3
1	C	113	LEU	2.3
1	C	90	TYR	2.3
1	B	26	GLY	2.3
1	C	183	ASP	2.3
1	B	207	ALA	2.3
1	C	108	ALA	2.3
1	D	14	LYS	2.3
1	D	24	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	138	ASN	2.3
1	D	176	ASN	2.3
1	B	100	ASP	2.3
1	B	121	GLY	2.3
1	B	92	ILE	2.3
1	B	182	LEU	2.3
1	A	48	SER	2.3
1	D	76	CYS	2.3
1	B	144	VAL	2.3
1	B	45	THR	2.3
1	A	82	GLN	2.3
1	D	142	HIS	2.3
1	A	159	LYS	2.3
1	A	136	LEU	2.3
1	B	86	PRO	2.2
1	D	135	GLY	2.2
1	A	19	SER	2.2
1	D	202	LEU	2.2
1	D	140	THR	2.2
1	B	82	GLN	2.2
1	A	179	LEU	2.2
1	B	21	GLU	2.2
1	B	57	GLN	2.2
1	A	170	VAL	2.2
1	B	142	HIS	2.2
1	A	182	LEU	2.1
1	C	105	PRO	2.1
1	C	128	PRO	2.1
1	C	129	ALA	2.1
1	C	92	ILE	2.1
1	C	126	CYS	2.1
1	C	155	ASN	2.1
1	C	60	ASP	2.1
1	C	85	PRO	2.1
1	B	35	THR	2.1
1	C	192	THR	2.1
1	C	166	GLU	2.1
1	D	21	GLU	2.1
1	D	93	GLU	2.1
1	C	123	ILE	2.1
1	A	74	TYR	2.1
1	B	90	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	97	GLY	2.1
1	D	103	GLU	2.1
1	C	186	VAL	2.1
1	C	132	MET	2.1
1	A	156	ALA	2.1
1	C	153	ALA	2.1
1	B	68	LEU	2.1
1	C	191	LEU	2.1
1	D	42	LYS	2.1
1	A	85	PRO	2.1
1	B	174	PRO	2.1
1	A	35	THR	2.0
1	C	94	PHE	2.0
1	D	30	LYS	2.0
1	A	207	ALA	2.0
1	B	63	ALA	2.0
1	C	57	GLN	2.0
1	D	47	GLU	2.0
1	B	141	ILE	2.0
1	D	198	TYR	2.0
1	B	164	ASP	2.0
1	C	164	ASP	2.0
1	A	192	THR	2.0
1	C	47	GLU	2.0
1	B	156	ALA	2.0
1	C	156	ALA	2.0
1	D	126	CYS	2.0
1	C	151	ASP	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
4	EDO	B	302	4/4	0.70	0.19	40,40,40,40	0
3	K31	A	303	14/14	0.73	0.27	62,63,63,63	0
2	MG	B	304	1/1	0.75	0.16	81,81,81,81	0
2	MG	A	302	1/1	0.81	0.11	74,74,74,74	0
4	EDO	C	301	4/4	0.82	0.13	41,42,42,42	0
3	K31	B	305	14/14	0.85	0.17	38,38,38,39	14
5	CL	B	301	1/1	0.85	0.13	57,57,57,57	0
4	EDO	A	304	4/4	0.86	0.13	30,30,30,30	4
2	MG	C	302	1/1	0.88	0.12	50,50,50,50	0
2	MG	D	302	1/1	0.88	0.13	52,52,52,52	0
2	MG	D	301	1/1	0.90	0.09	35,35,35,35	0
2	MG	A	301	1/1	0.92	0.08	29,29,29,29	0
4	EDO	B	306	4/4	0.92	0.14	36,36,36,36	4
2	MG	C	303	1/1	0.95	0.09	38,38,38,38	0
2	MG	B	303	1/1	0.98	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.