



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:57 PM UTC

PDB ID : 4PNL / pdb_00004pnl
Title : Crystal structure of TNKS-2 in complex with DR2313.
Authors : Qiu, W.; Lam, R.; Romanov, V.; Gordon, R.; Gebremeskel, S.; Vodsedalek, J.; Thompson, C.; Beletskaya, I.; Battaile, K.P.; Pai, E.F.; Chirgadze, N.Y.
Deposited on : 2014-05-23
Resolution : 1.50 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

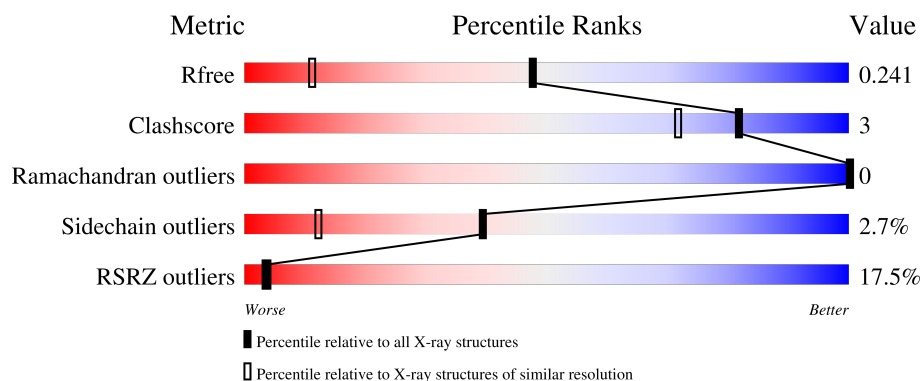
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	227	10% 82% 5% 13%
1	B	227	12% 81% 10% 9%
1	C	227	10% 84% 8% 8%
1	D	227	30% 77% 9% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7554 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	4	0
			1617	1021	299	285	12			
1	B	206	Total	C	N	O	S	0	3	0
			1681	1063	308	298	12			
1	C	208	Total	C	N	O	S	0	3	0
			1696	1072	310	303	11			
1	D	194	Total	C	N	O	S	0	7	0
			1601	1015	295	278	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	938	MET	-	initiating methionine	UNP Q9H2K2
A	939	GLY	-	expression tag	UNP Q9H2K2
A	940	SER	-	expression tag	UNP Q9H2K2
A	941	SER	-	expression tag	UNP Q9H2K2
A	942	HIS	-	expression tag	UNP Q9H2K2
A	943	HIS	-	expression tag	UNP Q9H2K2
A	944	HIS	-	expression tag	UNP Q9H2K2
A	945	HIS	-	expression tag	UNP Q9H2K2
A	946	HIS	-	expression tag	UNP Q9H2K2
A	947	HIS	-	expression tag	UNP Q9H2K2
A	948	SER	-	expression tag	UNP Q9H2K2
A	949	SER	-	expression tag	UNP Q9H2K2
A	950	GLY	-	expression tag	UNP Q9H2K2
A	951	ARG	-	expression tag	UNP Q9H2K2
A	952	GLU	-	expression tag	UNP Q9H2K2
A	953	ASN	-	expression tag	UNP Q9H2K2
A	954	LEU	-	expression tag	UNP Q9H2K2
A	955	TYR	-	expression tag	UNP Q9H2K2
A	956	PHE	-	expression tag	UNP Q9H2K2
A	957	GLN	-	expression tag	UNP Q9H2K2
A	958	GLY	-	expression tag	UNP Q9H2K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	938	MET	-	initiating methionine	UNP Q9H2K2
B	939	GLY	-	expression tag	UNP Q9H2K2
B	940	SER	-	expression tag	UNP Q9H2K2
B	941	SER	-	expression tag	UNP Q9H2K2
B	942	HIS	-	expression tag	UNP Q9H2K2
B	943	HIS	-	expression tag	UNP Q9H2K2
B	944	HIS	-	expression tag	UNP Q9H2K2
B	945	HIS	-	expression tag	UNP Q9H2K2
B	946	HIS	-	expression tag	UNP Q9H2K2
B	947	HIS	-	expression tag	UNP Q9H2K2
B	948	SER	-	expression tag	UNP Q9H2K2
B	949	SER	-	expression tag	UNP Q9H2K2
B	950	GLY	-	expression tag	UNP Q9H2K2
B	951	ARG	-	expression tag	UNP Q9H2K2
B	952	GLU	-	expression tag	UNP Q9H2K2
B	953	ASN	-	expression tag	UNP Q9H2K2
B	954	LEU	-	expression tag	UNP Q9H2K2
B	955	TYR	-	expression tag	UNP Q9H2K2
B	956	PHE	-	expression tag	UNP Q9H2K2
B	957	GLN	-	expression tag	UNP Q9H2K2
B	958	GLY	-	expression tag	UNP Q9H2K2
C	938	MET	-	initiating methionine	UNP Q9H2K2
C	939	GLY	-	expression tag	UNP Q9H2K2
C	940	SER	-	expression tag	UNP Q9H2K2
C	941	SER	-	expression tag	UNP Q9H2K2
C	942	HIS	-	expression tag	UNP Q9H2K2
C	943	HIS	-	expression tag	UNP Q9H2K2
C	944	HIS	-	expression tag	UNP Q9H2K2
C	945	HIS	-	expression tag	UNP Q9H2K2
C	946	HIS	-	expression tag	UNP Q9H2K2
C	947	HIS	-	expression tag	UNP Q9H2K2
C	948	SER	-	expression tag	UNP Q9H2K2
C	949	SER	-	expression tag	UNP Q9H2K2
C	950	GLY	-	expression tag	UNP Q9H2K2
C	951	ARG	-	expression tag	UNP Q9H2K2
C	952	GLU	-	expression tag	UNP Q9H2K2
C	953	ASN	-	expression tag	UNP Q9H2K2
C	954	LEU	-	expression tag	UNP Q9H2K2
C	955	TYR	-	expression tag	UNP Q9H2K2
C	956	PHE	-	expression tag	UNP Q9H2K2
C	957	GLN	-	expression tag	UNP Q9H2K2
C	958	GLY	-	expression tag	UNP Q9H2K2

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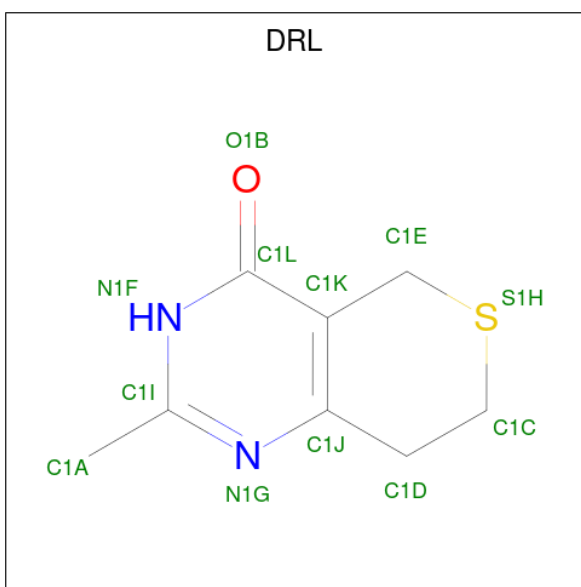
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression tag	UNP Q9H2K2
D	945	HIS	-	expression tag	UNP Q9H2K2
D	946	HIS	-	expression tag	UNP Q9H2K2
D	947	HIS	-	expression tag	UNP Q9H2K2
D	948	SER	-	expression tag	UNP Q9H2K2
D	949	SER	-	expression tag	UNP Q9H2K2
D	950	GLY	-	expression tag	UNP Q9H2K2
D	951	ARG	-	expression tag	UNP Q9H2K2
D	952	GLU	-	expression tag	UNP Q9H2K2
D	953	ASN	-	expression tag	UNP Q9H2K2
D	954	LEU	-	expression tag	UNP Q9H2K2
D	955	TYR	-	expression tag	UNP Q9H2K2
D	956	PHE	-	expression tag	UNP Q9H2K2
D	957	GLN	-	expression tag	UNP Q9H2K2
D	958	GLY	-	expression tag	UNP Q9H2K2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

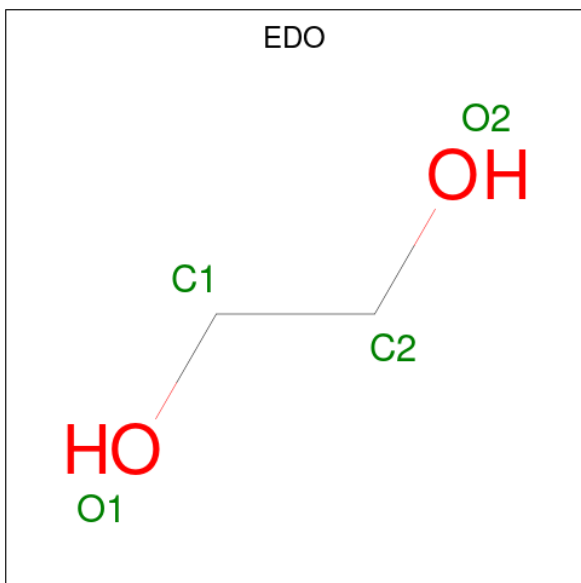
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 2-methyl-3,5,7,8-tetrahydro-4H-thiopyrano[4,3-d]pyrimidin-4-one (CCD ID: DRL) (formula: C₈H₁₀N₂OS).



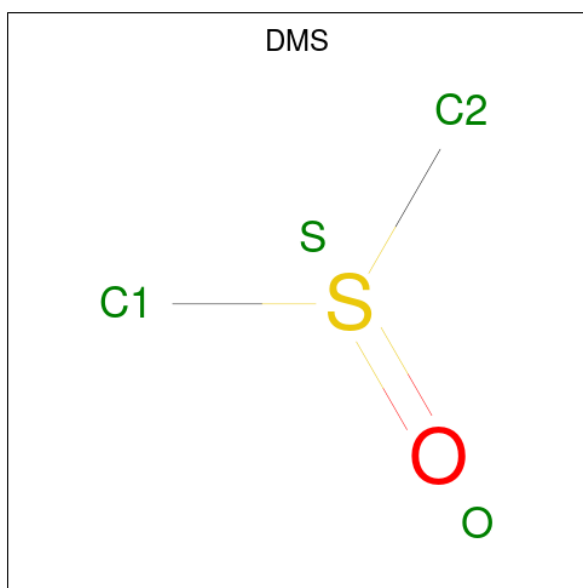
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	8	2	1	1		
3	B	1	Total	C	N	O	S	0	0
			12	8	2	1	1		
3	C	1	Total	C	N	O	S	0	0
			12	8	2	1	1		
3	D	1	Total	C	N	O	S	0	0
			12	8	2	1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
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 DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O S 4 2 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	235	Total O 235 235	0	0

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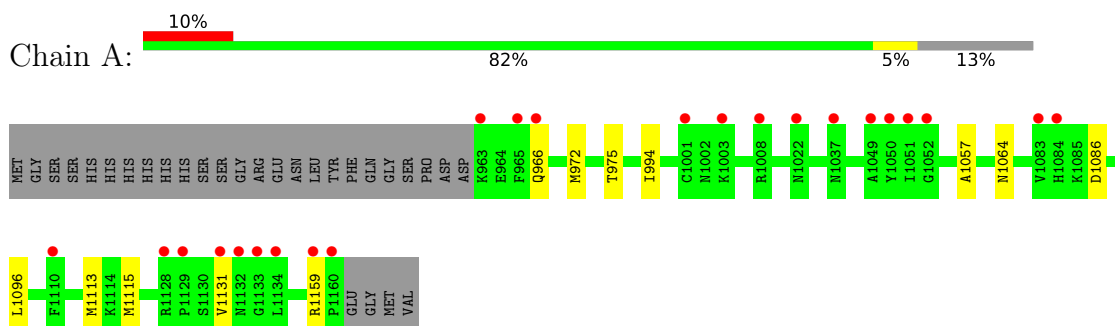
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	222	Total 222	O 222	0	0
6	C	243	Total 243	O 243	0	0
6	D	171	Total 171	O 171	0	0

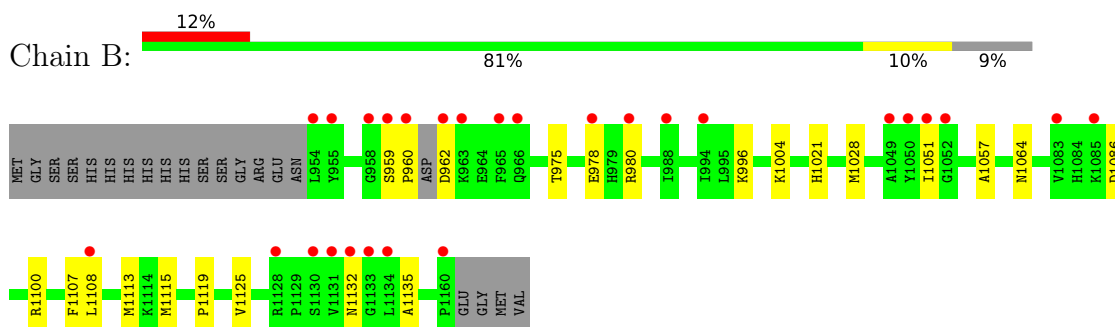
3 Residue-property plots [i](#)

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.

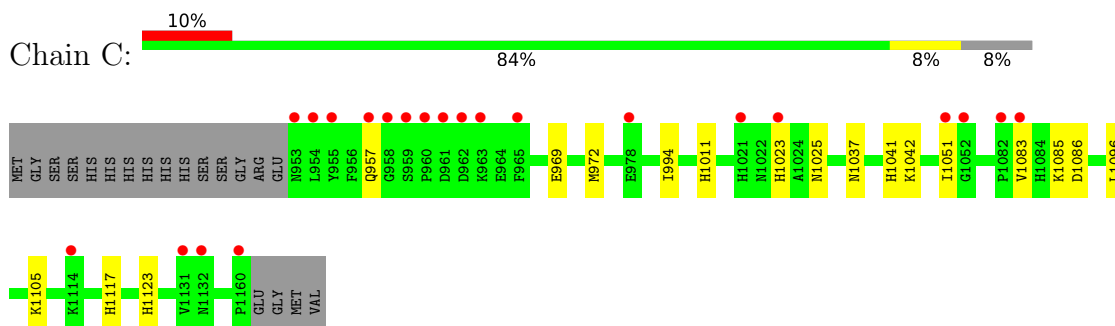
• Molecule 1: Tankyrase-2



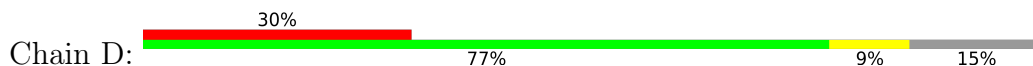
• Molecule 1: Tankyrase-2

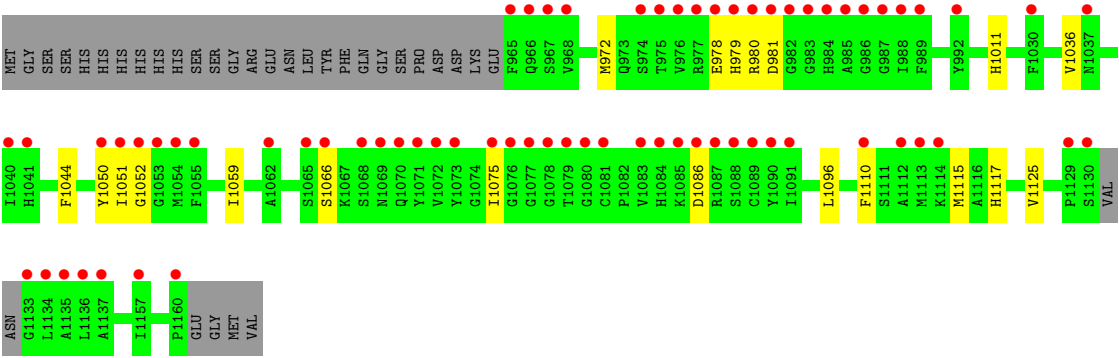


• Molecule 1: Tankyrase-2



• Molecule 1: Tankyrase-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.00Å 79.77Å 153.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 1.50 44.32 – 1.50	Depositor EDS
% Data completeness (in resolution range)	87.4 (44.32-1.50) 87.4 (44.32-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.50Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.244 0.211 , 0.241	Depositor DCC
R_{free} test set	1268 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7554	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% 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: DMS, DRL, ZN, 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	0.69	0/1669	1.10	1/2244 (0.0%)
1	B	0.67	0/1735	1.08	3/2330 (0.1%)
1	C	0.68	0/1752	1.10	2/2357 (0.1%)
1	D	0.69	0/1666	1.15	8/2238 (0.4%)
All	All	0.68	0/6822	1.11	14/9169 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1086	ASP	CA-CB-CG	6.29	118.89	112.60
1	D	1052	GLY	N-CA-C	6.22	120.42	112.83
1	D	1086	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	1086	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	1110	PHE	CA-CB-CG	5.71	119.50	113.80
1	D	1050	TYR	CA-C-N	5.51	129.66	120.62
1	D	1050	TYR	C-N-CA	5.51	129.66	120.62
1	D	1051	ILE	CA-C-N	5.50	126.19	120.03
1	D	1051	ILE	C-N-CA	5.50	126.19	120.03
1	B	1086	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	981	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	1021	HIS	CA-C-N	5.06	129.73	122.35
1	B	1021	HIS	C-N-CA	5.06	129.73	122.35
1	C	969	GLU	CB-CG-CD	5.03	121.14	112.60

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	1617	0	1563	7	0
1	B	1681	0	1620	10	0
1	C	1696	0	1627	11	0
1	D	1601	0	1550	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	10	0	0
3	B	12	0	10	0	0
3	C	12	0	10	0	0
3	D	12	0	10	0	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	C	16	0	24	2	0
4	D	4	0	6	0	0
5	D	4	0	6	0	0
6	A	235	0	0	0	0
6	B	222	0	0	0	0
6	C	243	0	0	2	0
6	D	171	0	0	2	0
All	All	7554	0	6454	33	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 (33) 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:1113:MET:HE3	1:A:1115[A]:MET:HE1	1.52	0.89
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.27	0.79
1:B:1115[A]:MET:HE1	1:B:1125:VAL:HG21	1.70	0.73
1:C:972:MET:HE1	1:C:1096[A]:LEU:HD12	1.80	0.64
1:A:1113:MET:HE3	1:A:1115[A]:MET:CE	2.29	0.61
1:C:1023[A]:HIS:HD2	1:C:1025:ASN:H	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:MET:HE3	1:B:1115[A]:MET:CE	2.29	0.61
1:A:972:MET:HE1	1:A:1096[A]:LEU:HD12	1.85	0.58
1:C:1042:LYS:HE2	4:C:1206:EDO:H22	1.87	0.57
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.89	0.56
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.88	0.55
1:D:979:HIS:HE1	1:D:1066:SER:HB2	1.71	0.54
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.92	0.53
1:C:1037:ASN:HB2	4:C:1205:EDO:H21	1.91	0.52
1:D:1115[A]:MET:HE1	1:D:1125:VAL:HG21	1.93	0.51
1:D:1117:HIS:HD2	6:D:1330:HOH:O	1.96	0.48
1:D:1011:HIS:HE1	6:D:1349:HOH:O	1.98	0.47
1:B:959:SER:HB3	1:B:960:PRO:HD2	1.96	0.47
1:B:1113:MET:HE3	1:B:1115[A]:MET:HE2	1.97	0.47
1:C:1117:HIS:HD2	6:C:1360:HOH:O	1.97	0.46
1:C:1011:HIS:HE1	6:C:1456:HOH:O	1.99	0.46
1:A:1113:MET:CE	1:A:1115[A]:MET:HE1	2.37	0.45
1:B:1028:MET:SD	1:B:1100:ARG:HG2	2.56	0.45
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.98	0.45
1:D:972:MET:HE1	1:D:1096[A]:LEU:HD12	1.98	0.44
1:D:1044:PHE:HB3	1:D:1059:ILE:HD13	1.99	0.44
1:C:1023[A]:HIS:CD2	1:C:1025:ASN:H	2.33	0.42
1:B:1115[A]:MET:HE3	1:B:1115[A]:MET:HB2	1.84	0.42
1:C:1037:ASN:O	1:C:1041:HIS:HD2	2.03	0.42
1:B:980:ARG:HE	1:B:1135:ALA:HB2	1.84	0.42
1:A:975:THR:HB	1:A:1064:ASN:HA	2.02	0.41
1:B:1107:PHE:CG	1:B:1119:PRO:HG2	2.56	0.41
1:B:975:THR:HB	1:B:1064:ASN:HA	2.04	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	200/227 (88%)	199 (100%)	1 (0%)	0	100	100
1	B	205/227 (90%)	204 (100%)	1 (0%)	0	100	100
1	C	209/227 (92%)	208 (100%)	1 (0%)	0	100	100
1	D	197/227 (87%)	193 (98%)	4 (2%)	0	100	100
All	All	811/908 (89%)	804 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	170/192 (88%)	166 (98%)	4 (2%)	43	15
1	B	177/192 (92%)	170 (96%)	7 (4%)	28	5
1	C	179/192 (93%)	175 (98%)	4 (2%)	45	17
1	D	169/192 (88%)	165 (98%)	4 (2%)	43	15
All	All	695/768 (90%)	676 (97%)	19 (3%)	39	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	966	GLN
1	A	1131	VAL
1	A	1159[A]	ARG
1	A	1159[B]	ARG
1	B	962	ASP
1	B	978	GLU
1	B	996	LYS
1	B	1004	LYS
1	B	1051	ILE
1	B	1108	LEU
1	B	1132	ASN
1	C	957	GLN
1	C	1051	ILE

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Mol	Chain	Res	Type
1	C	1083	VAL
1	C	1085	LYS
1	D	978	GLU
1	D	980	ARG
1	D	1036	VAL
1	D	1075	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	998	GLN
1	A	1011	HIS
1	A	1020	ASN
1	A	1022	ASN
1	A	1023	HIS
1	B	1037	ASN
1	B	1109	GLN
1	C	1011	HIS
1	C	1041	HIS
1	C	1109	GLN
1	C	1117	HIS
1	C	1123	HIS
1	D	979	HIS
1	D	998	GLN
1	D	1011	HIS
1	D	1117	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

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	1206	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	D	1204	-	3,3,3	0.52	0	2,2,2	0.36	0
4	EDO	C	1203	-	3,3,3	0.52	0	2,2,2	0.23	0
5	DMS	D	1203	-	3,3,3	0.34	0	3,3,3	0.36	0
3	DRL	C	1202	-	13,13,13	1.84	4 (30%)	10,18,18	2.24	4 (40%)
3	DRL	B	1202	-	13,13,13	1.81	4 (30%)	10,18,18	2.48	4 (40%)
4	EDO	C	1204	-	3,3,3	0.54	0	2,2,2	0.33	0
3	DRL	A	1202	-	13,13,13	1.77	4 (30%)	10,18,18	2.56	4 (40%)
4	EDO	B	1204	-	3,3,3	0.48	0	2,2,2	0.43	0
3	DRL	D	1202	-	13,13,13	1.80	4 (30%)	10,18,18	2.54	4 (40%)
4	EDO	B	1203	-	3,3,3	0.53	0	2,2,2	0.34	0
4	EDO	C	1205	-	3,3,3	0.43	0	2,2,2	0.32	0
4	EDO	A	1203	-	3,3,3	0.52	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	C	1206	-	-	0/1/1/1	-
4	EDO	D	1204	-	-	0/1/1/1	-
3	DRL	C	1202	-	-	-	0/2/2/2
3	DRL	B	1202	-	-	-	0/2/2/2
4	EDO	C	1204	-	-	0/1/1/1	-
4	EDO	A	1203	-	-	0/1/1/1	-
3	DRL	A	1202	-	-	-	0/2/2/2
4	EDO	B	1204	-	-	0/1/1/1	-
3	DRL	D	1202	-	-	-	0/2/2/2
4	EDO	B	1203	-	-	0/1/1/1	-
4	EDO	C	1205	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	1203	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	DRL	C1D-C1J	3.13	1.55	1.50
3	B	1202	DRL	C1D-C1J	3.11	1.55	1.50
3	C	1202	DRL	C1E-C1K	3.11	1.54	1.50
3	A	1202	DRL	C1E-C1K	3.10	1.54	1.50
3	B	1202	DRL	C1E-C1K	3.09	1.54	1.50
3	D	1202	DRL	C1E-C1K	3.05	1.54	1.50
3	C	1202	DRL	C1K-C1J	3.03	1.43	1.37
3	C	1202	DRL	C1D-C1J	2.95	1.55	1.50
3	A	1202	DRL	C1D-C1J	2.78	1.55	1.50
3	A	1202	DRL	C1K-C1J	2.77	1.42	1.37
3	B	1202	DRL	C1K-C1J	2.71	1.42	1.37
3	D	1202	DRL	C1K-C1J	2.66	1.42	1.37
3	B	1202	DRL	C1L-C1K	-2.30	1.40	1.44
3	A	1202	DRL	C1L-C1K	-2.21	1.41	1.44
3	C	1202	DRL	C1L-C1K	-2.17	1.41	1.44
3	D	1202	DRL	C1L-C1K	-2.10	1.41	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	DRL	C1K-C1L-N1F	6.44	120.60	115.70
3	D	1202	DRL	C1K-C1L-N1F	6.08	120.32	115.70
3	B	1202	DRL	C1K-C1L-N1F	6.01	120.27	115.70
3	C	1202	DRL	C1K-C1L-N1F	5.46	119.85	115.70
3	D	1202	DRL	N1F-C1I-N1G	-2.93	119.16	122.96
3	B	1202	DRL	N1F-C1I-N1G	-2.76	119.39	122.96
3	A	1202	DRL	C1K-C1J-N1G	-2.61	119.97	123.68
3	B	1202	DRL	O1B-C1L-C1K	-2.58	121.38	124.56
3	D	1202	DRL	C1K-C1J-N1G	-2.51	120.11	123.68
3	B	1202	DRL	C1K-C1J-N1G	-2.45	120.20	123.68
3	C	1202	DRL	C1K-C1J-N1G	-2.42	120.24	123.68
3	D	1202	DRL	O1B-C1L-C1K	-2.40	121.61	124.56
3	A	1202	DRL	N1F-C1I-N1G	-2.38	119.88	122.96
3	A	1202	DRL	O1B-C1L-C1K	-2.31	121.72	124.56
3	C	1202	DRL	N1F-C1I-N1G	-2.17	120.15	122.96
3	C	1202	DRL	O1B-C1L-C1K	-2.09	121.99	124.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1205	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1206	EDO	1	0
4	C	1205	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	198/227 (87%)	0.57	23 (11%) 9 9	10, 21, 41, 52	4 (2%)
1	B	206/227 (90%)	0.67	27 (13%) 7 7	10, 22, 43, 64	3 (1%)
1	C	208/227 (91%)	0.54	22 (10%) 11 11	10, 20, 41, 56	3 (1%)
1	D	194/227 (85%)	1.52	69 (35%) 1 1	14, 29, 48, 69	7 (3%)
All	All	806/908 (88%)	0.82	141 (17%) 4 3	10, 22, 45, 69	17 (2%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1052	GLY	6.4
1	D	1110	PHE	6.1
1	D	983	GLY	6.0
1	D	979	HIS	5.6
1	B	960	PRO	5.4
1	B	1131	VAL	5.0
1	D	1136	LEU	5.0
1	D	1051	ILE	4.7
1	D	985	ALA	4.7
1	D	1135	ALA	4.7
1	C	965	PHE	4.7
1	A	1050	TYR	4.6
1	B	1051	ILE	4.6
1	D	1130	SER	4.5
1	A	965	PHE	4.5
1	D	965	PHE	4.3
1	D	976	VAL	4.3
1	C	1051	ILE	4.3
1	D	1129	PRO	4.2
1	D	1134	LEU	4.1
1	B	1083	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	1076	GLY	4.0
1	D	1083	VAL	4.0
1	D	1080	GLY	3.9
1	A	1131	VAL	3.9
1	D	1071	TYR	3.9
1	B	1050	TYR	3.8
1	C	1083	VAL	3.8
1	C	960	PRO	3.7
1	D	1137	ALA	3.7
1	D	984	HIS	3.7
1	D	1133	GLY	3.7
1	D	1072	VAL	3.6
1	D	981	ASP	3.6
1	C	955	TYR	3.4
1	D	1113	MET	3.4
1	D	1075	ILE	3.4
1	A	1133	GLY	3.4
1	D	1114	LYS	3.3
1	A	1132	ASN	3.3
1	D	1077	GLY	3.3
1	B	1160	PRO	3.3
1	D	975	THR	3.2
1	B	954	LEU	3.2
1	B	1133	GLY	3.2
1	C	959	SER	3.2
1	D	988	ILE	3.2
1	D	989	PHE	3.1
1	D	980	ARG	3.1
1	C	962	ASP	3.1
1	A	1160	PRO	3.1
1	D	986	GLY	3.1
1	D	1081	CYS	3.1
1	D	982	GLY	3.1
1	A	1052	GLY	3.0
1	C	1160	PRO	3.0
1	B	1128	ARG	2.9
1	C	1132	ASN	2.9
1	D	977	ARG	2.9
1	D	1078	GLY	2.9
1	A	1049	ALA	2.9
1	C	963	LYS	2.9
1	D	1065	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	954	LEU	2.8
1	D	1089	CYS	2.8
1	B	965	PHE	2.8
1	D	974	SER	2.8
1	D	1079	THR	2.8
1	C	958	GLY	2.8
1	D	1037[A]	ASN	2.8
1	D	1085	LYS	2.8
1	B	980	ARG	2.8
1	B	959	SER	2.7
1	D	1066	SER	2.7
1	C	961	ASP	2.7
1	A	966	GLN	2.7
1	D	1050	TYR	2.7
1	D	1090	TYR	2.7
1	A	1159[A]	ARG	2.7
1	D	987	GLY	2.7
1	D	1052	GLY	2.7
1	D	1087	ARG	2.7
1	D	1062	ALA	2.6
1	C	1023[A]	HIS	2.6
1	C	1131	VAL	2.6
1	A	1134	LEU	2.6
1	B	1085	LYS	2.6
1	B	958	GLY	2.6
1	D	1160	PRO	2.6
1	A	1110	PHE	2.5
1	C	953	ASN	2.5
1	D	1084	HIS	2.5
1	D	1086	ASP	2.5
1	D	968	VAL	2.5
1	B	978	GLU	2.5
1	D	1054	MET	2.5
1	D	1112	ALA	2.4
1	D	1070	GLN	2.4
1	B	1132	ASN	2.4
1	A	1051	ILE	2.4
1	B	988	ILE	2.4
1	D	1091	ILE	2.4
1	D	1157	ILE	2.4
1	D	992	TYR	2.4
1	D	1041[A]	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1134	LEU	2.3
1	B	1130	SER	2.3
1	A	963	LYS	2.3
1	B	1052	GLY	2.3
1	B	994	ILE	2.3
1	A	1037	ASN	2.2
1	C	1114	LYS	2.2
1	D	1040	ILE	2.2
1	A	1022	ASN	2.2
1	B	1049	ALA	2.2
1	C	957	GLN	2.2
1	A	1084	HIS	2.2
1	C	1021	HIS	2.2
1	A	1129	PRO	2.2
1	B	963	LYS	2.2
1	B	962	ASP	2.2
1	C	1082	PRO	2.1
1	D	1073	TYR	2.1
1	A	1001	CYS	2.1
1	D	1068	SER	2.1
1	A	1003	LYS	2.1
1	D	967	SER	2.1
1	D	1030	PHE	2.1
1	D	1088	SER	2.1
1	C	978	GLU	2.1
1	A	1083	VAL	2.1
1	D	1053	GLY	2.1
1	B	955	TYR	2.1
1	D	966	GLN	2.1
1	A	1008	ARG	2.0
1	A	1128	ARG	2.0
1	B	1108	LEU	2.0
1	D	1069	ASN	2.0
1	B	966	GLN	2.0
1	D	978	GLU	2.0
1	D	1055	PHE	2.0

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

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	B	1203	4/4	0.59	0.28	53,54,55,57	0
4	EDO	A	1203	4/4	0.60	0.23	60,60,61,61	0
4	EDO	B	1204	4/4	0.70	0.24	53,54,54,54	0
4	EDO	C	1206	4/4	0.72	0.21	72,73,73,73	0
5	DMS	D	1203	4/4	0.72	0.27	85,85,85,85	0
4	EDO	D	1204	4/4	0.74	0.21	45,45,46,46	0
4	EDO	C	1205	4/4	0.78	0.21	42,44,45,45	0
4	EDO	C	1204	4/4	0.82	0.14	27,28,28,30	0
3	DRL	D	1202	12/12	0.90	0.11	27,30,31,33	0
2	ZN	D	1201	1/1	0.92	0.10	38,38,38,38	0
4	EDO	C	1203	4/4	0.94	0.09	24,28,28,30	0
2	ZN	B	1201	1/1	0.94	0.07	30,30,30,30	0
2	ZN	A	1201	1/1	0.95	0.07	25,25,25,25	0
2	ZN	C	1201	1/1	0.96	0.06	27,27,27,27	0
3	DRL	B	1202	12/12	0.97	0.07	19,20,21,22	0
3	DRL	A	1202	12/12	0.98	0.05	14,17,17,18	0
3	DRL	C	1202	12/12	0.99	0.05	13,14,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.