



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:22 PM UTC

PDB ID : 4PNQ / pdb_00004pnq
Title : Crystal Structure of human Tankyrase 2 in complex with 5AIQ.
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 : 2014-05-24
Resolution : 1.85 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

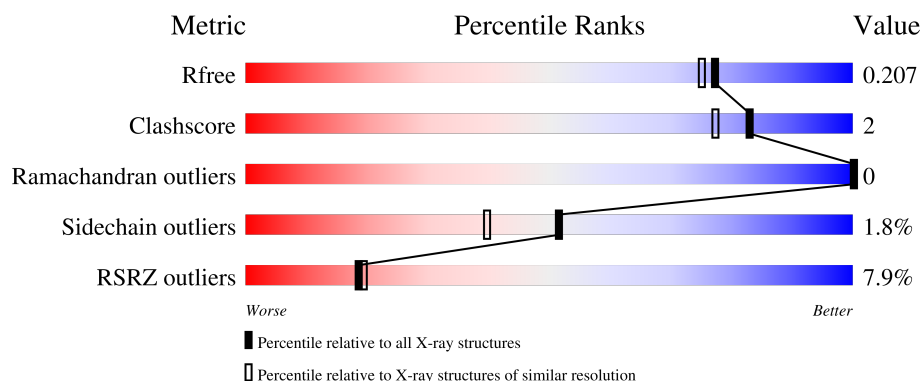
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	5% 83% 5% 11%
1	B	227	9% 86% •• 8%
1	C	227	6% 84% 7% 8%
1	D	227	8% 76% 7% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7421 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	202	Total	C	N	O	S	0	1	0
			1634	1029	300	293	12			
1	B	208	Total	C	N	O	S	0	1	0
			1687	1067	307	302	11			
1	C	208	Total	C	N	O	S	0	1	0
			1686	1066	308	301	11			
1	D	190	Total	C	N	O	S	0	0	0
			1543	973	286	273	11			

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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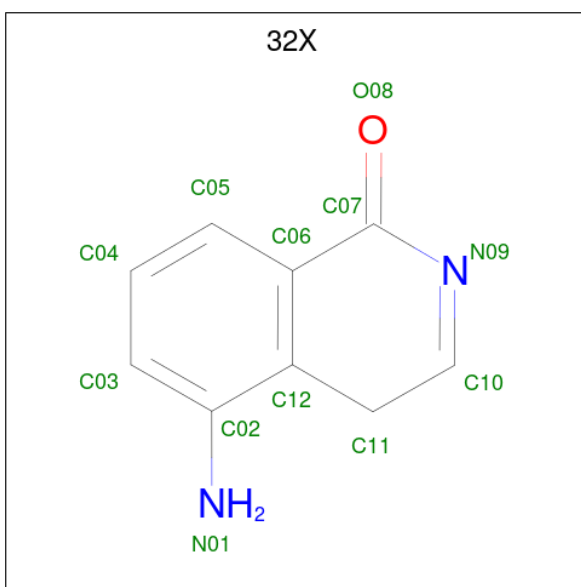
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	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).

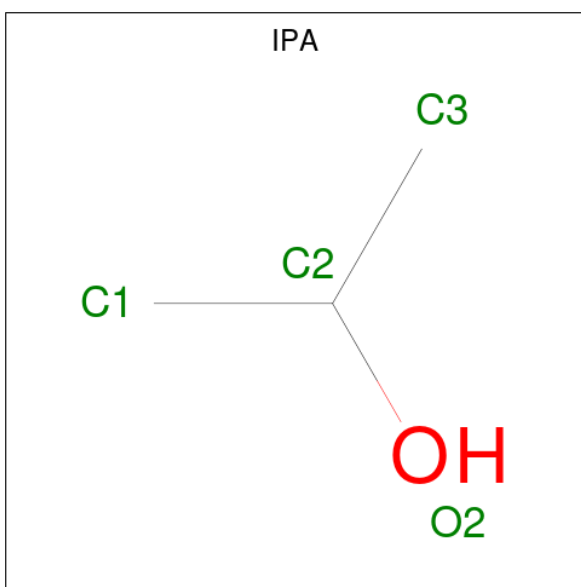
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 5-aminoisoquinolin-1(4H)-one (CCD ID: 32X) (formula: C₉H₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	2	1		
3	B	1	Total	C	N	O	0	0
			12	9	2	1		
3	C	1	Total	C	N	O	0	0
			12	9	2	1		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is water.

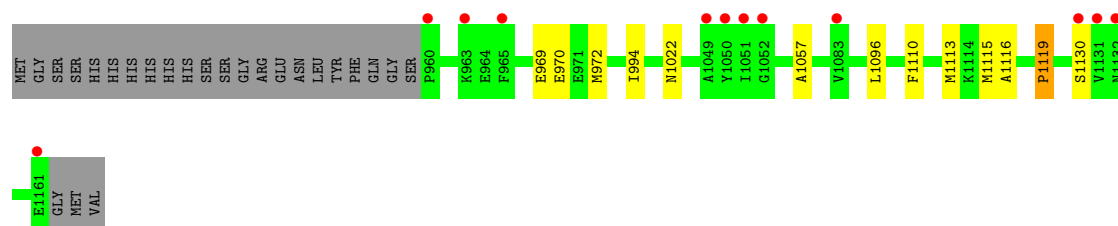
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0
5	B	191	Total 191	O 191	0	0
5	C	252	Total 252	O 252	0	0
5	D	178	Total 178	O 178	0	0

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.

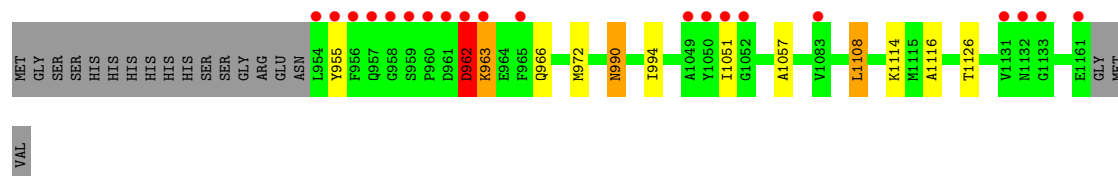
• Molecule 1: Tankyrase-2

Chain A: 



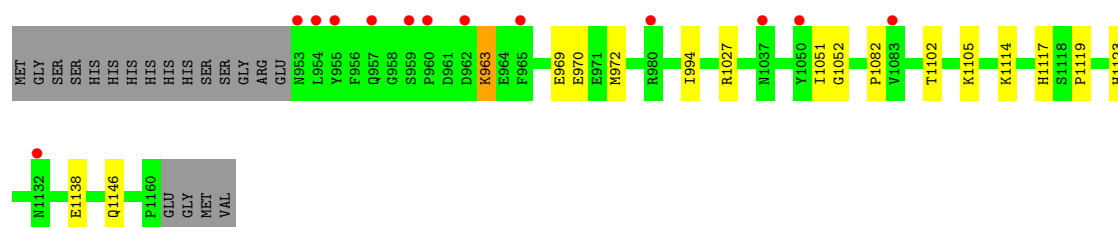
• Molecule 1: Tankyrase-2

Chain B: 



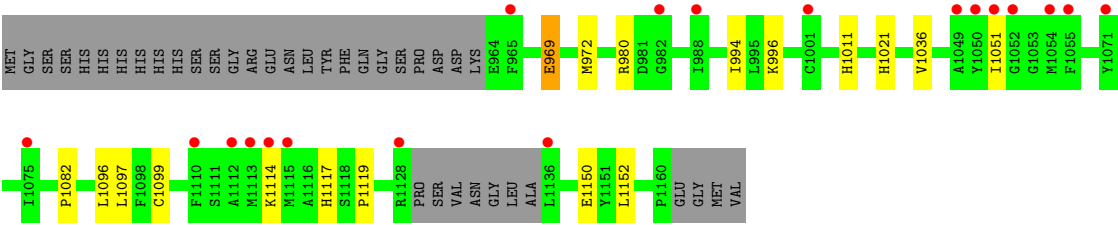
• Molecule 1: Tankyrase-2

Chain C: 



• Molecule 1: Tankyrase-2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.03Å 79.47Å 153.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.73 – 1.85 76.72 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (76.73-1.85) 99.6 (76.72-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.84Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.188 , 0.227 (Not available) , 0.207	Depositor DCC
R_{free} test set	990 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7421	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.59% 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: 32X, ZN, IPA

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	0.82	1/1681 (0.1%)	1.15	4/2259 (0.2%)
1	B	0.82	0/1737	1.15	7/2336 (0.3%)
1	C	0.81	1/1736 (0.1%)	1.14	5/2335 (0.2%)
1	D	0.82	1/1584 (0.1%)	1.14	3/2126 (0.1%)
All	All	0.82	3/6738 (0.0%)	1.14	19/9056 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1119	PRO	CA-C	5.63	1.54	1.51
1	A	1119	PRO	CA-C	5.45	1.54	1.51
1	D	1119	PRO	CA-C	5.02	1.54	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	990	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	955	TYR	N-CA-C	6.27	119.69	109.59
1	B	963	LYS	CA-C-N	6.04	128.65	120.44
1	B	963	LYS	C-N-CA	6.04	128.65	120.44
1	D	969	GLU	CB-CG-CD	5.93	122.69	112.60
1	C	969	GLU	CB-CG-CD	5.77	122.42	112.60
1	B	962	ASP	CA-C-N	5.76	128.79	120.38
1	B	962	ASP	C-N-CA	5.76	128.79	120.38
1	D	1150	GLU	N-CA-C	5.71	117.58	111.36
1	C	963	LYS	CA-C-N	5.67	127.81	120.44
1	C	963	LYS	C-N-CA	5.67	127.81	120.44
1	A	1116	ALA	N-CA-C	-5.44	105.77	112.90
1	B	1116	ALA	N-CA-C	-5.32	105.06	112.45
1	C	1052	GLY	N-CA-C	5.29	120.17	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1099	CYS	N-CA-C	5.26	118.31	109.95
1	A	969	GLU	CB-CG-CD	5.23	121.49	112.60
1	A	970	GLU	CB-CG-CD	5.07	121.21	112.60
1	A	1022	ASN	CA-CB-CG	5.02	117.62	112.60
1	C	970	GLU	CB-CG-CD	5.00	121.10	112.60

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	1634	0	1568	8	0
1	B	1687	0	1612	4	0
1	C	1686	0	1612	10	0
1	D	1543	0	1477	11	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	8	0	0
3	B	12	0	8	0	0
3	C	12	0	8	1	0
4	C	4	0	8	1	0
5	A	206	0	0	0	0
5	B	191	0	0	0	0
5	C	252	0	0	3	0
5	D	178	0	0	4	0
All	All	7421	0	6301	31	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 2.

All (31) 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:1105:LYS:H	1:C:1123:HIS:HD2	1.24	0.85
1:C:1138:GLU:OE1	4:C:1203:IPA:H11	1.91	0.70
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.78	0.65
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.80	0.63
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.82	0.61
1:D:1117:HIS:HD2	5:D:1441:HOH:O	1.86	0.59
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.88	0.57
1:D:996:LYS:HE2	5:D:1353:HOH:O	2.08	0.54
1:C:1105:LYS:H	1:C:1123:HIS:CD2	2.16	0.53
1:A:1115[A]:MET:HE1	1:A:1119:PRO:HG3	1.91	0.52
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.93	0.50
1:C:1117:HIS:HD2	5:C:1503:HOH:O	1.92	0.50
1:C:972:MET:HG2	1:C:994:ILE:CD1	2.45	0.47
1:D:1011:HIS:HE1	5:D:1366:HOH:O	1.97	0.46
1:C:1027:ARG:HD2	1:D:1021:HIS:CE1	2.52	0.45
1:C:1102:THR:HB	1:C:1146:GLN:HG2	1.99	0.45
1:D:1082:PRO:HD2	5:D:1416:HOH:O	2.17	0.45
1:A:1110:PHE:HD1	1:A:1130:SER:HB3	1.83	0.44
1:D:969:GLU:HG3	1:D:994:ILE:HD12	2.00	0.44
1:A:1113:MET:HE3	1:A:1115[A]:MET:SD	2.59	0.43
1:C:1082:PRO:HD2	5:C:1475:HOH:O	2.18	0.43
1:D:1036:VAL:HG13	1:D:1097:LEU:HD21	2.01	0.43
1:D:972:MET:HE1	1:D:1096:LEU:HD12	1.99	0.43
1:B:1108:LEU:HD12	1:B:1126:THR:HB	2.01	0.42
1:A:1115[A]:MET:HE2	1:A:1115[A]:MET:HB3	1.79	0.41
1:A:972:MET:HE1	1:A:1096:LEU:HD12	2.01	0.41
3:C:1201:32X:H1	5:C:1393:HOH:O	2.21	0.41
1:D:1036:VAL:HG11	1:D:1152:LEU:CD1	2.50	0.41
1:B:962:ASP:O	1:B:966:GLN:HG2	2.21	0.40
1:D:1036:VAL:HG11	1:D:1152:LEU:HD13	2.04	0.40
1:A:972:MET:HG2	1:A:994:ILE:CD1	2.48	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	201/227 (88%)	197 (98%)	4 (2%)	0	100	100
1	B	207/227 (91%)	201 (97%)	6 (3%)	0	100	100
1	C	207/227 (91%)	204 (99%)	3 (1%)	0	100	100
1	D	186/227 (82%)	181 (97%)	5 (3%)	0	100	100
All	All	801/908 (88%)	783 (98%)	18 (2%)	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	172/192 (90%)	172 (100%)	0	100	100
1	B	177/192 (92%)	171 (97%)	6 (3%)	32	17
1	C	177/192 (92%)	174 (98%)	3 (2%)	53	42
1	D	161/192 (84%)	158 (98%)	3 (2%)	50	38
All	All	687/768 (90%)	675 (98%)	12 (2%)	51	42

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	962	ASP
1	B	963	LYS
1	B	990	ASN
1	B	1051	ILE
1	B	1108	LEU
1	B	1114	LYS
1	C	963	LYS
1	C	1051	ILE
1	C	1114	LYS
1	D	980	ARG

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Mol	Chain	Res	Type
1	D	1051	ILE
1	D	1114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1095	GLN
1	A	1132	ASN
1	B	957	GLN
1	B	984	HIS
1	B	1037	ASN
1	B	1048	HIS
1	C	953	ASN
1	C	984	HIS
1	C	990	ASN
1	C	1011	HIS
1	C	1037	ASN
1	C	1048	HIS
1	C	1064	ASN
1	C	1095	GLN
1	C	1117	HIS
1	C	1123	HIS
1	C	1132	ASN
1	D	1011	HIS
1	D	1021	HIS
1	D	1064	ASN
1	D	1117	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	IPA	C	1203	-	3,3,3	0.76	0	3,3,3	0.92	0
3	32X	B	1201	-	12,13,13	3.61	5 (41%)	12,18,18	1.32	2 (16%)
3	32X	C	1201	-	12,13,13	4.91	5 (41%)	12,18,18	1.24	2 (16%)
3	32X	A	1202	-	12,13,13	4.18	4 (33%)	12,18,18	1.45	3 (25%)

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
3	32X	B	1201	-	-	-	0/2/2/2
3	32X	C	1201	-	-	-	0/2/2/2
3	32X	A	1202	-	-	-	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1201	32X	C02-C12	15.00	1.47	1.40
3	A	1202	32X	C02-C12	11.26	1.45	1.40
3	B	1201	32X	C02-C12	9.83	1.45	1.40
3	C	1201	32X	C10-N09	5.69	1.41	1.28
3	B	1201	32X	C10-N09	5.69	1.41	1.28
3	A	1202	32X	C04-C03	5.55	1.48	1.38
3	A	1202	32X	C10-N09	5.53	1.41	1.28
3	C	1201	32X	C04-C03	3.11	1.44	1.38
3	C	1201	32X	C11-C12	-2.70	1.45	1.51
3	B	1201	32X	C05-C06	2.58	1.43	1.39
3	B	1201	32X	C11-C12	-2.56	1.46	1.51
3	A	1202	32X	C04-C05	2.35	1.42	1.38
3	B	1201	32X	C04-C03	2.32	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1201	32X	C05-C06	2.23	1.43	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1201	32X	O08-C07-C06	3.01	126.18	121.33
3	A	1202	32X	O08-C07-C06	3.00	126.16	121.33
3	C	1201	32X	O08-C07-C06	2.98	126.14	121.33
3	A	1202	32X	O08-C07-N09	-2.31	116.67	120.23
3	B	1201	32X	O08-C07-N09	-2.28	116.72	120.23
3	A	1202	32X	C05-C06-C12	2.16	122.53	119.78
3	C	1201	32X	O08-C07-N09	-2.10	117.00	120.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1203	IPA	1	0
3	C	1201	32X	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	202/227 (88%)	0.09	12 (5%)	28 31	15, 27, 54, 81	2 (0%)
1	B	208/227 (91%)	0.23	20 (9%)	13 13	14, 26, 60, 92	1 (0%)
1	C	208/227 (91%)	0.00	13 (6%)	26 28	14, 24, 48, 65	1 (0%)
1	D	190/227 (83%)	0.45	19 (10%)	12 12	18, 32, 57, 78	0
All	All	808/908 (88%)	0.19	64 (7%)	18 19	14, 27, 57, 92	4 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1113	MET	5.4
1	C	965[A]	PHE	5.3
1	B	1049	ALA	5.0
1	A	1050	TYR	5.0
1	B	965[A]	PHE	4.9
1	B	960	PRO	4.8
1	A	960	PRO	4.4
1	B	1051	ILE	4.3
1	B	1050	TYR	4.1
1	B	954	LEU	4.1
1	B	958	GLY	3.9
1	A	1049	ALA	3.9
1	B	1131	VAL	3.8
1	D	1051	ILE	3.8
1	D	965	PHE	3.7
1	A	1131	VAL	3.5
1	A	1052	GLY	3.5
1	D	1050	TYR	3.4
1	B	961	ASP	3.3
1	B	1083	VAL	3.2
1	D	1136	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	954	LEU	3.1
1	B	962	ASP	3.1
1	D	1115	MET	3.0
1	D	1049	ALA	3.0
1	D	1054	MET	3.0
1	B	956	PHE	3.0
1	A	963	LYS	2.9
1	C	957	GLN	2.8
1	B	959	SER	2.8
1	A	1132	ASN	2.8
1	D	1001	CYS	2.7
1	B	1161	GLU	2.6
1	C	955	TYR	2.6
1	C	953	ASN	2.6
1	C	1083	VAL	2.6
1	A	1083	VAL	2.5
1	A	1051	ILE	2.5
1	C	1132	ASN	2.4
1	A	965	PHE	2.4
1	B	955	TYR	2.4
1	A	1130	SER	2.4
1	A	1161	GLU	2.3
1	C	962	ASP	2.3
1	B	957	GLN	2.3
1	D	1110	PHE	2.3
1	B	1132	ASN	2.2
1	D	982	GLY	2.2
1	D	1112	ALA	2.2
1	D	1075	ILE	2.2
1	C	1037	ASN	2.2
1	C	959	SER	2.2
1	B	1052	GLY	2.2
1	D	1114	LYS	2.2
1	C	1050	TYR	2.1
1	D	1052	GLY	2.1
1	D	1055	PHE	2.1
1	D	1128	ARG	2.1
1	C	960	PRO	2.1
1	C	980	ARG	2.1
1	B	963	LYS	2.0
1	D	988	ILE	2.0
1	B	1133	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1071	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IPA	C	1203	4/4	0.82	0.17	23,31,31,40	0
3	32X	A	1202	12/12	0.88	0.09	20,26,29,29	0
3	32X	B	1201	12/12	0.93	0.07	23,27,28,29	0
3	32X	C	1201	12/12	0.97	0.04	18,20,21,22	0
2	ZN	C	1202	1/1	0.99	0.02	32,32,32,32	0
2	ZN	D	1200	1/1	0.99	0.03	41,41,41,41	0
2	ZN	A	1201	1/1	1.00	0.01	34,34,34,34	0
2	ZN	B	1202	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.