



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:52 am GMT

PDB ID : 4TKI  
Title : Crystal Structure of human Tankyrase 2 in complex with BSI-201.  
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 : 2014-05-26  
Resolution : 2.15 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

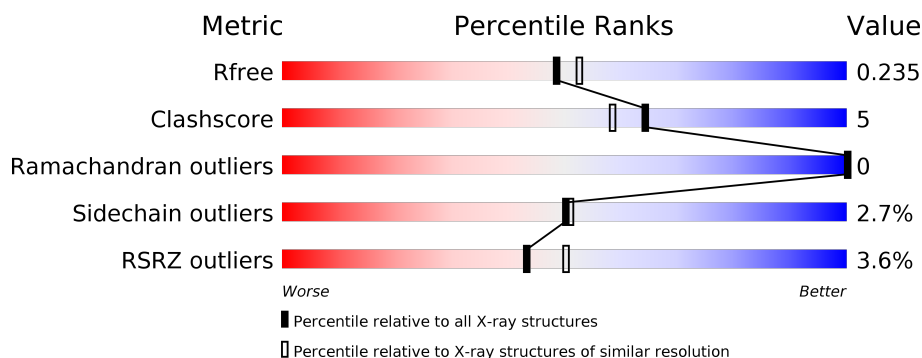
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>12%</div> </div> </div>
1	B	227	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	227	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	D	227	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>15%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	33E	A	1204	-	-	-	X
3	33E	D	1202	-	-	-	X
3	33E	D	1204	-	-	-	X
4	IPA	A	1205	-	-	-	X
4	IPA	B	1204	-	-	-	X
4	IPA	C	1204	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7194 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	199	Total	C	N	O	S	0	1	0
			1609	1015	297	286	11			
1	B	204	Total	C	N	O	S	0	0	0
			1649	1042	303	293	11			
1	C	208	Total	C	N	O	S	0	0	0
			1673	1055	308	299	11			
1	D	193	Total	C	N	O	S	0	0	0
			1560	982	290	277	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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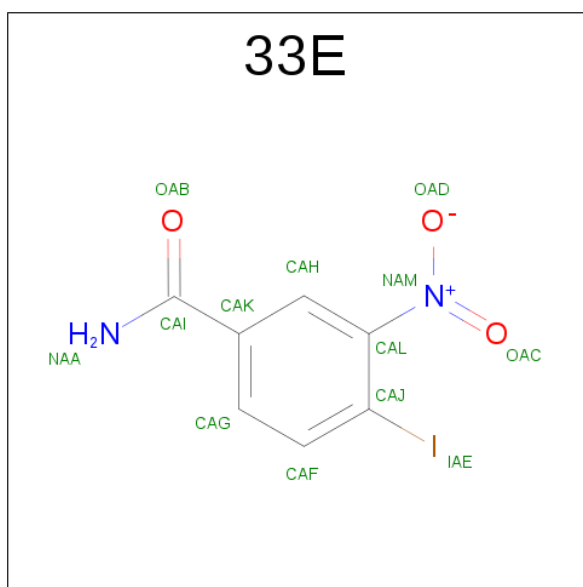
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	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 (three-letter code: ZN) (formula: Zn).

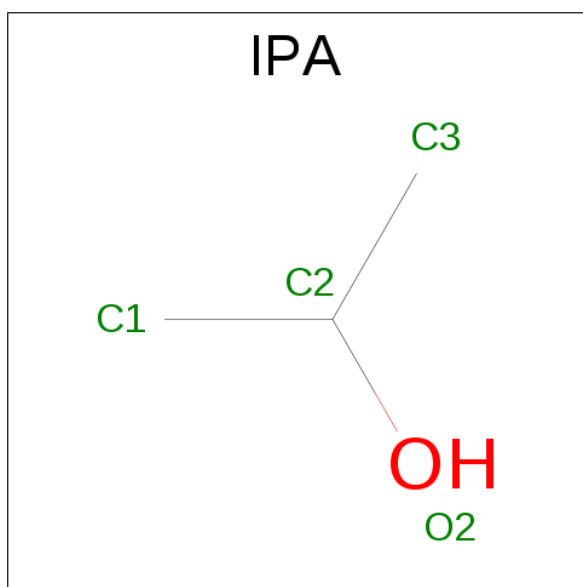
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 4-iodo-3-nitrobenzamide (three-letter code: 33E) (formula: C<sub>7</sub>H<sub>5</sub>IN<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	A	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	A	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	B	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	B	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	C	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	C	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	D	1	Total	C	I	N	O	
			13	7	1	2	3	0
3	D	1	Total	C	I	N	O	
			13	7	1	2	3	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

- Molecule 5 is water.

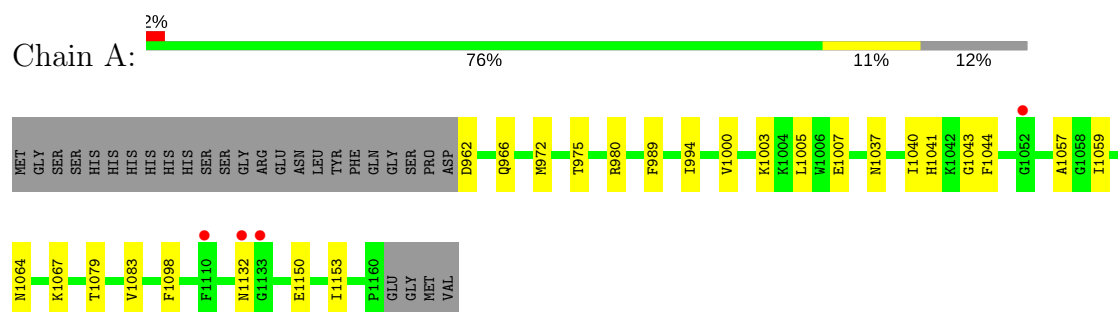
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	149	Total O 149 149	0	0
5	B	139	Total O 139 139	0	0
5	C	139	Total O 139 139	0	0
5	D	126	Total O 126 126	0	0



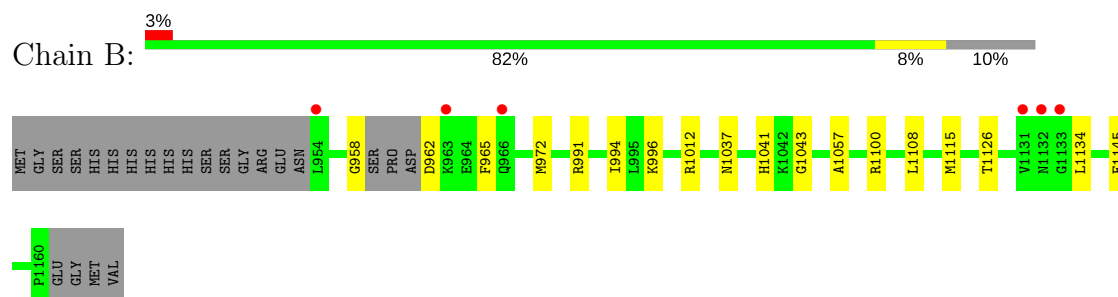
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

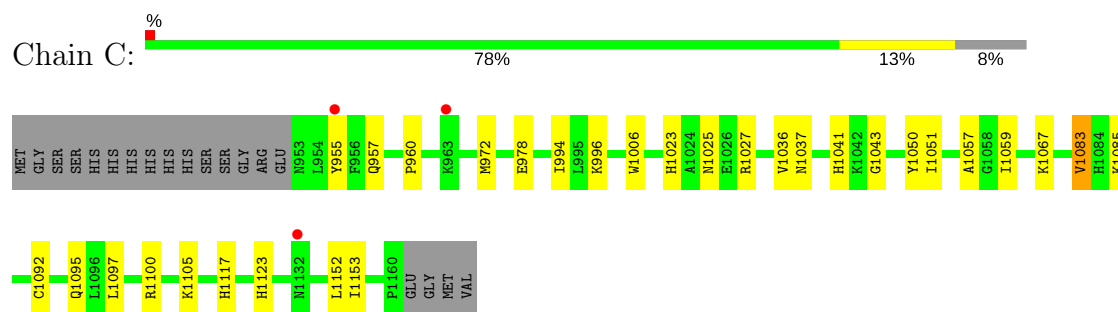
#### • Molecule 1: Tankyrase-2



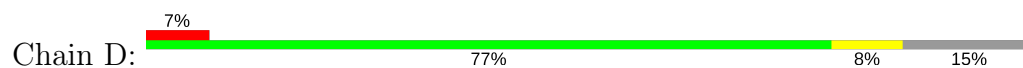
#### • Molecule 1: Tankyrase-2

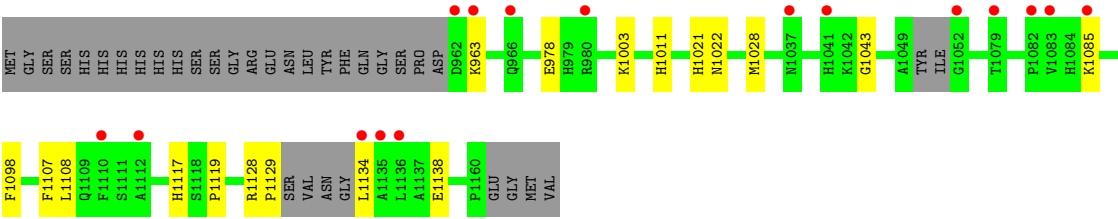


#### • Molecule 1: Tankyrase-2



#### • Molecule 1: Tankyrase-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.01Å 79.47Å 153.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.39 – 2.15 19.35 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.39-2.15) 99.2 (19.35-2.15)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.15Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.178 , 0.228 0.184 , 0.235	Depositor DCC
$R_{free}$ test set	1141 reflections (2.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 33E, 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	0.53	0/1655	0.73	1/2225 (0.0%)
1	B	0.52	0/1693	0.70	0/2274
1	C	0.55	0/1718	0.72	1/2310 (0.0%)
1	D	0.50	0/1600	0.68	0/2146
All	All	0.52	0/6666	0.71	2/8955 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	960	PRO	N-CA-CB	5.75	110.20	103.30
1	A	1132	ASN	C-N-CA	5.07	132.94	122.30

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	1609	0	1550	15	0
1	B	1649	0	1580	8	0
1	C	1673	0	1595	23	0
1	D	1560	0	1496	10	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	39	0	15	5	0
3	B	26	0	10	3	0
3	C	26	0	10	6	0
3	D	39	0	15	4	0
4	A	8	0	16	3	0
4	B	4	0	8	0	0
4	C	4	0	8	2	0
5	A	149	0	0	1	0
5	B	139	0	0	1	0
5	C	139	0	0	2	0
5	D	126	0	0	1	0
All	All	7194	0	6303	62	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 5.

All (62) 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)
3:A:1202:33E:OAC	3:A:1202:33E:IAE	2.70	0.78
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.32	0.76
1:C:1023:HIS:HD2	1:C:1025:ASN:H	1.36	0.73
3:C:1202:33E:OAC	3:C:1202:33E:IAE	2.82	0.68
1:B:1115:MET:SD	5:B:1389:HOH:O	2.53	0.66
1:A:1037:ASN:O	1:A:1041:HIS:HD2	1.80	0.65
3:D:1202:33E:IAE	3:D:1202:33E:OAC	2.85	0.65
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.81	0.64
1:C:1037:ASN:O	1:C:1041:HIS:HD2	1.82	0.62
3:D:1204:33E:IAE	3:D:1204:33E:OAC	2.87	0.61
1:D:1108:LEU:HD11	1:D:1128:ARG:HD3	1.81	0.61
3:B:1203:33E:OAC	3:B:1203:33E:IAE	2.89	0.61
1:C:1043:GLY:O	3:C:1203:33E:IAE	2.91	0.59
1:A:1059:ILE:HG23	4:A:1205:IPA:H2	1.85	0.59
1:C:1027:ARG:HD2	1:D:1021:HIS:CE1	2.38	0.58
1:A:1005:LEU:HD21	1:A:1043:GLY:HA3	1.84	0.58
1:A:1150:GLU:HG3	3:A:1204:33E:H5	1.69	0.57
1:A:989:PHE:H	4:A:1206:IPA:H33	1.71	0.55
1:B:1037:ASN:O	1:B:1041:HIS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1043:GLY:O	3:D:1203:33E:IAE	2.99	0.51
1:C:1023:HIS:CD2	1:C:1025:ASN:H	2.24	0.50
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.94	0.49
1:C:1083:VAL:HG13	1:C:1092:CYS:SG	2.53	0.49
3:B:1202:33E:IAE	3:B:1202:33E:OAC	3.01	0.49
1:A:1000:VAL:HG21	1:A:1040:ILE:HD12	1.95	0.49
1:B:1043:GLY:O	3:B:1202:33E:IAE	3.02	0.48
3:C:1203:33E:IAE	3:C:1203:33E:OAC	3.03	0.47
1:A:1067:LYS:HE2	3:A:1202:33E:IAE	2.85	0.47
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.98	0.46
1:C:1006:TRP:HZ3	1:C:1100:ARG:HD2	1.81	0.46
3:A:1204:33E:OAC	3:A:1204:33E:IAE	3.05	0.45
3:C:1203:33E:OAC	4:C:1204:IPA:H12	2.16	0.45
1:B:958:GLY:HA3	1:B:965:PHE:CD1	2.52	0.45
1:C:1059:ILE:HG23	4:C:1204:IPA:H2	1.99	0.45
1:A:1003:LYS:O	1:A:1007:GLU:HG2	2.18	0.44
1:C:1117:HIS:HD2	5:C:1326:HOH:O	2.00	0.44
1:C:996:LYS:HD3	5:C:1420:HOH:O	2.18	0.44
1:C:1023:HIS:CE1	1:D:1022:ASN:O	2.71	0.44
1:D:1028:MET:HB3	1:D:1098:PHE:CZ	2.53	0.43
1:A:1043:GLY:O	3:A:1203:33E:IAE	3.07	0.43
1:B:1108:LEU:HD12	1:B:1126:THR:HB	2.00	0.43
1:C:1095:GLN:HA	1:C:1153:ILE:O	2.19	0.42
1:B:1012:ARG:HG2	1:B:1145:GLU:HG2	2.02	0.42
1:A:1037:ASN:O	1:A:1041:HIS:CD2	2.68	0.42
1:C:1051:ILE:HD13	1:C:1057:ALA:CB	2.50	0.42
1:C:1037:ASN:O	1:C:1041:HIS:CD2	2.68	0.42
1:C:1050:TYR:CD2	3:C:1202:33E:H3	2.55	0.42
1:D:1107:PHE:CG	1:D:1119:PRO:HG2	2.55	0.41
1:A:972:MET:HG2	1:A:994:ILE:HD11	2.03	0.41
1:C:1036:VAL:HG22	1:C:1097:LEU:HG	2.02	0.41
1:D:1129:PRO:HA	1:D:1134:LEU:HB3	2.02	0.41
1:A:975:THR:HB	1:A:1064:ASN:HA	2.02	0.41
1:A:1044:PHE:HB3	1:A:1059:ILE:HD13	2.03	0.41
1:C:955:TYR:HE1	1:C:1152:LEU:HD22	1.85	0.41
1:D:1011:HIS:HE1	5:D:1399:HOH:O	2.04	0.41
1:C:1067:LYS:HE2	3:C:1202:33E:IAE	2.90	0.41
1:C:1051:ILE:HD13	1:C:1057:ALA:HB2	2.03	0.40
1:A:1098:PHE:HB2	1:A:1153:ILE:HD11	2.03	0.40
4:A:1206:IPA:H2	5:A:1403:HOH:O	2.20	0.40
1:C:1095:GLN:HB3	1:C:1152:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:MET:HG2	1:C:994:ILE:HD11	2.03	0.40
1:D:1138:GLU:OE1	3:D:1202:33E:IAE	3.10	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/227 (87%)	195 (98%)	3 (2%)	0	100	100
1	B	200/227 (88%)	197 (98%)	3 (2%)	0	100	100
1	C	206/227 (91%)	200 (97%)	6 (3%)	0	100	100
1	D	187/227 (82%)	183 (98%)	4 (2%)	0	100	100
All	All	791/908 (87%)	775 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	169/192 (88%)	164 (97%)	5 (3%)	46	45
1	B	172/192 (90%)	167 (97%)	5 (3%)	48	46
1	C	174/192 (91%)	170 (98%)	4 (2%)	56	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	163/192 (85%)	159 (98%)	4 (2%)	53	55
All	All	678/768 (88%)	660 (97%)	18 (3%)	50	51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	962	ASP
1	A	966	GLN
1	A	980	ARG
1	A	1079	THR
1	A	1083	VAL
1	B	962	ASP
1	B	991	ARG
1	B	996	LYS
1	B	1100	ARG
1	B	1134	LEU
1	C	957	GLN
1	C	978	GLU
1	C	1083	VAL
1	C	1085	LYS
1	D	963	LYS
1	D	978	GLU
1	D	1003	LYS
1	D	1085	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1037	ASN
1	A	1041	HIS
1	A	1070	GLN
1	A	1132	ASN
1	B	1011	HIS
1	B	1041	HIS
1	C	1023	HIS
1	C	1041	HIS
1	C	1117	HIS
1	C	1123	HIS
1	D	1023	HIS
1	D	1070	GLN
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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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$
3	33E	A	1202	-	11,13,13	2.20	1 (9%)	13,18,18	1.94	3 (23%)
3	33E	A	1203	-	11,13,13	2.29	2 (18%)	13,18,18	1.28	3 (23%)
3	33E	A	1204	-	11,13,13	2.14	1 (9%)	13,18,18	1.32	1 (7%)
4	IPA	A	1205	-	3,3,3	0.93	0	3,3,3	0.47	0
4	IPA	A	1206	-	3,3,3	0.74	0	3,3,3	0.09	0
3	33E	B	1202	-	11,13,13	2.47	2 (18%)	13,18,18	1.27	2 (15%)
3	33E	B	1203	-	11,13,13	2.23	1 (9%)	13,18,18	1.69	2 (15%)
4	IPA	B	1204	-	3,3,3	0.79	0	3,3,3	0.07	0
3	33E	C	1202	-	11,13,13	2.19	2 (18%)	13,18,18	1.36	2 (15%)
3	33E	C	1203	-	11,13,13	2.20	1 (9%)	13,18,18	0.95	0
4	IPA	C	1204	-	3,3,3	0.75	0	3,3,3	0.37	0
3	33E	D	1202	-	11,13,13	2.44	2 (18%)	13,18,18	1.47	2 (15%)
3	33E	D	1203	-	11,13,13	2.49	2 (18%)	13,18,18	1.29	2 (15%)
3	33E	D	1204	-	11,13,13	2.12	1 (9%)	13,18,18	1.05	1 (7%)

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	33E	A	1202	-	-	0/6/8/8	0/1/1/1
3	33E	A	1203	-	-	0/6/8/8	0/1/1/1
3	33E	A	1204	-	-	0/6/8/8	0/1/1/1
4	IPA	A	1205	-	-	0/0/0/0	0/0/0/0
4	IPA	A	1206	-	-	0/0/0/0	0/0/0/0
3	33E	B	1202	-	-	0/6/8/8	0/1/1/1
3	33E	B	1203	-	-	0/6/8/8	0/1/1/1
4	IPA	B	1204	-	-	0/0/0/0	0/0/0/0
3	33E	C	1202	-	-	0/6/8/8	0/1/1/1
3	33E	C	1203	-	-	0/6/8/8	0/1/1/1
4	IPA	C	1204	-	-	0/0/0/0	0/0/0/0
3	33E	D	1202	-	-	0/6/8/8	0/1/1/1
3	33E	D	1203	-	-	0/6/8/8	0/1/1/1
3	33E	D	1204	-	-	0/6/8/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	33E	CAK-CAI	2.23	1.54	1.50
3	C	1202	33E	CAK-CAI	2.81	1.54	1.50
3	B	1202	33E	CAK-CAI	2.83	1.54	1.50
3	D	1203	33E	CAK-CAI	3.01	1.55	1.50
3	A	1203	33E	CAK-CAI	3.15	1.55	1.50
3	C	1202	33E	OAC-NAM	5.87	1.33	1.22
3	A	1203	33E	OAC-NAM	6.56	1.34	1.22
3	A	1202	33E	OAC-NAM	6.58	1.34	1.22
3	D	1204	33E	OAC-NAM	6.63	1.34	1.22
3	C	1203	33E	OAC-NAM	6.68	1.34	1.22
3	A	1204	33E	OAC-NAM	6.70	1.34	1.22
3	B	1203	33E	OAC-NAM	6.94	1.35	1.22
3	B	1202	33E	OAC-NAM	7.35	1.36	1.22
3	D	1202	33E	OAC-NAM	7.37	1.36	1.22
3	D	1203	33E	OAC-NAM	7.40	1.36	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1203	33E	CAK-CAI-NAA	-4.04	113.16	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	33E	CAK-CAI-NAA	-3.79	113.44	117.77
3	A	1203	33E	CAK-CAI-NAA	-2.51	114.91	117.77
3	B	1202	33E	CAK-CAI-NAA	-2.49	114.93	117.77
3	D	1202	33E	CAK-CAI-NAA	-2.43	115.00	117.77
3	C	1202	33E	CAL-CAJ-IAE	2.02	124.56	120.73
3	A	1202	33E	OAB-CAI-CAK	2.09	122.07	119.62
3	B	1202	33E	CAK-CAH-CAL	2.18	121.55	118.83
3	A	1204	33E	CAL-CAJ-IAE	2.23	124.94	120.73
3	A	1203	33E	CAL-CAJ-IAE	2.23	124.94	120.73
3	A	1203	33E	CAK-CAH-CAL	2.23	121.61	118.83
3	B	1203	33E	CAH-CAL-NAM	2.34	118.54	115.82
3	D	1204	33E	CAK-CAH-CAL	2.40	121.82	118.83
3	D	1203	33E	CAL-CAJ-IAE	2.41	125.28	120.73
3	D	1203	33E	CAK-CAH-CAL	2.67	122.16	118.83
3	D	1202	33E	CAH-CAL-NAM	3.24	119.58	115.82
3	C	1202	33E	CAH-CAL-NAM	3.30	119.65	115.82
3	A	1202	33E	CAH-CAL-NAM	4.27	120.77	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	33E	2	0
3	A	1203	33E	1	0
3	A	1204	33E	2	0
4	A	1205	IPA	1	0
4	A	1206	IPA	2	0
3	B	1202	33E	2	0
3	B	1203	33E	1	0
3	C	1202	33E	3	0
3	C	1203	33E	3	0
4	C	1204	IPA	2	0
3	D	1202	33E	2	0
3	D	1203	33E	1	0
3	D	1204	33E	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	199/227 (87%)	-0.22	4 (2%) 65 72	14, 24, 45, 69	0
1	B	204/227 (89%)	-0.19	6 (2%) 52 60	13, 24, 47, 74	0
1	C	208/227 (91%)	-0.14	3 (1%) 75 80	13, 25, 49, 65	0
1	D	193/227 (85%)	0.06	16 (8%) 12 16	16, 29, 51, 75	0
All	All	804/908 (88%)	-0.12	29 (3%) 43 50	13, 25, 49, 75	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1132	ASN	4.7
1	D	962	ASP	4.6
1	D	963	LYS	4.0
1	B	1131	VAL	3.9
1	C	955	TYR	3.8
1	D	1110	PHE	3.6
1	A	1132	ASN	3.6
1	D	1052	GLY	3.5
1	A	1133	GLY	3.3
1	C	963	LYS	3.1
1	B	1133	GLY	3.0
1	C	1132	ASN	3.0
1	D	1083	VAL	2.9
1	D	1082	PRO	2.9
1	D	1112	ALA	2.9
1	D	980	ARG	2.9
1	D	1135	ALA	2.8
1	A	1052	GLY	2.7
1	A	1110	PHE	2.6
1	D	1134	LEU	2.6
1	D	1041	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	963	LYS	2.5
1	B	954	LEU	2.4
1	D	966	GLN	2.3
1	D	1079	THR	2.3
1	D	1037	ASN	2.1
1	B	966	GLN	2.1
1	D	1136	LEU	2.1
1	D	1085	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	IPA	B	1204	4/4	0.67	0.22	5.95	28,31,34,35	0
4	IPA	C	1204	4/4	0.70	0.23	3.35	19,29,30,34	0
3	33E	D	1204	13/13	0.90	0.23	3.20	44,59,70,83	0
3	33E	D	1202	13/13	0.97	0.15	3.19	30,44,50,52	0
3	33E	A	1204	13/13	0.88	0.18	2.40	51,59,71,86	0
4	IPA	A	1205	4/4	0.71	0.19	2.06	16,16,23,26	0
3	33E	C	1203	13/13	0.96	0.18	1.68	50,55,65,65	0
4	IPA	A	1206	4/4	0.83	0.17	0.92	37,37,37,38	0
3	33E	B	1202	13/13	0.98	0.13	0.27	37,42,52,55	0
3	33E	A	1203	13/13	0.99	0.10	0.20	35,36,44,46	0
3	33E	D	1203	13/13	0.99	0.13	0.05	49,50,54,55	0
3	33E	C	1202	13/13	0.98	0.10	-0.19	22,25,35,38	0
3	33E	A	1202	13/13	0.99	0.08	-0.88	21,24,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	33E	B	1203	13/13	0.99	0.08	-1.11	25,30,37,40	0
2	ZN	D	1201	1/1	0.98	0.03	-1.71	41,41,41,41	0
2	ZN	A	1201	1/1	0.99	0.03	-2.06	29,29,29,29	0
2	ZN	B	1201	1/1	0.99	0.03	-2.26	35,35,35,35	0
2	ZN	C	1201	1/1	0.98	0.03	-2.32	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.