



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 PM GMT

PDB ID : 4N4V  
Title : Co-crystal structure of tankyrase 1 with compound 4 [(4S)-3-{trans-4-[6-amino-5-(pyrimidin-2-yl)pyridin-3-yl]cyclohexyl}-5,5-dimethyl-4-phenyl-1,3-oxazolidin-2-one]  
Authors : Huang, X.  
Deposited on : 2013-10-08  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

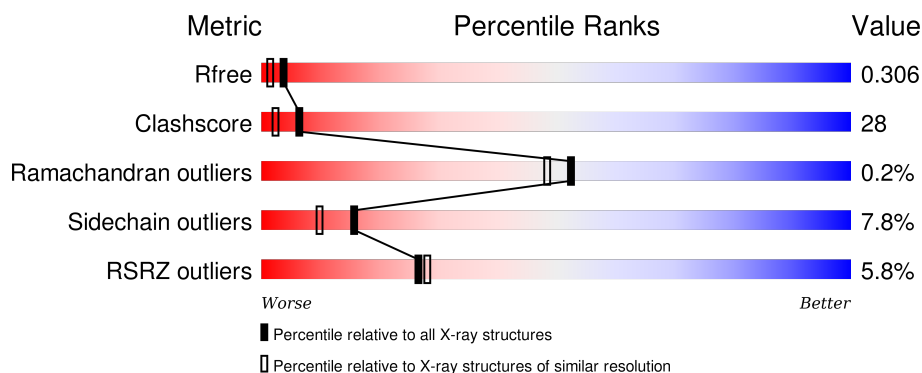
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	217	<div> <div>3%</div> <div>65%</div> <div>27%</div> <div>• •</div> </div>
1	B	217	<div> <div>8%</div> <div>54%</div> <div>30%</div> <div>6% • 7%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2GY	A	1402	-	-	-	X
3	2GY	B	1402	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3734 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1697	1068	310	307	12			
1	B	202	Total	C	N	O	S	0	0	0
			1615	1016	294	294	11			

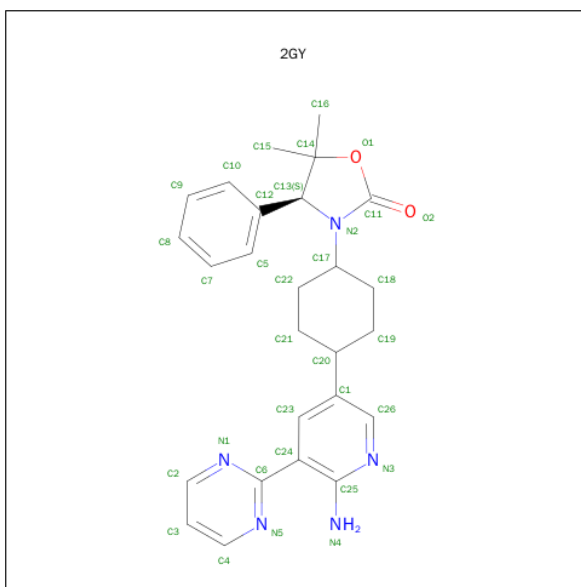
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	HIS	-	EXPRESSION TAG	UNP O95271
A	1316	HIS	-	EXPRESSION TAG	UNP O95271
A	1317	HIS	-	EXPRESSION TAG	UNP O95271
A	1318	HIS	-	EXPRESSION TAG	UNP O95271
A	1319	HIS	-	EXPRESSION TAG	UNP O95271
A	1320	HIS	-	EXPRESSION TAG	UNP O95271
B	1315	HIS	-	EXPRESSION TAG	UNP O95271
B	1316	HIS	-	EXPRESSION TAG	UNP O95271
B	1317	HIS	-	EXPRESSION TAG	UNP O95271
B	1318	HIS	-	EXPRESSION TAG	UNP O95271
B	1319	HIS	-	EXPRESSION TAG	UNP O95271
B	1320	HIS	-	EXPRESSION TAG	UNP O95271

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is (4S)-3-{TRANS-4-[6-AMINO-5-(PYRIMIDIN-2-YL)PYRIDIN-3-YL]CYCLOHEXYL}-5,5-DIMETHYL-4-PHENYL-1,3-OXAZOLIDIN-2-ONE (three-letter code: 2GY) (formula: C<sub>26</sub>H<sub>29</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 33	C 26	N 5	O 2	0	0
3	B	1	Total 33	C 26	N 5	O 2	0	0

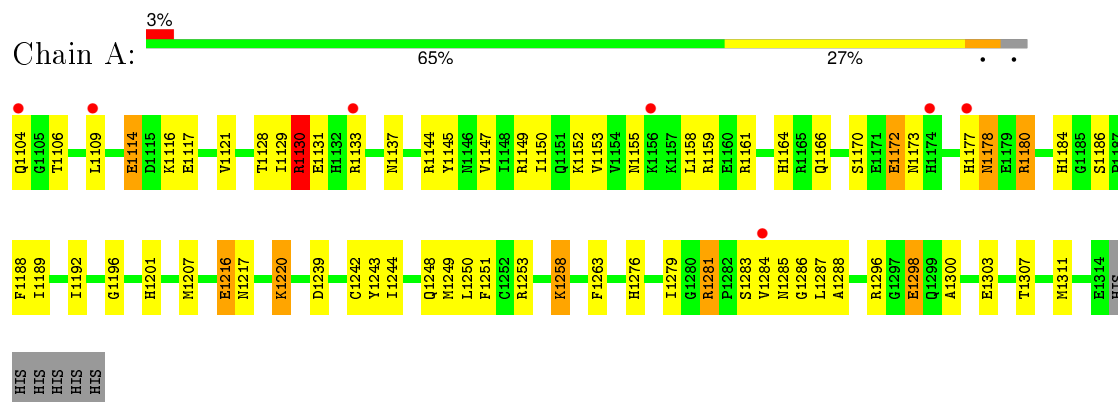
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	201	Total O 201 201	0	0
4	B	153	Total O 153 153	0	0

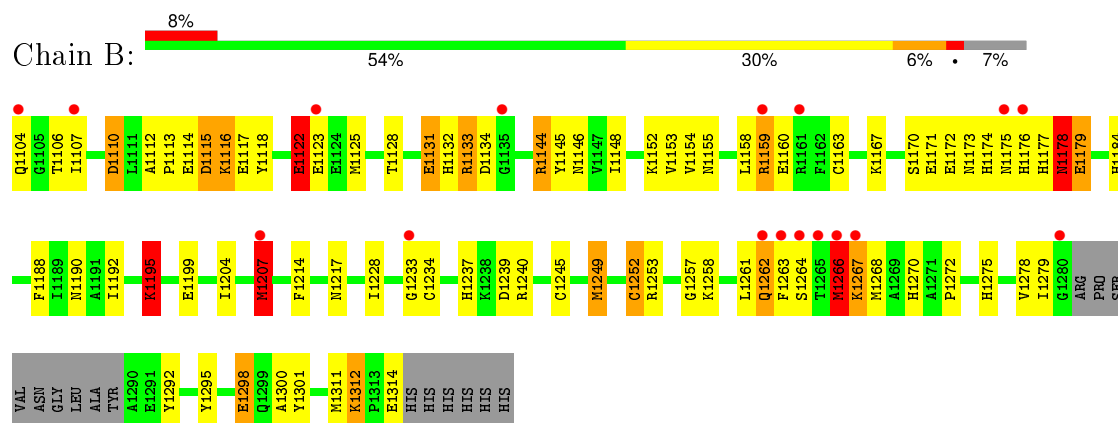
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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-1



#### • Molecule 1: Tankyrase-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.99 Å 77.72 Å 147.78 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 41.61 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 93.4 (41.61-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.97 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.290 0.280 , 0.306	Depositor DCC
$R_{free}$ test set	1601 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	5 of 32865 reflections (0.015%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2GY, ZN

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	0.58	1/1740 (0.1%)	0.89	8/2339 (0.3%)
1	B	0.70	4/1655 (0.2%)	1.26	18/2225 (0.8%)
All	All	0.64	5/3395 (0.1%)	1.08	26/4564 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1266	MET	C-N	8.65	1.53	1.34
1	B	1122	GLU	CB-CG	7.03	1.65	1.52
1	B	1179	GLU	CB-CG	-6.21	1.40	1.52
1	B	1131	GLU	CB-CG	5.14	1.61	1.52
1	A	1130	ARG	CG-CD	5.09	1.64	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1133	ARG	NE-CZ-NH1	-26.86	106.87	120.30
1	B	1133	ARG	NE-CZ-NH2	18.87	129.74	120.30
1	B	1159	ARG	NE-CZ-NH1	-15.21	112.69	120.30
1	A	1130	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	B	1159	ARG	NE-CZ-NH2	10.82	125.71	120.30
1	A	1130	ARG	NE-CZ-NH2	-9.71	115.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1172	GLU	CA-CB-CG	9.35	133.97	113.40
1	B	1133	ARG	CD-NE-CZ	-9.19	110.74	123.60
1	B	1195	LYS	CA-CB-CG	7.04	128.88	113.40
1	B	1133	ARG	CA-CB-CG	7.03	128.86	113.40
1	B	1115	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	1171	GLU	CA-CB-CG	6.39	127.46	113.40
1	B	1267	LYS	O-C-N	6.34	132.84	122.70
1	B	1116	LYS	CA-CB-CG	6.30	127.26	113.40
1	A	1249	MET	CA-CB-CG	6.29	123.98	113.30
1	B	1133	ARG	CG-CD-NE	6.25	124.92	111.80
1	B	1266	MET	CA-C-N	-6.13	103.71	117.20
1	A	1258	LYS	CA-CB-CG	6.09	126.79	113.40
1	B	1115	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	1267	LYS	C-N-CA	-5.91	106.93	121.70
1	B	1178	ASN	CB-CA-C	5.90	122.20	110.40
1	B	1249	MET	CA-CB-CG	5.81	123.18	113.30
1	A	1130	ARG	CA-CB-CG	5.55	125.62	113.40
1	A	1287	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	B	1207	MET	CA-CB-CG	5.20	122.14	113.30
1	A	1251	PHE	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1159	ARG	Sidechain
1	B	1266	MET	Mainchain

## 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	1697	0	1630	83	0
1	B	1615	0	1532	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	29	4	0
4	A	201	0	0	27	2
4	B	153	0	0	37	2
All	All	3734	0	3219	182	2

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 28.

All (182) 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:B:1190:ASN:HB2	4:B:1613:HOH:O	1.25	1.28
1:B:1175:ASN:HB3	4:B:1543:HOH:O	1.40	1.20
1:B:1263:PHE:HB2	4:B:1577:HOH:O	1.38	1.19
1:B:1176:HIS:HD2	4:B:1633:HOH:O	1.26	1.19
1:B:1314:GLU:HB2	4:B:1599:HOH:O	1.49	1.10
1:A:1133:ARG:HD2	4:A:1694:HOH:O	1.48	1.10
1:B:1176:HIS:CD2	4:B:1633:HOH:O	2.01	1.08
1:A:1248:GLN:OE1	4:A:1570:HOH:O	1.74	1.06
1:B:1107:ILE:HG13	4:B:1621:HOH:O	1.55	1.05
1:A:1298:GLU:CG	4:A:1549:HOH:O	2.06	1.03
1:A:1296:ARG:CZ	4:A:1647:HOH:O	2.09	0.98
1:A:1161:ARG:NH2	1:A:1298:GLU:OE2	1.97	0.97
1:B:1263:PHE:CB	4:B:1577:HOH:O	2.01	0.96
1:B:1262:GLN:NE2	4:B:1612:HOH:O	1.89	0.95
1:B:1153:VAL:O	4:B:1596:HOH:O	1.84	0.95
1:A:1116:LYS:HE3	4:A:1685:HOH:O	1.68	0.93
1:A:1172:GLU:OE1	1:A:1276:HIS:NE2	2.01	0.92
1:A:1298:GLU:HG3	4:A:1549:HOH:O	1.68	0.87
1:A:1296:ARG:NH2	4:A:1647:HOH:O	2.08	0.86
1:A:1281:ARG:HG2	1:A:1281:ARG:HH11	1.39	0.86
1:A:1283:SER:HA	1:B:1263:PHE:CE1	2.11	0.85
1:A:1220:LYS:NZ	4:A:1512:HOH:O	1.92	0.83
1:B:1314:GLU:C	4:B:1599:HOH:O	2.17	0.81
1:B:1228:ILE:HD11	3:B:1402:2GY:H9	1.64	0.80
1:B:1252:CYS:HB3	1:B:1301:TYR:O	1.83	0.79
1:B:1178:ASN:ND2	1:B:1257:GLY:O	2.17	0.78
1:A:1130:ARG:HH11	1:A:1217:ASN:HD21	1.31	0.76
1:B:1270:HIS:HD2	4:B:1524:HOH:O	1.66	0.76
1:B:1239:ASP:OD1	4:B:1640:HOH:O	2.04	0.75
1:A:1144:ARG:HG2	1:A:1145:TYR:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:GLU:HB3	4:A:1658:HOH:O	1.86	0.75
1:B:1152:LYS:NZ	4:B:1649:HOH:O	2.20	0.74
1:B:1115:ASP:OD2	1:B:1117:GLU:HB3	1.88	0.74
1:A:1253:ARG:HG3	1:A:1303:GLU:HG2	1.70	0.73
1:B:1314:GLU:CA	4:B:1599:HOH:O	2.39	0.71
1:B:1170:SER:O	1:B:1175:ASN:HA	1.88	0.71
1:A:1220:LYS:HE3	4:A:1535:HOH:O	1.90	0.71
1:B:1264:SER:O	4:B:1612:HOH:O	2.08	0.71
1:A:1284:VAL:HG23	1:B:1263:PHE:HE2	1.56	0.71
1:B:1314:GLU:CB	4:B:1599:HOH:O	2.18	0.71
1:A:1201:HIS:HE1	4:A:1629:HOH:O	1.74	0.71
1:A:1284:VAL:HG23	1:B:1263:PHE:CE2	2.25	0.70
1:A:1298:GLU:H	1:A:1298:GLU:CD	1.93	0.70
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.73	0.70
1:B:1176:HIS:HB3	4:B:1604:HOH:O	1.91	0.70
1:B:1144:ARG:HD2	1:B:1311:MET:SD	2.31	0.70
1:A:1130:ARG:NH1	4:A:1679:HOH:O	2.23	0.70
1:A:1133:ARG:CZ	1:A:1288:ALA:HB2	2.22	0.70
1:A:1283:SER:OG	1:A:1286:GLY:HA3	1.92	0.70
1:B:1312:LYS:HD3	4:B:1525:HOH:O	1.92	0.69
1:B:1114:GLU:H	1:B:1114:GLU:CD	1.95	0.68
1:B:1175:ASN:CB	4:B:1543:HOH:O	2.15	0.68
1:A:1281:ARG:HG2	1:A:1281:ARG:NH1	2.06	0.68
1:A:1117:GLU:OE2	1:A:1152:LYS:HE2	1.93	0.68
1:A:1104:GLN:HB3	4:A:1560:HOH:O	1.92	0.67
1:A:1114:GLU:OE2	4:A:1561:HOH:O	2.10	0.67
1:A:1173:ASN:ND2	1:A:1258:LYS:HE3	2.09	0.67
1:B:1268:MET:HE1	1:B:1272:PRO:HD3	1.76	0.67
1:A:1153:VAL:O	4:A:1529:HOH:O	2.12	0.67
1:B:1132:HIS:C	1:B:1134:ASP:H	1.97	0.67
1:B:1311:MET:O	4:B:1552:HOH:O	2.12	0.66
1:B:1268:MET:HE1	1:B:1278:VAL:HG21	1.77	0.66
1:B:1228:ILE:HD11	3:B:1402:2GY:C15	2.26	0.65
1:A:1149:ARG:HB3	1:A:1307:THR:HB	1.78	0.65
1:B:1207:MET:H	1:B:1207:MET:HE2	1.61	0.65
1:A:1161:ARG:CZ	1:A:1298:GLU:OE2	2.45	0.64
1:B:1113:PRO:HD2	1:B:1114:GLU:OE2	1.96	0.64
1:A:1216:GLU:HG3	4:A:1567:HOH:O	1.98	0.63
1:A:1128:THR:HB	1:A:1217:ASN:HA	1.81	0.63
1:A:1298:GLU:HG2	4:A:1549:HOH:O	1.87	0.62
1:B:1207:MET:N	1:B:1207:MET:HE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:PHE:CD1	1:A:1283:SER:HB3	2.35	0.61
1:B:1146:ASN:ND2	1:B:1148:ILE:HD11	2.15	0.61
1:A:1158:LEU:HD21	1:A:1196:GLY:CA	2.31	0.61
1:A:1173:ASN:HD22	1:A:1258:LYS:HE3	1.67	0.60
1:B:1114:GLU:CG	4:B:1508:HOH:O	2.49	0.60
1:B:1228:ILE:CD1	3:B:1402:2GY:H9	2.31	0.60
1:A:1279:ILE:HG22	1:A:1281:ARG:HD2	1.83	0.60
1:A:1188:PHE:O	1:A:1192:ILE:HG13	2.01	0.59
1:A:1130:ARG:HD2	1:A:1217:ASN:ND2	2.17	0.59
1:B:1268:MET:CE	1:B:1278:VAL:HG21	2.33	0.59
1:B:1163:CYS:SG	4:B:1502:HOH:O	2.04	0.58
1:A:1284:VAL:CG2	1:B:1263:PHE:HE2	2.15	0.58
1:A:1159:ARG:NH2	1:A:1303:GLU:OE2	2.37	0.58
1:A:1117:GLU:O	1:A:1121:VAL:HG23	2.04	0.58
1:B:1199:GLU:HG2	1:B:1295:TYR:O	2.04	0.58
1:A:1284:VAL:O	1:A:1285:ASN:CB	2.51	0.57
1:B:1245:CYS:HB2	4:B:1519:HOH:O	2.03	0.57
1:A:1159:ARG:HH12	1:A:1253:ARG:HE	1.50	0.57
1:A:1180:ARG:NH1	4:A:1668:HOH:O	2.39	0.56
1:A:1159:ARG:HH12	1:A:1253:ARG:NE	2.04	0.56
1:B:1114:GLU:HG3	4:B:1508:HOH:O	2.06	0.56
1:B:1268:MET:HE1	1:B:1278:VAL:CG2	2.35	0.55
1:A:1283:SER:HA	1:B:1263:PHE:CZ	2.41	0.55
1:B:1195:LYS:CA	1:B:1195:LYS:HE3	2.35	0.55
1:B:1190:ASN:CB	4:B:1613:HOH:O	2.06	0.54
1:B:1114:GLU:N	1:B:1114:GLU:CD	2.61	0.54
1:B:1146:ASN:HD21	1:B:1148:ILE:HD11	1.73	0.53
1:B:1262:GLN:HG3	1:B:1262:GLN:O	2.08	0.53
1:B:1144:ARG:HD3	1:B:1145:TYR:O	2.08	0.53
1:A:1155:ASN:ND2	1:A:1158:LEU:HD13	2.24	0.52
1:A:1137:ASN:ND2	4:A:1604:HOH:O	2.32	0.52
1:B:1123:GLU:OE1	4:B:1637:HOH:O	2.19	0.52
1:A:1164:HIS:HE1	4:A:1547:HOH:O	1.92	0.51
1:B:1234:CYS:SG	1:B:1237:HIS:HB2	2.50	0.51
1:B:1177:HIS:CD2	1:B:1178:ASN:N	2.79	0.50
1:A:1253:ARG:HG3	1:A:1303:GLU:CG	2.41	0.50
1:B:1160:GLU:HG2	4:B:1570:HOH:O	2.11	0.50
1:B:1132:HIS:C	1:B:1134:ASP:N	2.66	0.49
1:B:1144:ARG:HG3	1:B:1311:MET:HB2	1.95	0.49
1:B:1172:GLU:HB3	4:B:1588:HOH:O	2.12	0.49
1:B:1152:LYS:HE2	4:B:1593:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:PHE:HB3	4:B:1577:HOH:O	1.89	0.49
1:B:1177:HIS:HD2	1:B:1178:ASN:N	2.11	0.49
1:A:1166:GLN:HG3	1:A:1177:HIS:HB2	1.95	0.48
1:A:1186:SER:O	1:A:1189:ILE:HG12	2.13	0.48
1:B:1298:GLU:H	1:B:1298:GLU:HG3	1.30	0.48
1:B:1122:GLU:HG3	1:B:1122:GLU:O	2.12	0.48
1:A:1130:ARG:NH1	1:A:1217:ASN:HD21	2.07	0.48
1:A:1158:LEU:HD21	1:A:1196:GLY:HA2	1.96	0.48
1:A:1144:ARG:NE	1:A:1311:MET:SD	2.87	0.48
1:B:1268:MET:CE	1:B:1272:PRO:HD3	2.42	0.47
1:A:1180:ARG:CZ	1:B:1174:HIS:CE1	2.97	0.47
1:B:1228:ILE:CD1	3:B:1402:2GY:C15	2.90	0.47
1:B:1112:ALA:HB1	1:B:1114:GLU:OE2	2.15	0.47
1:B:1110:ASP:N	1:B:1110:ASP:OD2	2.48	0.47
1:B:1115:ASP:HB2	4:B:1558:HOH:O	2.15	0.46
1:B:1233:GLY:CA	1:B:1240:ARG:HG2	2.45	0.46
1:B:1115:ASP:CB	4:B:1558:HOH:O	2.64	0.46
1:A:1114:GLU:H	1:A:1114:GLU:HG3	1.30	0.46
1:A:1133:ARG:CD	4:A:1694:HOH:O	2.29	0.46
1:A:1133:ARG:NH1	1:A:1288:ALA:HB2	2.30	0.45
1:B:1258:LYS:HG2	1:B:1275:HIS:CD2	2.51	0.45
1:A:1144:ARG:HG2	1:A:1145:TYR:H	1.80	0.45
1:B:1188:PHE:O	1:B:1192:ILE:HG13	2.16	0.45
1:B:1134:ASP:HB2	4:B:1530:HOH:O	2.17	0.45
1:A:1220:LYS:HZ2	1:A:1220:LYS:HG2	1.56	0.45
1:A:1220:LYS:CE	4:A:1535:HOH:O	2.57	0.45
1:B:1117:GLU:OE2	1:B:1152:LYS:NZ	2.45	0.45
1:B:1233:GLY:HA2	1:B:1240:ARG:HG2	1.99	0.44
1:B:1177:HIS:HD2	1:B:1179:GLU:H	1.66	0.44
1:A:1243:TYR:HB3	4:A:1523:HOH:O	2.18	0.44
1:B:1116:LYS:HE3	1:B:1116:LYS:HB3	1.52	0.44
1:B:1155:ASN:HB3	1:B:1158:LEU:HB2	1.99	0.44
1:B:1312:LYS:HB2	1:B:1312:LYS:HE2	1.65	0.43
1:A:1106:THR:HG21	1:A:1153:VAL:HG13	1.98	0.43
1:B:1195:LYS:CE	1:B:1195:LYS:HA	2.48	0.43
1:B:1184:HIS:HB2	1:B:1214:PHE:CD1	2.52	0.43
1:B:1106:THR:HG22	1:B:1107:ILE:N	2.32	0.43
1:B:1106:THR:HA	1:B:1154:VAL:O	2.19	0.43
1:B:1262:GLN:NE2	1:B:1264:SER:O	2.52	0.43
1:A:1130:ARG:HG3	4:A:1666:HOH:O	2.18	0.43
1:B:1253:ARG:O	1:B:1300:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1268:MET:HE3	1:B:1270:HIS:O	2.18	0.43
1:B:1295:TYR:N	1:B:1295:TYR:CD2	2.87	0.43
1:B:1115:ASP:CG	1:B:1117:GLU:H	2.22	0.43
1:A:1239:ASP:HB3	1:A:1242:CYS:HB2	2.01	0.43
1:B:1146:ASN:HB2	1:B:1311:MET:SD	2.58	0.43
1:A:1284:VAL:HG22	4:A:1677:HOH:O	2.19	0.42
1:A:1189:ILE:HD12	1:A:1250:LEU:HG	2.00	0.42
1:B:1279:ILE:HG12	1:B:1292:TYR:CD1	2.54	0.42
1:A:1253:ARG:O	1:A:1300:ALA:HA	2.20	0.42
1:A:1178:ASN:HD22	1:B:1176:HIS:CE1	2.38	0.42
1:A:1220:LYS:NZ	4:A:1535:HOH:O	2.53	0.42
1:A:1263:PHE:CZ	1:B:1263:PHE:HB3	2.55	0.42
1:B:1106:THR:HG21	1:B:1153:VAL:HG13	2.02	0.42
1:B:1207:MET:C	1:B:1267:LYS:HE3	2.39	0.41
1:A:1129:ILE:HD11	1:A:1145:TYR:CE2	2.56	0.41
1:B:1207:MET:H	1:B:1207:MET:CE	2.31	0.41
1:A:1184:HIS:HE1	3:A:1402:2GY:H15	1.84	0.41
1:A:1281:ARG:CG	1:A:1281:ARG:NH1	2.78	0.41
1:B:1125:MET:HG2	1:B:1145:TYR:CD2	2.56	0.41
1:B:1173:ASN:ND2	1:B:1176:HIS:HB2	2.35	0.41
1:A:1184:HIS:CE1	3:A:1402:2GY:H15	2.55	0.41
1:B:1314:GLU:N	4:B:1580:HOH:O	2.44	0.41
1:A:1242:CYS:SG	1:A:1244:ILE:HB	2.60	0.41
1:A:1147:VAL:HG11	1:A:1150:ILE:HD11	2.02	0.41
1:B:1107:ILE:CG1	4:B:1621:HOH:O	2.37	0.41
1:B:1173:ASN:O	1:B:1174:HIS:C	2.59	0.41
1:A:1184:HIS:HA	4:A:1508:HOH:O	2.20	0.41
1:A:1263:PHE:CZ	1:B:1261:LEU:HG	2.56	0.40
1:B:1104:GLN:N	4:B:1624:HOH:O	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1516:HOH:O	4:B:1508:HOH:O[4_455]	2.10	0.10
4:A:1579:HOH:O	4:B:1607:HOH:O[4_455]	2.16	0.04

## 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	209/217 (96%)	203 (97%)	6 (3%)	0	100	100
1	B	198/217 (91%)	190 (96%)	7 (4%)	1 (0%)	34	26
All	All	407/434 (94%)	393 (97%)	13 (3%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1266	MET

### 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	178/185 (96%)	167 (94%)	11 (6%)	23	16
1	B	168/185 (91%)	152 (90%)	16 (10%)	11	6
All	All	346/370 (94%)	319 (92%)	27 (8%)	16	10

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1109	LEU
1	A	1114	GLU
1	A	1130	ARG
1	A	1170	SER
1	A	1178	ASN

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Mol	Chain	Res	Type
1	A	1180	ARG
1	A	1207	MET
1	A	1216	GLU
1	A	1220	LYS
1	A	1281	ARG
1	A	1298	GLU
1	B	1110	ASP
1	B	1118	TYR
1	B	1122	GLU
1	B	1131	GLU
1	B	1133	ARG
1	B	1144	ARG
1	B	1167	LYS
1	B	1178	ASN
1	B	1195	LYS
1	B	1204	ILE
1	B	1207	MET
1	B	1249	MET
1	B	1252	CYS
1	B	1262	GLN
1	B	1298	GLU
1	B	1312	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1164	HIS
1	A	1166	GLN
1	A	1173	ASN
1	A	1178	ASN
1	A	1201	HIS
1	A	1217	ASN
1	A	1248	GLN
1	B	1104	GLN
1	B	1174	HIS
1	B	1177	HIS
1	B	1178	ASN
1	B	1270	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	2GY	A	1402	-	37,37,37	3.41	20 (54%)	48,54,54	4.16	27 (56%)
3	2GY	B	1402	-	37,37,37	4.38	24 (64%)	48,54,54	4.28	24 (50%)

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	2GY	A	1402	-	-	0/16/45/45	0/5/5/5
3	2GY	B	1402	-	-	0/16/45/45	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	2GY	O1-C14	-6.20	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	2GY	C11-N2	-5.20	1.28	1.35
3	A	1402	2GY	C1-C20	-4.84	1.43	1.52
3	B	1402	2GY	C17-N2	-4.38	1.41	1.48
3	A	1402	2GY	C17-N2	-4.13	1.41	1.48
3	B	1402	2GY	C11-N2	-3.68	1.30	1.35
3	B	1402	2GY	O2-C11	-2.85	1.16	1.21
3	B	1402	2GY	C1-C20	-2.27	1.47	1.52
3	A	1402	2GY	C13-N2	-2.23	1.45	1.47
3	B	1402	2GY	C15-C14	2.18	1.56	1.52
3	A	1402	2GY	C3-C2	2.25	1.44	1.37
3	B	1402	2GY	C23-C24	2.36	1.43	1.39
3	B	1402	2GY	C3-C4	2.40	1.44	1.37
3	B	1402	2GY	C24-C25	2.40	1.46	1.43
3	B	1402	2GY	C3-C2	2.59	1.45	1.37
3	A	1402	2GY	C3-C4	2.63	1.45	1.37
3	B	1402	2GY	C2-N1	2.67	1.40	1.34
3	A	1402	2GY	C4-N5	2.73	1.40	1.34
3	B	1402	2GY	C4-N5	2.75	1.40	1.34
3	B	1402	2GY	C9-C10	2.87	1.44	1.38
3	A	1402	2GY	C2-N1	3.13	1.41	1.34
3	B	1402	2GY	C23-C1	3.17	1.44	1.39
3	A	1402	2GY	C23-C1	3.21	1.44	1.39
3	B	1402	2GY	C8-C7	3.21	1.46	1.38
3	B	1402	2GY	C8-C9	3.37	1.46	1.38
3	A	1402	2GY	C26-C1	3.41	1.43	1.38
3	A	1402	2GY	C8-C9	3.42	1.46	1.38
3	A	1402	2GY	C7-C5	3.49	1.46	1.38
3	A	1402	2GY	C8-C7	3.55	1.47	1.38
3	B	1402	2GY	C7-C5	3.63	1.46	1.38
3	A	1402	2GY	O1-C14	3.75	1.54	1.48
3	A	1402	2GY	C9-C10	3.79	1.46	1.38
3	B	1402	2GY	O1-C11	4.68	1.43	1.35
3	B	1402	2GY	C5-C12	4.76	1.46	1.39
3	B	1402	2GY	C26-C1	5.10	1.45	1.38
3	A	1402	2GY	C5-C12	5.63	1.48	1.39
3	B	1402	2GY	C6-N5	5.88	1.42	1.34
3	B	1402	2GY	C10-C12	6.10	1.49	1.39
3	A	1402	2GY	O1-C11	6.19	1.45	1.35
3	A	1402	2GY	C10-C12	6.24	1.49	1.39
3	A	1402	2GY	C6-N5	6.49	1.43	1.34
3	A	1402	2GY	C6-N1	8.37	1.45	1.34
3	B	1402	2GY	C6-N1	8.79	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	2GY	C14-C13	17.18	1.73	1.55

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	2GY	C1-C26-N3	-8.40	113.17	124.87
3	B	1402	2GY	C1-C26-N3	-8.26	113.37	124.87
3	A	1402	2GY	O1-C14-C13	-8.11	95.78	102.73
3	B	1402	2GY	N1-C6-N5	-7.43	112.87	125.78
3	B	1402	2GY	C23-C1-C20	-7.07	110.51	120.89
3	B	1402	2GY	O1-C14-C15	-6.83	98.88	106.83
3	A	1402	2GY	N1-C6-N5	-6.75	114.05	125.78
3	B	1402	2GY	O1-C14-C13	-6.23	97.39	102.73
3	A	1402	2GY	O1-C14-C16	-5.94	99.91	106.83
3	A	1402	2GY	C22-C17-N2	-5.62	102.17	112.65
3	B	1402	2GY	C22-C17-N2	-4.79	103.72	112.65
3	A	1402	2GY	C23-C1-C20	-4.73	113.94	120.89
3	B	1402	2GY	C14-C13-C12	-4.59	111.59	115.58
3	A	1402	2GY	O1-C11-N2	-3.70	107.98	110.05
3	A	1402	2GY	O2-C11-N2	-3.54	123.71	128.21
3	B	1402	2GY	O1-C14-C16	-3.50	102.75	106.83
3	A	1402	2GY	C19-C20-C1	-2.75	107.04	112.89
3	A	1402	2GY	C5-C12-C13	-2.72	114.93	120.69
3	B	1402	2GY	C12-C13-N2	-2.66	110.56	113.83
3	A	1402	2GY	N4-C25-N3	-2.48	113.44	118.39
3	B	1402	2GY	C15-C14-C16	-2.45	104.06	110.99
3	A	1402	2GY	C15-C14-C16	-2.24	104.65	110.99
3	B	1402	2GY	C8-C7-C5	-2.08	117.13	120.19
3	A	1402	2GY	C18-C17-N2	-2.07	108.78	112.65
3	A	1402	2GY	C18-C19-C20	2.46	115.46	110.42
3	A	1402	2GY	C10-C12-C5	2.50	121.50	118.31
3	B	1402	2GY	C9-C8-C7	2.60	124.50	119.93
3	B	1402	2GY	C18-C17-C22	2.94	118.14	111.22
3	A	1402	2GY	C24-C6-N5	3.34	119.81	116.85
3	B	1402	2GY	C10-C12-C5	3.36	122.59	118.31
3	A	1402	2GY	C15-C14-C13	3.37	121.29	113.44
3	A	1402	2GY	C24-C25-N3	3.45	124.75	119.77
3	B	1402	2GY	C24-C25-N3	3.76	125.19	119.77
3	B	1402	2GY	C24-C6-N5	4.12	120.50	116.85
3	B	1402	2GY	C26-N3-C25	4.16	123.70	118.88
3	B	1402	2GY	C14-O1-C11	4.31	114.96	110.05
3	A	1402	2GY	C18-C17-C22	4.71	122.33	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	2GY	C26-N3-C25	4.88	124.54	118.88
3	A	1402	2GY	C16-C14-C13	4.98	125.03	113.44
3	A	1402	2GY	O1-C11-O2	5.45	128.23	122.53
3	B	1402	2GY	C19-C20-C21	5.63	121.78	109.31
3	B	1402	2GY	C23-C1-C26	6.90	124.34	116.78
3	A	1402	2GY	C19-C20-C21	7.00	124.81	109.31
3	A	1402	2GY	C2-N1-C6	7.31	122.93	115.93
3	A	1402	2GY	C23-C1-C26	7.43	124.93	116.78
3	A	1402	2GY	C4-N5-C6	7.88	123.47	115.93
3	B	1402	2GY	C15-C14-C13	8.09	132.27	113.44
3	B	1402	2GY	C4-N5-C6	8.55	124.11	115.93
3	B	1402	2GY	C2-N1-C6	9.25	124.78	115.93
3	A	1402	2GY	C24-C6-N1	10.28	125.96	116.85
3	B	1402	2GY	C24-C6-N1	10.76	126.37	116.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	2GY	2	0
3	B	1402	2GY	4	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, 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	211/217 (97%)	0.36	7 (3%) 50 51	18, 25, 34, 42	0
1	B	202/217 (93%)	0.59	17 (8%) 14 14	20, 28, 36, 43	0
All	All	413/434 (95%)	0.47	24 (5%) 26 28	18, 26, 36, 43	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1104	GLN	8.6
1	A	1104	GLN	8.2
1	B	1265	THR	7.5
1	B	1263	PHE	7.4
1	B	1107	ILE	3.6
1	B	1207	MET	3.3
1	B	1176	HIS	3.2
1	A	1177	HIS	3.2
1	A	1174	HIS	3.1
1	A	1133	ARG	3.1
1	A	1284	VAL	3.1
1	B	1264	SER	2.8
1	B	1123	GLU	2.6
1	A	1109	LEU	2.4
1	B	1280	GLY	2.4
1	B	1161	ARG	2.4
1	B	1267	LYS	2.3
1	B	1262	GLN	2.3
1	B	1233	GLY	2.2
1	B	1159	ARG	2.2
1	B	1175	ASN	2.1
1	B	1135	GLY	2.1
1	B	1266	MET	2.0
1	A	1156	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( $\text{\AA}^2$ )	Q<0.9
3	2GY	A	1402	33/33	0.84	0.26	3.65	29,42,59,63	0
3	2GY	B	1402	33/33	0.85	0.23	2.58	35,47,64,68	0
2	ZN	A	1401	1/1	0.99	0.07	-1.76	26,26,26,26	0
2	ZN	B	1401	1/1	0.99	0.06	-3.05	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.