



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2016 – 10:54 AM EDT

PDB ID : 5DLV  
Title : Crystal structure of Autotaxin (ENPP2) with tauroursodeoxycholic acid (TUDCA)  
Authors : Keune, W.J.; Heidebrecht, T.; von Castelmur, E.; Joosten, R.P.; Perrakis, A.  
Deposited on : 2015-09-07  
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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027257  
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) : rb-20027257

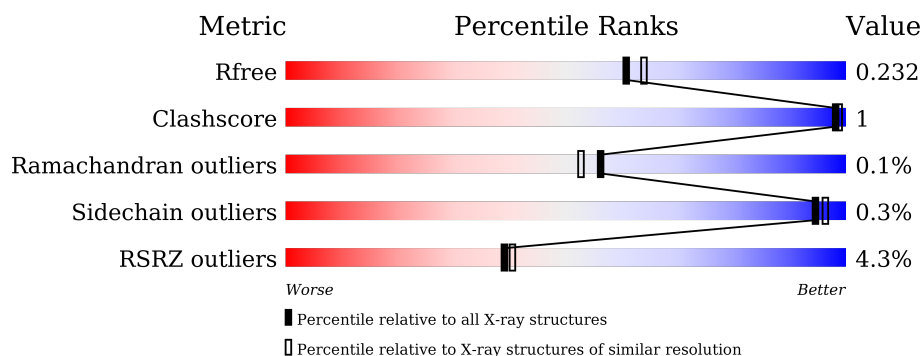
# 1 Overall quality at a glance

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	827	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
1	B	827	<div> <div>4%</div> <div>91%</div> <div>6%</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
10	5D5	A	930[A]	-	-	-	X
11	SCN	A	931	-	-	-	X
12	GOL	A	933	-	-	-	X
12	GOL	A	934	-	-	-	X
12	GOL	A	935	-	-	-	X
12	GOL	A	937	-	-	-	X
12	GOL	A	938	-	-	-	X
12	GOL	B	930	-	-	-	X
12	GOL	B	931	-	-	-	X
12	GOL	B	933	-	-	-	X
12	GOL	B	934	-	-	-	X
7	IOD	A	913	-	-	-	X
7	IOD	A	921	-	-	X	-
7	IOD	B	923	-	-	X	-
8	PO4	A	927	-	-	-	X
8	PO4	B	924	-	-	-	X
9	NA	B	926	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 13814 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.

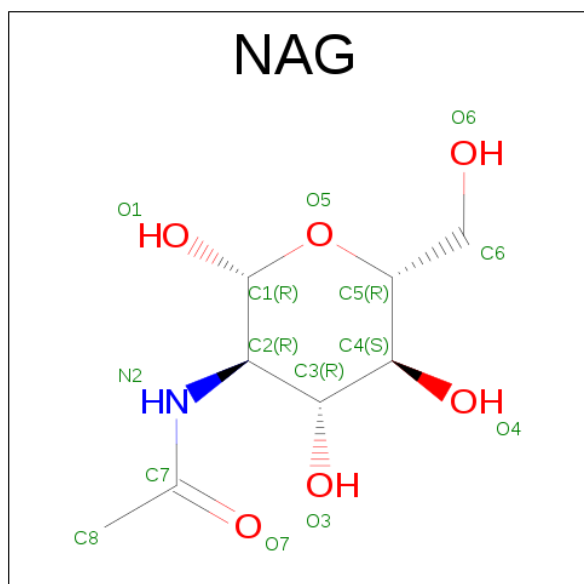
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	5	0
			6354	4035	1095	1175	49			
1	B	781	Total	C	N	O	S	0	5	0
			6354	4035	1095	1175	49			

There are 6 discrepancies between the modelled and reference sequences:

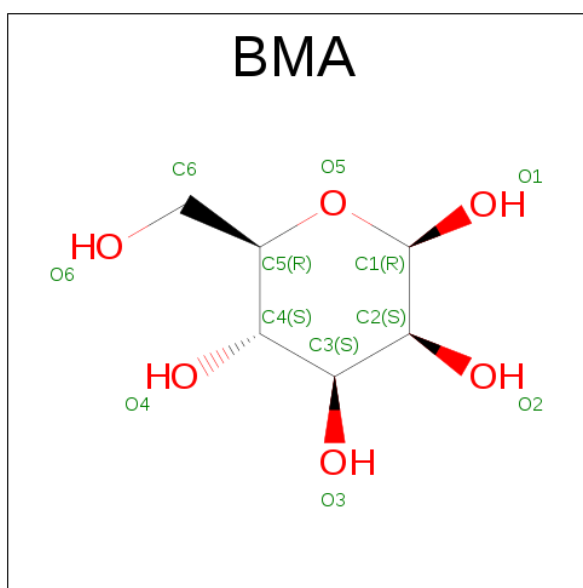
Chain	Residue	Modelled	Actual	Comment	Reference
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	cloning artefact	UNP Q64610
A	806	ALA	ASN	engineered mutation	UNP Q64610
B	410	ALA	ASN	engineered mutation	UNP Q64610
B	591	THR	ARG	cloning artefact	UNP Q64610
B	806	ALA	ASN	engineered mutation	UNP Q64610

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



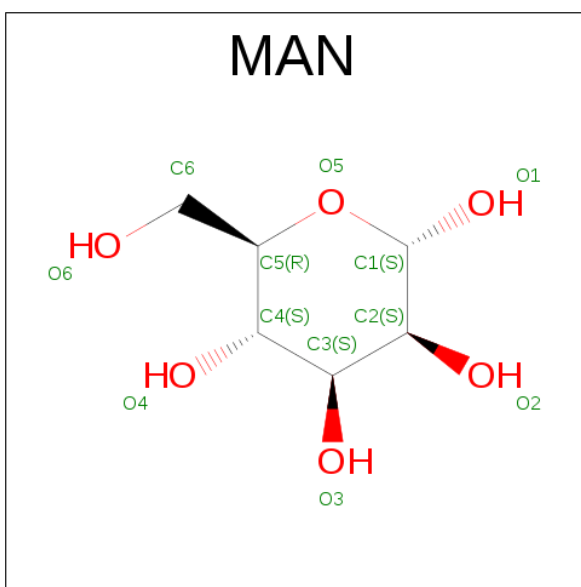
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

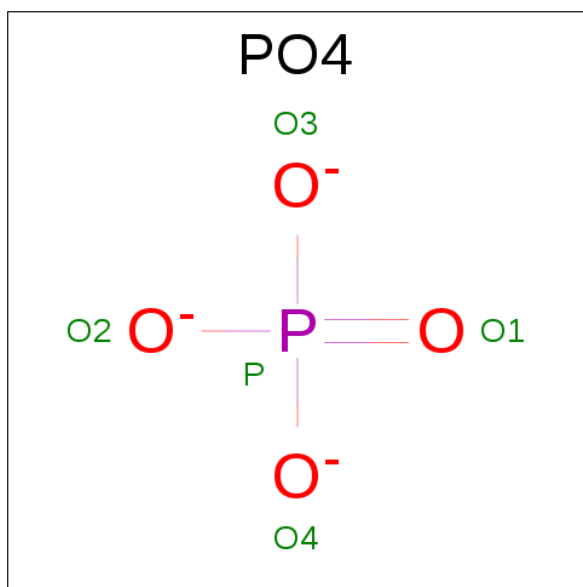
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	13	Total	I	0	0
			13	13		
7	A	14	Total	I	0	0
			14	14		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

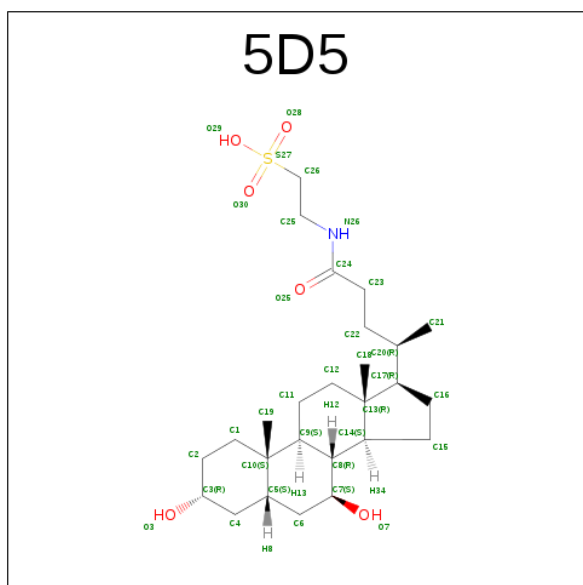


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

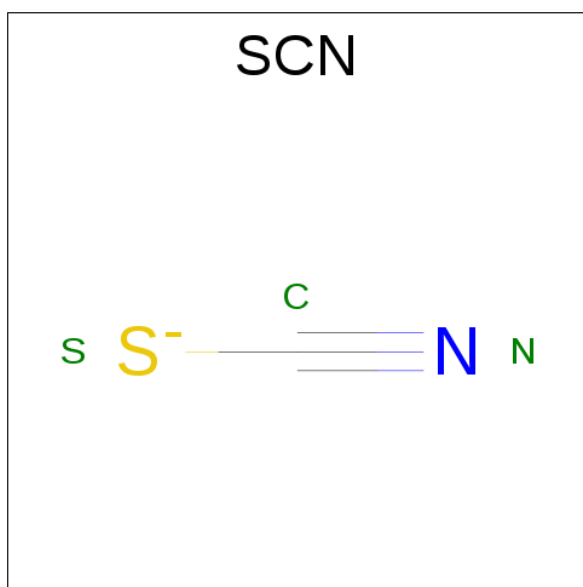
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Na 2 2	0	0
9	A	2	Total Na 2 2	0	0

- Molecule 10 is 2-{[(3alpha,5beta,7alpha,8alpha,14beta,17alpha)-3,7-dihydroxy-24-oxocholan-24-yl]amino}ethanesulfonic acid (three-letter code: 5D5) (formula: C<sub>26</sub>H<sub>45</sub>NO<sub>6</sub>S).



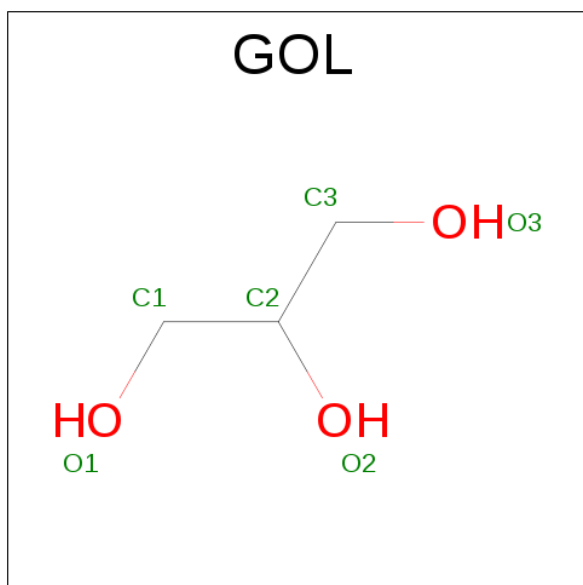
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O S 102 78 3 18 3	0	1
10	B	1	Total C N O S 102 78 3 18 3	0	1

- Molecule 11 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		

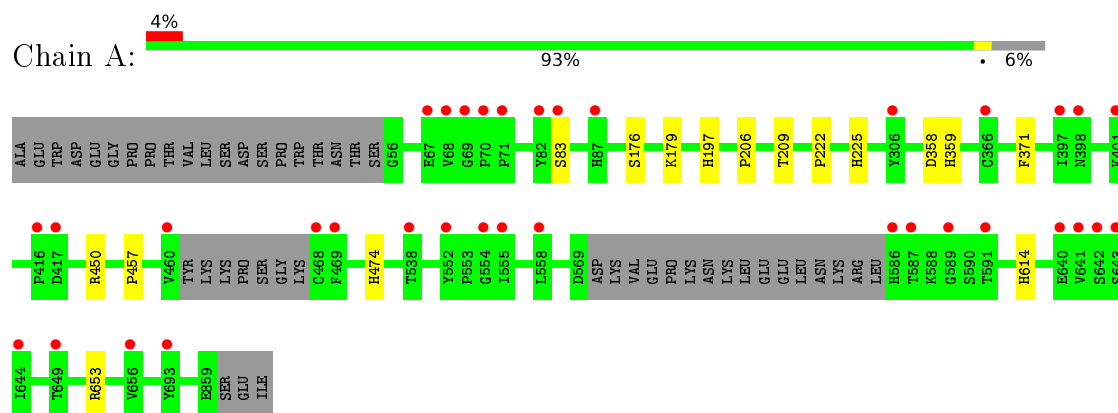
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	299	Total	O	0	1
			300	300		
13	B	288	Total	O	0	1
			289	289		

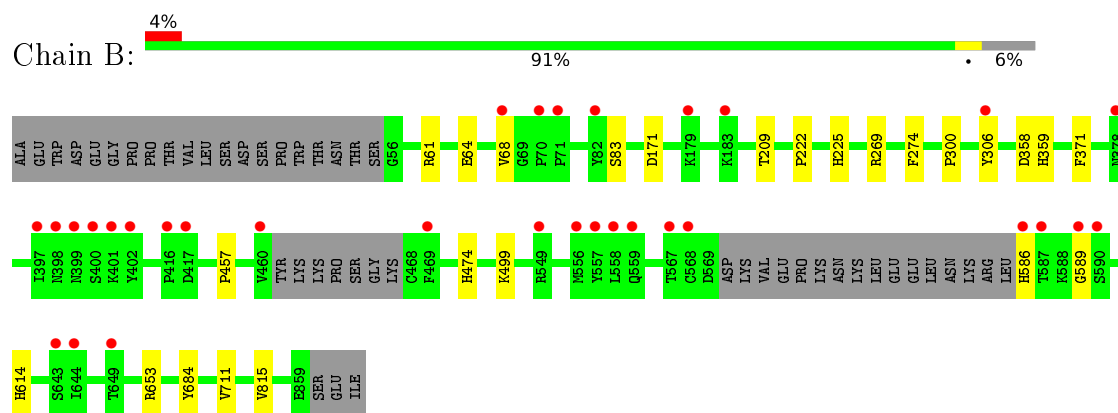
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.88Å 77.83Å 92.44Å 83.84° 79.29° 77.08°	Depositor
Resolution (Å)	90.61 – 2.00 46.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (90.61-2.00) 95.8 (46.80-2.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.227 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	5310 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: GOL, ZN, BMA, NAG, 5D5, NA, CA, SCN, IOD, PO4, MAN

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	0.50	0/6544	0.69	3/8876 (0.0%)
1	B	0.50	0/6544	0.70	2/8876 (0.0%)
All	All	0.50	0/13088	0.70	5/17752 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	358	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	653	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	653	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	450	ARG	NE-CZ-NH2	5.12	122.86	120.30

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	6354	0	6112	7	0
1	B	6354	0	6112	12	0
2	A	28	0	24	0	0
2	B	28	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	8	0	0
3	B	11	0	8	0	0
4	A	66	0	56	0	0
4	B	44	0	38	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	14	0	0	3	0
7	B	13	0	0	2	0
8	A	5	0	0	1	0
8	B	5	0	0	1	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	102	0	0	2	0
10	B	102	0	0	4	0
11	A	6	0	0	0	0
11	B	6	0	0	0	0
12	A	36	0	48	0	0
12	B	30	0	40	1	0
13	A	300	0	0	1	0
13	B	289	0	0	1	0
All	All	13814	0	12470	26	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (26) 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)
10:A:930[B]:5D5:O25	10:A:930[B]:5D5:C26	2.30	0.80
7:B:923:IOD:I	13:B:1269:HOH:O	2.73	0.76
1:A:197:HIS:CD2	7:A:921:IOD:I	3.16	0.69
7:A:923:IOD:I	13:A:1298:HOH:O	2.86	0.63
1:A:197:HIS:NE2	7:A:921:IOD:I	3.04	0.60
10:A:930[A]:5D5:O30	10:A:930[A]:5D5:N26	2.35	0.59
10:B:927[A]:5D5:O25	10:B:927[A]:5D5:C26	2.50	0.57
1:B:209:THR:OG1	8:B:924:PO4:P	2.67	0.52
1:B:499:LYS:HE2	7:B:923:IOD:I	2.83	0.49
10:B:927[A]:5D5:C12	10:B:927[A]:5D5:C21	2.90	0.49
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:PHE:HA	10:B:927[B]:5D5:O29	2.14	0.48
1:B:222:PRO:HA	1:B:225:HIS:CE1	2.49	0.48
1:B:171:ASP:OD2	1:B:306[B]:TYR:OH	2.20	0.47
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.49	0.47
1:B:371:PHE:CE1	1:B:457:PRO:HA	2.49	0.46
1:A:176:SER:O	1:A:179:LYS:HB2	2.16	0.45
1:B:684:TYR:HE2	12:B:934:GOL:O2	1.99	0.45
1:A:359:HIS:CE1	1:A:474:HIS:CE1	3.06	0.44
1:A:209:THR:OG1	8:A:927:PO4:P	2.78	0.42
10:B:927[B]:5D5:C25	10:B:927[B]:5D5:C22	2.95	0.42
1:B:359:HIS:CE1	1:B:474:HIS:CE1	3.08	0.42
1:B:269[B]:ARG:HG2	1:B:300:PRO:HA	2.01	0.41
1:B:64:GLU:OE2	1:B:68:VAL:HG21	2.20	0.41
1:B:586:HIS:HB3	1:B:589:GLY:H	1.87	0.40
1:B:711:VAL:HG13	1:B:815:VAL:HG13	2.03	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	781/827 (94%)	756 (97%)	24 (3%)	1 (0%)	56	53
1	B	781/827 (94%)	755 (97%)	25 (3%)	1 (0%)	56	53
All	All	1562/1654 (94%)	1511 (97%)	49 (3%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	B	83	SER

### 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	712/749 (95%)	710 (100%)	2 (0%)	94	96
1	B	712/749 (95%)	710 (100%)	2 (0%)	94	96
All	All	1424/1498 (95%)	1420 (100%)	4 (0%)	94	96

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

Mol	Chain	Res	Type
1	A	206	PRO
1	A	614	HIS
1	B	61	ARG
1	B	614	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 37 are monoatomic - leaving 39 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	$\# Z  > 2$
2	NAG	A	901	1,2	14,14,15	0.36	0	15,19,21	0.86	0
2	NAG	A	902	3,2	14,14,15	0.64	0	15,19,21	1.26	2 (13%)
3	BMA	A	903	2,4	11,11,12	0.48	0	15,15,17	0.92	0
4	MAN	A	904	3,4	11,11,12	0.40	0	15,15,17	1.12	1 (6%)
4	MAN	A	905	4	11,11,12	0.47	0	15,15,17	0.74	0
4	MAN	A	906	4	11,11,12	0.46	0	15,15,17	1.21	1 (6%)
4	MAN	A	907	3	11,11,12	0.68	0	15,15,17	1.48	2 (13%)
4	MAN	A	908	4	11,11,12	0.66	0	15,15,17	1.60	3 (20%)
4	MAN	A	909	4	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
8	PO4	A	927	5	4,4,4	0.37	0	6,6,6	0.25	0
10	5D5	A	930[A]	-	37,37,37	1.43	1 (2%)	58,58,58	1.32	10 (17%)
10	5D5	A	930[B]	-	37,37,37	1.44	1 (2%)	58,58,58	1.38	8 (13%)
10	5D5	A	930[C]	-	37,37,37	1.39	1 (2%)	58,58,58	1.63	16 (27%)
11	SCN	A	931	-	2,2,2	0.65	0	1,1,1	0.56	0
11	SCN	A	932	-	2,2,2	0.85	0	1,1,1	0.51	0
12	GOL	A	933	-	5,5,5	0.24	0	5,5,5	0.15	0
12	GOL	A	934	-	5,5,5	0.47	0	5,5,5	0.71	0
12	GOL	A	935	-	5,5,5	0.22	0	5,5,5	0.29	0
12	GOL	A	936	-	5,5,5	0.30	0	5,5,5	0.20	0
12	GOL	A	937	-	5,5,5	0.23	0	5,5,5	0.16	0
12	GOL	A	938	-	5,5,5	0.14	0	5,5,5	0.38	0
2	NAG	B	901	1,2	14,14,15	0.53	0	15,19,21	1.05	1 (6%)
2	NAG	B	902	3,2	14,14,15	0.55	0	15,19,21	0.95	1 (6%)
3	BMA	B	903	2,4	11,11,12	0.46	0	15,15,17	0.96	0
4	MAN	B	904	3,4	11,11,12	0.67	0	15,15,17	1.52	2 (13%)
4	MAN	B	905	4	11,11,12	0.75	0	15,15,17	1.29	2 (13%)
4	MAN	B	906	4	11,11,12	0.69	0	15,15,17	0.86	0
4	MAN	B	907	3	11,11,12	0.38	0	15,15,17	1.14	2 (13%)
8	PO4	B	924	5	4,4,4	0.47	0	6,6,6	0.30	0
10	5D5	B	927[A]	-	37,37,37	1.47	1 (2%)	58,58,58	1.47	11 (18%)
10	5D5	B	927[B]	-	37,37,37	1.51	1 (2%)	58,58,58	1.62	11 (18%)
10	5D5	B	927[C]	-	37,37,37	1.40	1 (2%)	58,58,58	1.71	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SCN	B	928	-	2,2,2	0.59	0	1,1,1	0.55	0
11	SCN	B	929	-	2,2,2	0.71	0	1,1,1	0.50	0
12	GOL	B	930	-	5,5,5	0.24	0	5,5,5	0.08	0
12	GOL	B	931	-	5,5,5	0.48	0	5,5,5	0.63	0
12	GOL	B	932	-	5,5,5	0.20	0	5,5,5	0.39	0
12	GOL	B	933	-	5,5,5	0.28	0	5,5,5	0.41	0
12	GOL	B	934	-	5,5,5	0.21	0	5,5,5	0.53	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
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	905	4	-	0/2/19/22	0/1/1/1
4	MAN	A	906	4	-	0/2/19/22	0/1/1/1
4	MAN	A	907	3	-	0/2/19/22	0/1/1/1
4	MAN	A	908	4	-	0/2/19/22	0/1/1/1
4	MAN	A	909	4	-	0/2/19/22	0/1/1/1
8	PO4	A	927	5	-	0/0/0/0	0/0/0/0
10	5D5	A	930[A]	-	-	0/16/77/77	0/4/4/4
10	5D5	A	930[B]	-	-	0/16/77/77	0/4/4/4
10	5D5	A	930[C]	-	-	0/16/77/77	0/4/4/4
11	SCN	A	931	-	-	0/0/0/0	0/0/0/0
11	SCN	A	932	-	-	0/0/0/0	0/0/0/0
12	GOL	A	933	-	-	0/4/4/4	0/0/0/0
12	GOL	A	934	-	-	0/4/4/4	0/0/0/0
12	GOL	A	935	-	-	0/4/4/4	0/0/0/0
12	GOL	A	936	-	-	0/4/4/4	0/0/0/0
12	GOL	A	937	-	-	0/4/4/4	0/0/0/0
12	GOL	A	938	-	-	0/4/4/4	0/0/0/0
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	905	4	-	0/2/19/22	0/1/1/1
4	MAN	B	906	4	-	0/2/19/22	0/1/1/1
4	MAN	B	907	3	-	0/2/19/22	0/1/1/1
8	PO4	B	924	5	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	5D5	B	927[A]	-	-	0/16/77/77	0/4/4/4
10	5D5	B	927[B]	-	-	0/16/77/77	0/4/4/4
10	5D5	B	927[C]	-	-	0/16/77/77	0/4/4/4
11	SCN	B	928	-	-	0/0/0/0	0/0/0/0
11	SCN	B	929	-	-	0/0/0/0	0/0/0/0
12	GOL	B	930	-	-	0/4/4/4	0/0/0/0
12	GOL	B	931	-	-	0/4/4/4	0/0/0/0
12	GOL	B	932	-	-	0/4/4/4	0/0/0/0
12	GOL	B	933	-	-	0/4/4/4	0/0/0/0
12	GOL	B	934	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	927[B]	5D5	C26-S27	-8.21	1.65	1.77
10	B	927[A]	5D5	C26-S27	-7.64	1.66	1.77
10	A	930[A]	5D5	C26-S27	-7.58	1.66	1.77
10	A	930[B]	5D5	C26-S27	-7.50	1.66	1.77
10	B	927[C]	5D5	C26-S27	-7.43	1.66	1.77
10	A	930[C]	5D5	C26-S27	-7.08	1.66	1.77

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	930[C]	5D5	C13-C17-C20	-4.81	111.66	119.49
10	B	927[C]	5D5	C13-C17-C20	-4.33	112.44	119.49
10	A	930[A]	5D5	C13-C17-C20	-3.16	114.34	119.49
10	B	927[A]	5D5	C11-C9-C10	-3.02	110.01	113.88
10	B	927[C]	5D5	C9-C8-C7	-3.00	108.26	111.89
2	A	902	NAG	O5-C5-C4	-2.98	105.20	110.13
10	B	927[B]	5D5	C25-N26-C24	-2.94	116.96	122.79
10	B	927[C]	5D5	C10-C9-C8	-2.92	108.70	111.86
10	B	927[A]	5D5	C5-C4-C3	-2.90	108.59	112.88
10	B	927[C]	5D5	C13-C14-C8	-2.88	110.17	113.99
10	B	927[A]	5D5	C13-C17-C20	-2.78	114.96	119.49
10	A	930[C]	5D5	C5-C4-C3	-2.74	108.82	112.88
4	A	908	MAN	O5-C5-C4	-2.74	105.59	110.13
10	A	930[C]	5D5	C13-C14-C8	-2.72	110.38	113.99
10	B	927[C]	5D5	C21-C20-C17	-2.71	108.81	112.99
10	B	927[A]	5D5	C4-C3-C2	-2.66	107.13	110.53
2	A	902	NAG	O3-C3-C2	-2.65	103.71	109.37
10	B	927[B]	5D5	C4-C5-C10	-2.64	109.82	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	927[B]	5D5	C25-C26-S27	-2.64	105.79	113.66
10	A	930[C]	5D5	C21-C20-C17	-2.61	108.97	112.99
10	B	927[A]	5D5	C19-C10-C9	-2.60	107.75	111.20
10	B	927[A]	5D5	C5-C6-C7	-2.59	111.50	114.44
10	B	927[B]	5D5	C4-C3-C2	-2.58	107.22	110.53
10	A	930[B]	5D5	C5-C4-C3	-2.52	109.15	112.88
10	B	927[C]	5D5	C11-C12-C13	-2.48	108.35	112.81
10	B	927[A]	5D5	C13-C14-C8	-2.45	110.74	113.99
10	B	927[B]	5D5	C5-C4-C3	-2.42	109.30	112.88
10	A	930[C]	5D5	C14-C8-C9	-2.38	106.27	109.63
10	B	927[A]	5D5	C11-C12-C13	-2.34	108.61	112.81
10	B	927[B]	5D5	C23-C24-N26	-2.34	112.39	116.46
10	B	927[C]	5D5	C5-C4-C3	-2.34	109.42	112.88
10	B	927[C]	5D5	C4-C3-C2	-2.33	107.55	110.53
10	A	930[B]	5D5	C11-C12-C13	-2.31	108.67	112.81
10	B	927[C]	5D5	C11-C9-C10	-2.27	110.97	113.88
10	A	930[C]	5D5	C5-C6-C7	-2.26	111.88	114.44
10	A	930[B]	5D5	C13-C17-C20	-2.24	115.85	119.49
10	A	930[C]	5D5	C11-C12-C13	-2.19	108.87	112.81
10	A	930[C]	5D5	C19-C10-C9	-2.19	108.30	111.20
10	A	930[A]	5D5	C5-C4-C3	-2.18	109.64	112.88
10	B	927[C]	5D5	C19-C10-C9	-2.16	108.34	111.20
10	A	930[A]	5D5	C21-C20-C17	-2.15	109.67	112.99
4	B	905	MAN	O5-C5-C4	-2.15	106.57	110.13
10	A	930[A]	5D5	C11-C12-C13	-2.13	108.98	112.81
10	A	930[C]	5D5	C11-C9-C10	-2.12	111.17	113.88
10	A	930[C]	5D5	O29-S27-O30	-2.11	106.60	111.26
2	B	902	NAG	O4-C4-C5	-2.09	103.71	109.23
10	A	930[A]	5D5	C25-C26-S27	-2.08	107.46	113.66
10	A	930[B]	5D5	C4-C5-C10	-2.05	110.46	112.66
10	A	930[B]	5D5	C25-C26-S27	-2.04	107.58	113.66
10	B	927[B]	5D5	C23-C22-C20	-2.04	110.68	114.46
10	A	930[A]	5D5	C5-C6-C7	-2.04	112.12	114.44
10	B	927[C]	5D5	C23-C22-C20	-2.00	110.73	114.46
10	A	930[A]	5D5	C19-C10-C9	-2.00	108.55	111.20
4	B	907	MAN	O5-C5-C4	2.01	113.47	110.13
10	A	930[C]	5D5	C16-C17-C13	2.04	106.22	103.83
10	B	927[A]	5D5	O30-S27-C26	2.06	108.33	106.87
4	B	905	MAN	O3-C3-C2	2.08	113.81	110.01
4	A	904	MAN	O3-C3-C2	2.08	113.82	110.01
10	A	930[C]	5D5	O28-S27-C26	2.14	108.38	106.87
4	B	904	MAN	O5-C1-C2	2.14	114.32	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	908	MAN	O2-C2-C1	2.20	113.64	109.23
4	A	907	MAN	C2-C3-C4	2.26	115.00	111.05
4	A	906	MAN	C1-O5-C5	2.34	115.57	112.14
2	B	901	NAG	C3-C4-C5	2.38	114.47	110.23
10	A	930[B]	5D5	C1-C10-C5	2.46	110.48	107.76
10	A	930[A]	5D5	O29-S27-C26	2.48	110.15	104.99
10	B	927[A]	5D5	O29-S27-C26	2.51	110.20	104.99
10	B	927[C]	5D5	O29-S27-C26	2.60	110.39	104.99
10	A	930[C]	5D5	O29-S27-C26	2.74	110.69	104.99
10	A	930[A]	5D5	C1-C10-C5	2.80	110.85	107.76
4	B	907	MAN	C1-O5-C5	2.81	116.27	112.14
4	A	909	MAN	C1-O5-C5	2.82	116.29	112.14
10	B	927[B]	5D5	C1-C10-C5	2.94	111.00	107.76
10	A	930[A]	5D5	O30-S27-C26	2.94	108.94	106.87
10	B	927[B]	5D5	C6-C7-C8	3.00	114.64	111.46
10	A	930[C]	5D5	C1-C10-C5	3.01	111.07	107.76
10	B	927[A]	5D5	C1-C10-C5	3.02	111.09	107.76
10	B	927[B]	5D5	O29-S27-C26	3.03	111.28	104.99
10	A	930[C]	5D5	C17-C13-C14	3.23	103.87	100.09
10	A	930[B]	5D5	O28-S27-C26	3.29	109.19	106.87
4	A	907	MAN	C1-O5-C5	3.33	117.03	112.14
10	B	927[C]	5D5	C17-C13-C14	3.43	104.09	100.09
4	A	908	MAN	C6-C5-C4	3.56	121.90	112.99
10	B	927[C]	5D5	C1-C10-C5	3.72	111.86	107.76
4	B	904	MAN	C1-C2-C3	3.77	114.12	109.55
10	B	927[C]	5D5	O30-S27-C26	3.95	109.66	106.87
10	A	930[C]	5D5	O30-S27-C26	4.02	109.71	106.87
10	A	930[B]	5D5	O30-S27-C26	4.46	110.02	106.87
10	B	927[B]	5D5	O30-S27-C26	6.60	111.53	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	927	PO4	1	0
10	A	930[A]	5D5	1	0
10	A	930[B]	5D5	1	0
8	B	924	PO4	1	0
10	B	927[A]	5D5	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	927[B]	5D5	2	0
12	B	934	GOL	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, 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	781/827 (94%)	0.15	35 (4%) 37 38	15, 32, 66, 107	0
1	B	781/827 (94%)	0.12	32 (4%) 41 42	14, 33, 66, 110	0
All	All	1562/1654 (94%)	0.14	67 (4%) 39 40	14, 33, 66, 110	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	LYS	7.5
1	B	398	ASN	7.1
1	B	70	PRO	6.0
1	A	69	GLY	5.8
1	B	586	HIS	5.3
1	A	398	ASN	5.3
1	B	397	ILE	4.9
1	B	589	GLY	4.7
1	A	587	THR	4.6
1	B	587	THR	4.5
1	A	70	PRO	4.3
1	A	460	VAL	4.3
1	A	401	LYS	4.3
1	A	558	LEU	4.1
1	A	71	PRO	3.9
1	A	469	PHE	3.9
1	B	469	PHE	3.8
1	B	306[A]	TYR	3.8
1	A	306[A]	TYR	3.8
1	A	643	SER	3.7
1	B	71	PRO	3.7
1	B	400	SER	3.7
1	B	68	VAL	3.6
1	A	641	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	3.5
1	B	643	SER	3.5
1	A	67	GLU	3.4
1	A	87	HIS	3.4
1	B	378	ASN	3.4
1	A	586	HIS	3.1
1	A	397	ILE	3.1
1	A	640	GLU	3.0
1	B	558	LEU	3.0
1	A	644	ILE	2.8
1	A	468	CYS	2.8
1	B	567	THR	2.8
1	A	649	THR	2.8
1	B	179	LYS	2.8
1	A	416	PRO	2.8
1	A	693	TYR	2.7
1	A	591	THR	2.7
1	B	402	TYR	2.7
1	B	590	SER	2.7
1	B	568	CYS	2.6
1	B	460	VAL	2.6
1	A	589	GLY	2.5
1	A	555	ILE	2.5
1	B	556	MET	2.4
1	B	183	LYS	2.4
1	A	538	THR	2.4
1	B	399	ASN	2.4
1	A	552	TYR	2.4
1	A	554	GLY	2.4
1	A	82	TYR	2.3
1	B	416	PRO	2.3
1	B	549	ARG	2.3
1	B	417	ASP	2.3
1	A	83	SER	2.2
1	A	417	ASP	2.2
1	A	642	SER	2.2
1	B	557	TYR	2.2
1	B	82	TYR	2.1
1	B	649	THR	2.1
1	A	656	VAL	2.1
1	A	366	CYS	2.1
1	B	644	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	559	GLN	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
12	GOL	A	933	6/6	0.80	0.40	12.59	58,63,63,70	0
12	GOL	A	934	6/6	0.79	0.28	8.06	27,43,46,51	0
11	SCN	A	931	3/3	0.72	0.20	7.46	53,53,60,86	0
12	GOL	B	930	6/6	0.83	0.38	6.32	56,61,63,66	0
12	GOL	B	931	6/6	0.65	0.32	6.11	31,46,48,51	0
12	GOL	B	933	6/6	0.82	0.24	5.18	46,51,57,57	0
8	PO4	A	927	5/5	0.72	0.24	5.02	38,44,58,82	0
12	GOL	B	934	6/6	0.86	0.22	4.54	36,40,45,60	0
12	GOL	A	937	6/6	0.92	0.15	4.28	33,39,42,45	0
12	GOL	A	938	6/6	0.83	0.21	3.69	38,41,47,65	0
8	PO4	B	924	5/5	0.63	0.21	2.94	35,38,53,71	0
12	GOL	A	935	6/6	0.88	0.26	2.70	41,50,57,62	0
7	IOD	A	913	1/1	1.00	0.11	2.21	26,26,26,26	0
10	5D5	A	930[A]	34/34	0.84	0.25	2.18	41,58,59,60	34
9	NA	B	926	1/1	0.94	0.14	2.16	44,44,44,44	0
10	5D5	B	927[A]	34/34	0.88	0.24	1.86	26,27,28,29	34
12	GOL	B	932	6/6	0.78	0.30	1.84	49,58,59,70	0
4	MAN	A	905	11/12	0.88	0.15	1.66	39,47,55,64	0
10	5D5	A	930[B]	34/34	0.84	0.25	1.51	30,31,35,37	34
10	5D5	A	930[C]	34/34	0.84	0.25	1.43	32,55,57,57	34

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	SCN	B	928	3/3	0.89	0.16	1.25	39,39,40,63	0
10	5D5	B	927[C]	34/34	0.88	0.24	1.25	32,53,56,57	34
11	SCN	A	932	3/3	0.86	0.14	1.20	29,29,40,44	0
10	5D5	B	927[B]	34/34	0.88	0.24	1.19	13,15,16,16	34
7	IOD	B	911	1/1	1.00	0.11	0.79	25,25,25,25	0
2	NAG	A	901	14/15	0.97	0.14	0.66	17,18,20,21	0
6	CA	B	910	1/1	1.00	0.11	-0.49	20,20,20,20	0
7	IOD	A	921	1/1	0.98	0.13	-0.60	59,59,59,59	1
9	NA	B	925	1/1	0.88	0.13	-0.68	39,39,39,39	0
2	NAG	B	901	14/15	0.97	0.11	-0.72	18,19,22,24	0
6	CA	A	912	1/1	1.00	0.12	-0.78	23,23,23,23	0
5	ZN	A	911	1/1	0.98	0.06	-1.10	71,71,71,71	0
5	ZN	B	909	1/1	0.98	0.06	-1.11	63,63,63,63	0
5	ZN	B	908	1/1	0.99	0.08	-1.23	29,29,29,29	0
7	IOD	B	917	1/1	0.99	0.07	-1.72	55,55,55,55	1
7	IOD	A	919	1/1	1.00	0.05	-1.77	58,58,58,58	1
7	IOD	A	917	1/1	0.99	0.07	-1.92	43,43,43,43	1
9	NA	A	928	1/1	0.92	0.06	-1.92	37,37,37,37	0
7	IOD	B	915	1/1	0.99	0.08	-1.95	40,40,40,40	1
7	IOD	B	914	1/1	0.99	0.07	-2.17	40,40,40,40	1
5	ZN	A	910	1/1	1.00	0.08	-2.20	29,29,29,29	0
7	IOD	A	915	1/1	0.99	0.05	-2.51	68,68,68,68	1
7	IOD	A	922	1/1	0.99	0.07	-2.51	48,48,48,48	1
7	IOD	A	916	1/1	0.99	0.07	-2.73	37,37,37,37	1
7	IOD	B	916	1/1	1.00	0.06	-3.42	40,40,40,40	1
7	IOD	B	913	1/1	0.99	0.04	-4.04	67,67,67,67	1
7	IOD	B	920	1/1	1.00	0.04	-4.29	53,53,53,53	1
7	IOD	A	918	1/1	1.00	0.06	-4.83	39,39,39,39	1
3	BMA	B	903	11/12	0.89	0.12	-	51,59,66,66	0
7	IOD	B	919	1/1	0.95	0.07	-	67,67,67,67	1
4	MAN	A	908	11/12	0.86	0.17	-	33,44,47,48	0
7	IOD	A	914	1/1	0.99	0.07	-	50,50,50,50	1
7	IOD	A	924	1/1	0.99	0.05	-	51,51,51,51	1
9	NA	A	929	1/1	0.96	0.19	-	39,39,39,39	0
4	MAN	B	905	11/12	0.85	0.16	-	50,59,63,66	0
7	IOD	B	918	1/1	0.99	0.06	-	57,57,57,57	1
11	SCN	B	929	3/3	0.89	0.17	-	41,41,46,54	0
7	IOD	A	925	1/1	0.99	0.07	-	52,52,52,52	1
4	MAN	A	906	11/12	0.92	0.12	-	26,33,40,45	0
4	MAN	A	909	11/12	0.87	0.11	-	45,47,49,50	0
7	IOD	B	923	1/1	0.99	0.03	-	67,67,67,67	1
7	IOD	B	921	1/1	0.98	0.07	-	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	902	14/15	0.95	0.12	-	28,33,39,45	0
7	IOD	B	912	1/1	1.00	0.06	-	56,56,56,56	1
7	IOD	B	922	1/1	0.99	0.07	-	60,60,60,60	1
4	MAN	B	906	11/12	0.81	0.16	-	36,49,52,53	0
12	GOL	A	936	6/6	0.78	0.41	-	43,45,52,54	0
4	MAN	B	907	11/12	0.78	0.19	-	70,78,83,90	0
7	IOD	A	926	1/1	0.98	0.05	-	61,61,61,61	1
2	NAG	A	902	14/15	0.98	0.11	-	22,24,26,28	0
4	MAN	A	907	11/12	0.78	0.16	-	43,49,51,53	0
7	IOD	A	920	1/1	1.00	0.07	-	48,48,48,48	1
7	IOD	A	923	1/1	0.98	0.06	-	58,58,58,58	1
3	BMA	A	903	11/12	0.96	0.09	-	32,37,42,43	0
4	MAN	A	904	11/12	0.91	0.11	-	36,39,44,45	0
4	MAN	B	904	11/12	0.89	0.10	-	49,51,53,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.