



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:54 PM GMT

PDB ID : 4DT2  
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with Maybridge fragment CC27209  
Authors : Feder, D.; Hussein, W.M.; Clayton, D.J.; Kan, M.; Schenk, G.; McGeary, R.P.; Guddat, L.W.  
Deposited on : 2012-02-20  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

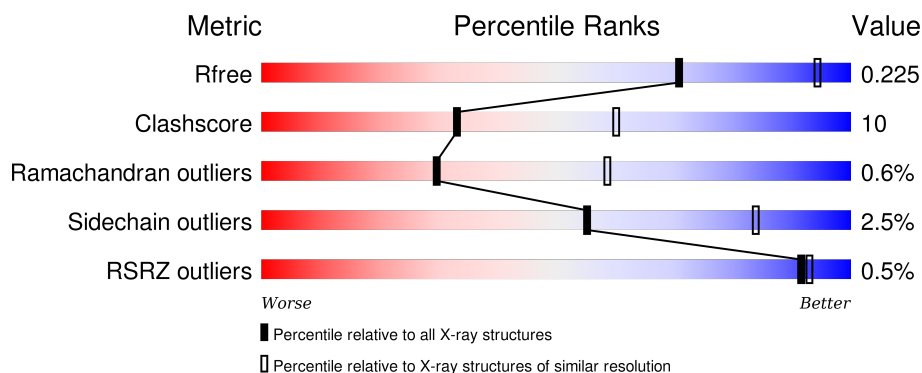
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	426	<div> <div></div> <div>77%22%</div> </div>
1	B	426	<div> <div>%</div> <div>77%22%</div> </div>
1	C	426	<div> <div></div> <div>73%26%.</div> </div>
1	D	426	<div> <div>%</div> <div>80%19%.</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	NAG	C	507	-	-	-	X
10	NAG	D	504	-	-	-	X
4	GOL	A	503	-	-	-	X
4	GOL	C	508	-	-	-	X
5	0LV	A	504	-	-	X	X
5	0LV	B	504	-	-	X	X
5	0LV	C	512	-	-	X	X
5	0LV	D	511	-	-	X	X
6	SO4	A	505	-	-	-	X
6	SO4	A	510	-	-	-	X
6	SO4	C	515	-	-	-	X
6	SO4	D	514	-	-	-	X
6	SO4	D	515	-	-	-	X
8	EDO	A	512	-	-	X	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 15025 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 Purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3510	2253	610	637	10			
1	B	426	Total	C	N	O	S	0	0	0
			3510	2253	610	637	10			
1	C	426	Total	C	N	O	S	1	0	0
			3510	2253	610	637	10			
1	D	426	Total	C	N	O	S	0	0	0
			3510	2253	610	637	10			

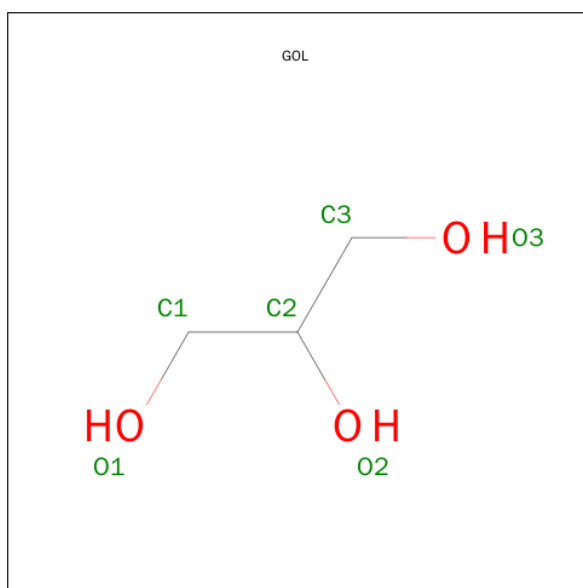
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

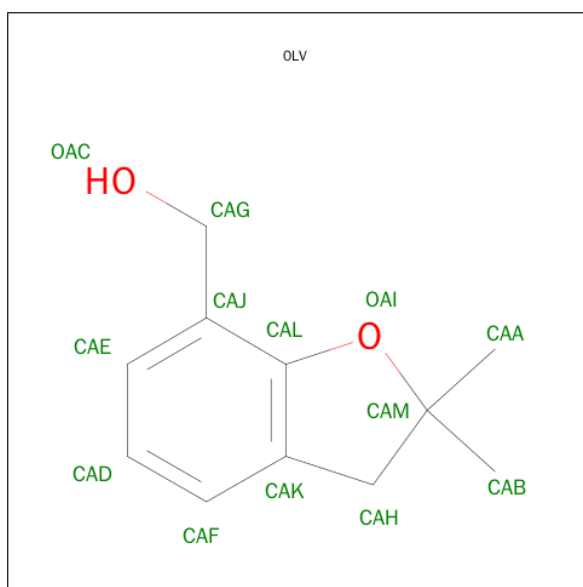
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



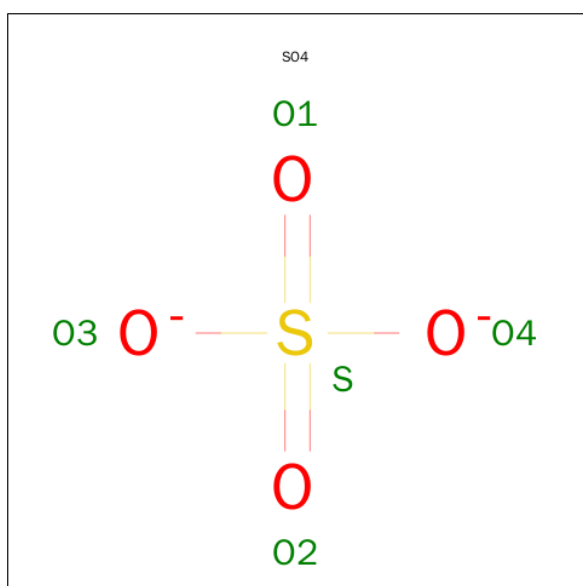
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (2,2-DIMETHYL-2,3-DIHYDRO-1-BENZOFURAN-7-YL)METHANOL (three-letter code: 0LV) (formula:  $C_{11}H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	11	2		
5	B	1	Total	C	O	0	0
			13	11	2		
5	C	1	Total	C	O	0	0
			13	11	2		
5	D	1	Total	C	O	0	0
			13	11	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



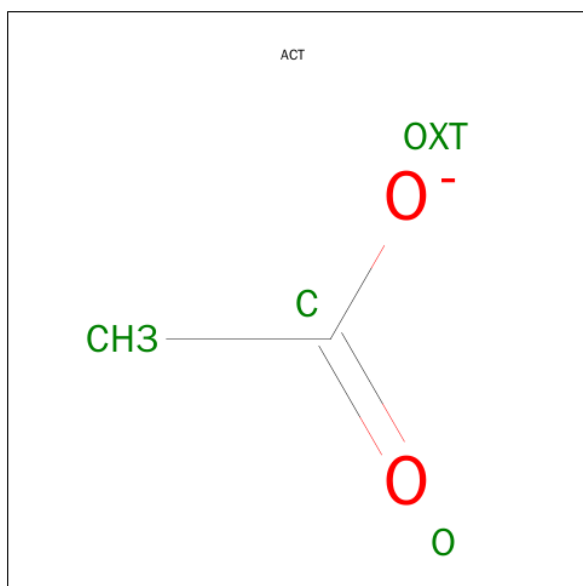
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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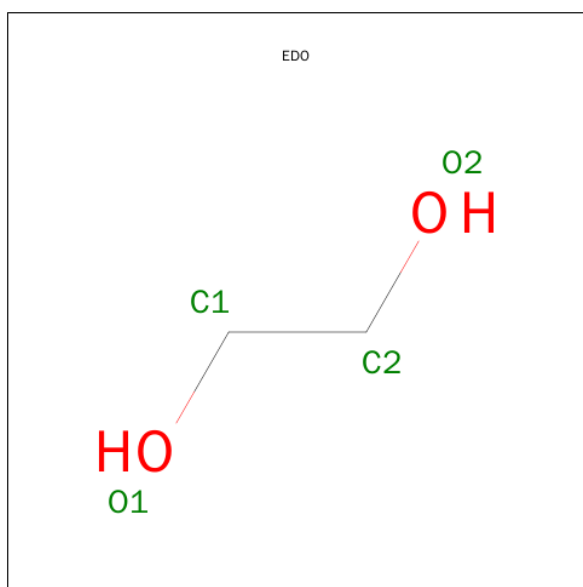
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

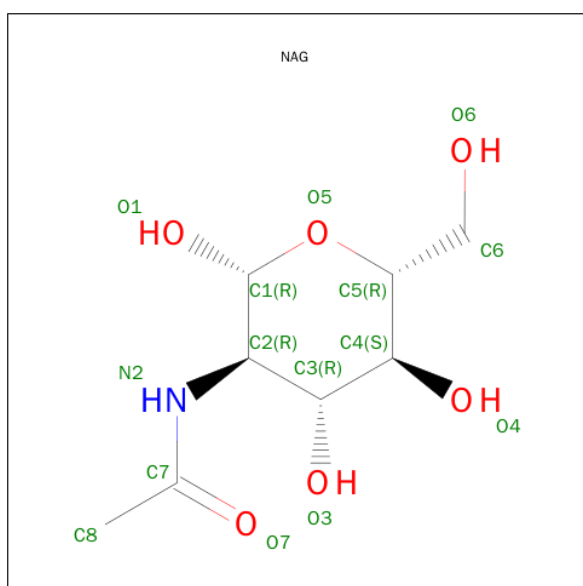


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	3	Total	C	N	O	0	0
			38	22	2	14		
11	A	3	Total	C	N	O	0	0
			38	22	2	14		
11	B	3	Total	C	N	O	0	0
			38	22	2	14		
11	C	3	Total	C	N	O	0	0
			38	22	2	14		
11	C	3	Total	C	N	O	0	0
			38	22	2	14		
11	D	3	Total	C	N	O	0	0
			38	22	2	14		
11	D	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 12 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	2	Total	C	N	O	0	0
			24	14	1	9		

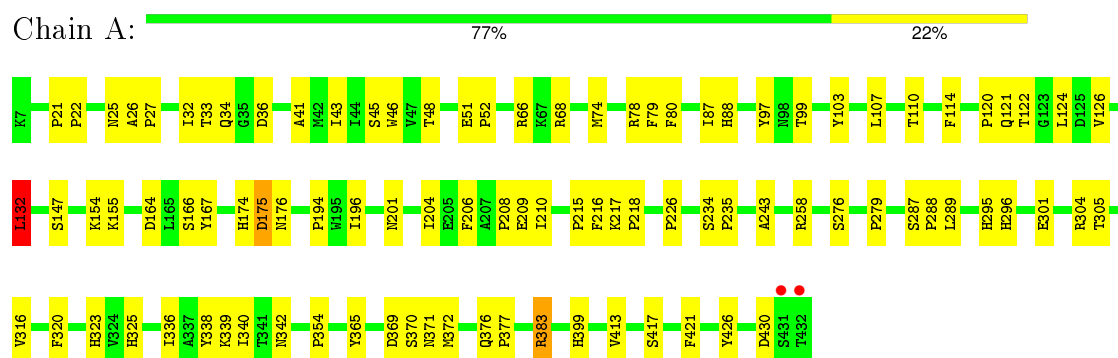
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	127	Total 127	O 127	0	0
13	B	85	Total 85	O 85	0	0
13	C	85	Total 85	O 85	0	0
13	D	96	Total 96	O 96	0	0

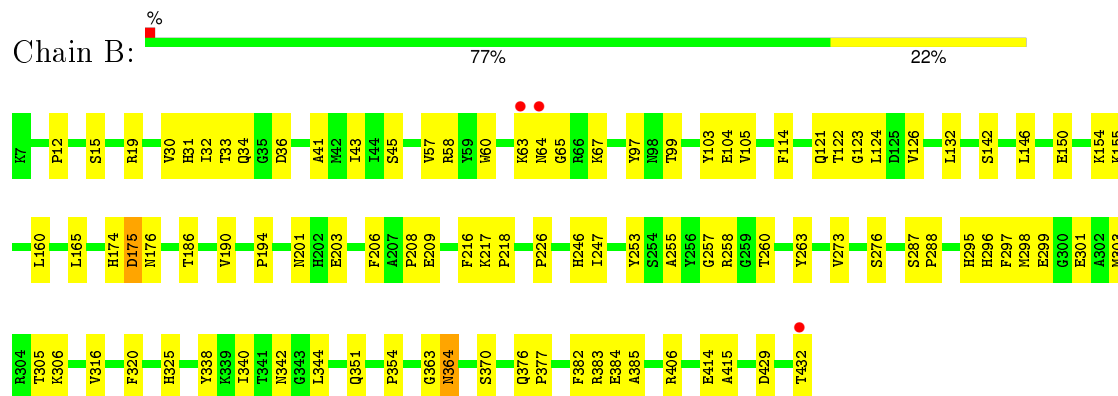
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

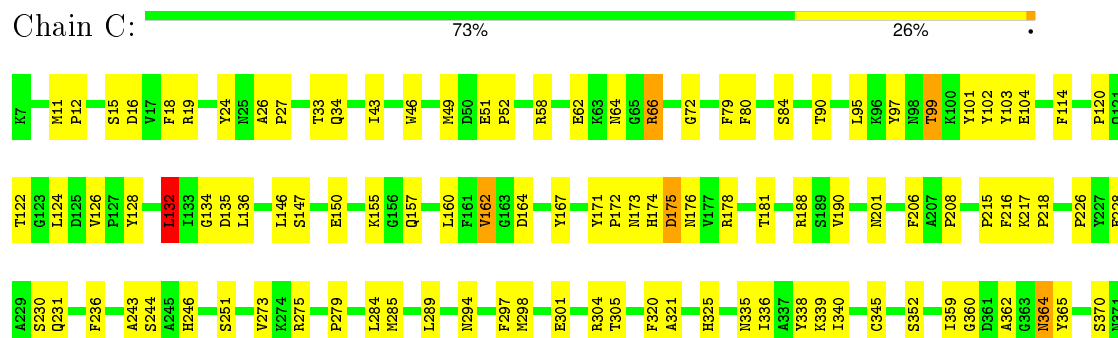
- Molecule 1: Purple acid phosphatase

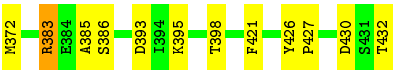


- Molecule 1: Purple acid phosphatase

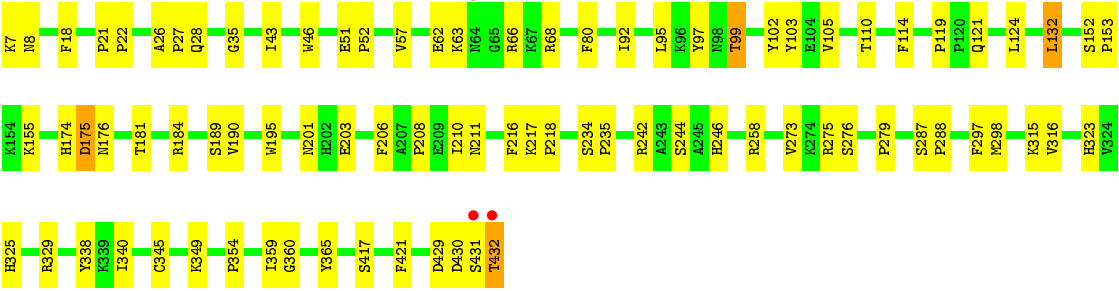
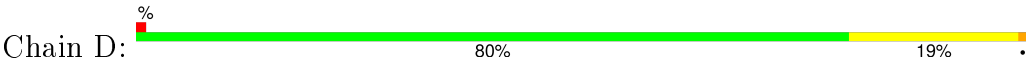


- Molecule 1: Purple acid phosphatase





● Molecule 1: Purple acid phosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.76Å 126.76Å 298.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.72 – 2.70 19.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.72-2.70) 99.8 (19.90-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.71Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, $R_{free}$	0.175 , 0.228 0.175 , 0.225	Depositor DCC
$R_{free}$ test set	3861 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.6	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 76900 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0LV, ZN, FE, NAG, GOL, EDO, SO4, ACT, FUC

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	0.46	0/3629	0.57	1/4934 (0.0%)
1	B	0.43	0/3629	0.55	0/4934
1	C	0.44	0/3629	0.55	1/4934 (0.0%)
1	D	0.44	0/3629	0.57	1/4934 (0.0%)
All	All	0.44	0/14516	0.56	3/19736 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	CA-CB-CG	-6.12	101.23	115.30
1	D	132	LEU	CA-CB-CG	-6.01	101.48	115.30
1	C	132	LEU	CA-CB-CG	-5.91	101.71	115.30

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	3510	0	3326	77	0
1	B	3510	0	3327	68	0
1	C	3510	0	3327	80	0
1	D	3510	0	3327	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	2	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	A	13	0	13	11	0
5	B	13	0	13	9	0
5	C	13	0	14	13	0
5	D	13	0	14	13	0
6	A	30	0	0	2	0
6	B	15	0	0	1	0
6	C	15	0	0	0	0
6	D	20	0	0	0	0
7	A	4	0	3	0	0
8	A	4	0	6	6	0
9	A	38	0	34	2	0
10	A	14	0	13	0	0
10	B	28	0	26	0	0
10	C	28	0	26	0	0
10	D	28	0	26	0	0
11	A	76	0	68	2	0
11	B	38	0	34	1	0
11	C	76	0	68	5	0
11	D	76	0	68	2	0
12	B	24	0	22	0	0
13	A	127	0	0	3	0
13	B	85	0	0	0	0
13	C	85	0	0	2	0
13	D	96	0	0	0	0
All	All	15025	0	13779	293	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 10.

The worst 5 of 293 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:258:ARG:HH22	5:C:512:0LV:H4	1.13	1.08
1:D:323:HIS:CE1	5:D:511:0LV:H9	1.93	1.03
1:C:124:LEU:HD12	1:C:279:PRO:HG3	1.46	0.95
1:A:296:HIS:HE1	5:A:504:0LV:H2	1.30	0.95
1:C:325:HIS:CE1	5:C:512:0LV:H11	2.02	0.94

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	424/426 (100%)	401 (95%)	22 (5%)	1 (0%)	52	80
1	B	424/426 (100%)	387 (91%)	33 (8%)	4 (1%)	21	49
1	C	424/426 (100%)	399 (94%)	22 (5%)	3 (1%)	26	55
1	D	424/426 (100%)	396 (93%)	26 (6%)	2 (0%)	34	63
All	All	1696/1704 (100%)	1583 (93%)	103 (6%)	10 (1%)	30	59

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	A	175	ASP
1	B	175	ASP
1	C	175	ASP
1	D	63	LYS

### 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	375/375 (100%)	369 (98%)	6 (2%)	70	91
1	B	375/375 (100%)	365 (97%)	10 (3%)	52	82
1	C	375/375 (100%)	361 (96%)	14 (4%)	41	72
1	D	375/375 (100%)	367 (98%)	8 (2%)	61	87
All	All	1500/1500 (100%)	1462 (98%)	38 (2%)	55	84

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	64	ASN
1	C	147	SER
1	D	359	ILE
1	C	99	THR
1	C	162	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	A	296	HIS
1	C	246	HIS
1	C	325	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 ⓘ

26 carbohydrates are modelled in this entry.

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	$\# Z  > 2$
9	NAG	A	513	9,1	14,14,15	0.62	0	15,19,21	1.02	1 (6%)
9	FUC	A	514	9	10,10,11	0.59	0	14,14,16	1.17	1 (7%)
9	NAG	A	515	9	14,14,15	0.72	0	15,19,21	2.95	4 (26%)
11	NAG	A	517	11,1	14,14,15	0.66	0	15,19,21	1.33	1 (6%)
11	NAG	A	518	11	14,14,15	0.55	0	15,19,21	1.28	3 (20%)
11	FUC	A	519	11	10,10,11	0.75	0	14,14,16	1.78	5 (35%)
11	NAG	A	520	11,1	14,14,15	0.57	0	15,19,21	1.15	1 (6%)
11	NAG	A	521	11	14,14,15	0.72	0	15,19,21	1.48	3 (20%)
11	FUC	A	522	11	10,10,11	0.56	0	14,14,16	1.44	3 (21%)
11	NAG	B	505	11,1	14,14,15	0.51	0	15,19,21	1.51	4 (26%)
11	NAG	B	506	11	14,14,15	0.51	0	15,19,21	1.01	0
11	FUC	B	507	11	10,10,11	0.51	0	14,14,16	1.31	1 (7%)
12	NAG	B	512	1,12	14,14,15	0.52	0	15,19,21	0.99	0
12	FUC	B	513	12	10,10,11	0.57	0	14,14,16	0.90	1 (7%)
11	NAG	C	503	11,1	14,14,15	0.50	0	15,19,21	1.01	1 (6%)
11	NAG	C	504	11	14,14,15	0.78	0	15,19,21	2.02	3 (20%)
11	FUC	C	505	11	10,10,11	0.52	0	14,14,16	1.04	0
11	NAG	C	509	11,1	14,14,15	0.53	0	15,19,21	0.74	0
11	NAG	C	510	11	14,14,15	0.57	0	15,19,21	1.05	1 (6%)
11	FUC	C	511	11	10,10,11	0.60	0	14,14,16	1.38	3 (21%)
11	NAG	D	501	11,1	14,14,15	0.59	0	15,19,21	0.92	0
11	NAG	D	502	11	14,14,15	0.60	0	15,19,21	1.54	2 (13%)
11	FUC	D	503	11	10,10,11	0.58	0	14,14,16	1.35	2 (14%)
11	NAG	D	505	11,1	14,14,15	0.59	0	15,19,21	1.00	2 (13%)
11	NAG	D	506	11	14,14,15	0.65	0	15,19,21	1.18	1 (6%)
11	FUC	D	507	11	10,10,11	0.56	0	14,14,16	0.71	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
9	NAG	A	513	9,1	-	0/6/23/26	0/1/1/1
9	FUC	A	514	9	-	0/0/17/20	0/1/1/1
9	NAG	A	515	9	-	0/6/23/26	0/1/1/1
11	NAG	A	517	11,1	-	0/6/23/26	0/1/1/1
11	NAG	A	518	11	-	0/6/23/26	0/1/1/1
11	FUC	A	519	11	-	0/0/17/20	0/1/1/1
11	NAG	A	520	11,1	-	0/6/23/26	0/1/1/1
11	NAG	A	521	11	-	0/6/23/26	0/1/1/1
11	FUC	A	522	11	-	0/0/17/20	0/1/1/1
11	NAG	B	505	11,1	-	0/6/23/26	0/1/1/1
11	NAG	B	506	11	-	0/6/23/26	0/1/1/1
11	FUC	B	507	11	-	0/0/17/20	0/1/1/1
12	NAG	B	512	1,12	-	0/6/23/26	0/1/1/1
12	FUC	B	513	12	-	0/0/17/20	0/1/1/1
11	NAG	C	503	11,1	-	0/6/23/26	0/1/1/1
11	NAG	C	504	11	-	2/6/23/26	0/1/1/1
11	FUC	C	505	11	-	0/0/17/20	0/1/1/1
11	NAG	C	509	11,1	-	0/6/23/26	0/1/1/1
11	NAG	C	510	11	-	0/6/23/26	0/1/1/1
11	FUC	C	511	11	-	0/0/17/20	0/1/1/1
11	NAG	D	501	11,1	-	0/6/23/26	0/1/1/1
11	NAG	D	502	11	-	0/6/23/26	0/1/1/1
11	FUC	D	503	11	-	0/0/17/20	0/1/1/1
11	NAG	D	505	11,1	-	0/6/23/26	0/1/1/1
11	NAG	D	506	11	-	0/6/23/26	0/1/1/1
11	FUC	D	507	11	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	515	NAG	C2-N2-C7	-7.01	114.04	123.04
11	C	504	NAG	C2-N2-C7	-4.94	116.70	123.04
11	D	506	NAG	C2-N2-C7	-3.46	118.60	123.04
11	A	521	NAG	C2-N2-C7	-3.32	118.78	123.04
9	A	515	NAG	O3-C3-C2	-3.20	102.78	109.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	504	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	C	504	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	514	FUC	2	0
9	A	515	NAG	2	0
11	A	517	NAG	1	0
11	A	520	NAG	1	0
11	A	521	NAG	1	0
11	B	505	NAG	1	0
11	B	507	FUC	1	0
11	C	503	NAG	2	0
11	C	504	NAG	4	0
11	C	505	FUC	1	0
11	D	502	NAG	2	0
11	D	503	FUC	2	0

## 5.6 Ligand geometry

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GOL	A	503	-	5,5,5	0.35	0	5,5,5	0.25	0
5	OLV	A	504	-	14,14,14	2.94	5 (35%)	21,21,21	2.75	8 (38%)
6	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.23	0
6	SO4	A	506	-	4,4,4	0.46	0	6,6,6	0.35	0
6	SO4	A	507	-	4,4,4	0.08	0	6,6,6	0.12	0
6	SO4	A	508	-	4,4,4	0.08	0	6,6,6	0.24	0
6	SO4	A	509	-	4,4,4	0.20	0	6,6,6	0.13	0
6	SO4	A	510	-	4,4,4	0.31	0	6,6,6	0.13	0
7	ACT	A	511	-	1,3,3	2.48	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	A	512	-	3,3,3	0.54	0	2,2,2	0.33	0
10	NAG	A	516	1	14,14,15	0.62	0	15,19,21	1.17	1 (6%)
10	NAG	B	503	1	14,14,15	0.52	0	15,19,21	1.24	2 (13%)
5	OLV	B	504	-	14,14,14	3.04	5 (35%)	21,21,21	2.69	6 (28%)
6	SO4	B	508	-	4,4,4	0.08	0	6,6,6	0.25	0
6	SO4	B	509	-	4,4,4	0.16	0	6,6,6	0.17	0
6	SO4	B	510	-	4,4,4	0.14	0	6,6,6	0.18	0
10	NAG	B	511	1	14,14,15	0.72	0	15,19,21	1.46	3 (20%)
10	NAG	C	501	1	14,14,15	0.49	0	15,19,21	0.78	0
10	NAG	C	507	1	14,14,15	0.49	0	15,19,21	1.78	3 (20%)
4	GOL	C	508	-	5,5,5	0.25	0	5,5,5	0.46	0
5	OLV	C	512	-	14,14,14	3.28	6 (42%)	21,21,21	2.84	7 (33%)
6	SO4	C	513	-	4,4,4	0.15	0	6,6,6	0.37	0
6	SO4	C	514	-	4,4,4	0.10	0	6,6,6	0.26	0
6	SO4	C	515	-	4,4,4	0.16	0	6,6,6	0.28	0
10	NAG	D	504	1	14,14,15	0.54	0	15,19,21	1.44	4 (26%)
4	GOL	D	510	-	5,5,5	0.28	0	5,5,5	0.43	0
5	OLV	D	511	-	14,14,14	3.16	6 (42%)	21,21,21	2.31	5 (23%)
6	SO4	D	512	-	4,4,4	0.10	0	6,6,6	0.11	0
6	SO4	D	513	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	D	514	-	4,4,4	0.29	0	6,6,6	0.36	0
6	SO4	D	515	-	4,4,4	0.15	0	6,6,6	0.31	0
10	NAG	D	516	1	14,14,15	0.54	0	15,19,21	1.14	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
5	OLV	A	504	-	-	0/2/12/12	0/2/2/2
6	SO4	A	505	-	-	0/0/0/0	0/0/0/0
6	SO4	A	506	-	-	0/0/0/0	0/0/0/0
6	SO4	A	507	-	-	0/0/0/0	0/0/0/0
6	SO4	A	508	-	-	0/0/0/0	0/0/0/0
6	SO4	A	509	-	-	0/0/0/0	0/0/0/0
6	SO4	A	510	-	-	0/0/0/0	0/0/0/0
7	ACT	A	511	-	-	0/0/0/0	0/0/0/0
8	EDO	A	512	-	-	0/1/1/1	0/0/0/0
10	NAG	A	516	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	503	1	-	0/6/23/26	0/1/1/1
5	0LV	B	504	-	-	0/2/12/12	0/2/2/2
6	SO4	B	508	-	-	0/0/0/0	0/0/0/0
6	SO4	B	509	-	-	0/0/0/0	0/0/0/0
6	SO4	B	510	-	-	0/0/0/0	0/0/0/0
10	NAG	B	511	1	-	0/6/23/26	0/1/1/1
10	NAG	C	501	1	-	0/6/23/26	0/1/1/1
10	NAG	C	507	1	-	0/6/23/26	0/1/1/1
4	GOL	C	508	-	-	0/4/4/4	0/0/0/0
5	0LV	C	512	-	-	0/2/12/12	0/2/2/2
6	SO4	C	513	-	-	0/0/0/0	0/0/0/0
6	SO4	C	514	-	-	0/0/0/0	0/0/0/0
6	SO4	C	515	-	-	0/0/0/0	0/0/0/0
10	NAG	D	504	1	-	0/6/23/26	0/1/1/1
4	GOL	D	510	-	-	0/4/4/4	0/0/0/0
5	0LV	D	511	-	-	0/2/12/12	0/2/2/2
6	SO4	D	512	-	-	0/0/0/0	0/0/0/0
6	SO4	D	513	-	-	0/0/0/0	0/0/0/0
6	SO4	D	514	-	-	0/0/0/0	0/0/0/0
6	SO4	D	515	-	-	0/0/0/0	0/0/0/0
10	NAG	D	516	1	-	0/6/23/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	511	0LV	OAI-CAM	-7.50	1.41	1.48
5	C	512	0LV	OAI-CAM	-7.21	1.41	1.48
5	A	504	0LV	OAI-CAM	-6.65	1.42	1.48
5	B	504	0LV	OAI-CAM	-6.59	1.42	1.48
5	C	512	0LV	CAH-CAM	-6.41	1.47	1.54

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	512	0LV	OAI-CAL-CAK	-6.21	108.88	113.81
5	B	504	0LV	OAI-CAL-CAK	-5.69	109.29	113.81
5	C	512	0LV	CAM-OAI-CAL	-4.50	104.64	107.20
5	D	511	0LV	OAI-CAL-CAK	-4.18	110.49	113.81
5	A	504	0LV	OAI-CAL-CAK	-3.63	110.93	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	GOL	2	0
5	A	504	0LV	11	0
6	A	505	SO4	1	0
6	A	508	SO4	1	0
8	A	512	EDO	6	0
5	B	504	0LV	9	0
6	B	509	SO4	1	0
4	C	508	GOL	1	0
5	C	512	0LV	13	0
5	D	511	0LV	13	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	426/426 (100%)	-0.77	2 (0%) 91 93	29, 37, 51, 78	0
1	B	426/426 (100%)	-0.69	3 (0%) 89 90	30, 44, 59, 88	0
1	C	426/426 (100%)	-0.67	0 100 100	31, 41, 58, 89	1 (0%)
1	D	426/426 (100%)	-0.69	3 (0%) 89 90	28, 40, 58, 85	0
All	All	1704/1704 (100%)	-0.70	8 (0%) 91 93	28, 40, 58, 89	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	THR	3.9
1	B	432	THR	3.4
1	D	64	ASN	3.2
1	D	432	THR	3.0
1	A	431	SER	2.7

### 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](#)

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
11	NAG	A	520	14/15	0.95	0.12	0.54	44,53,58,58	0
11	NAG	C	509	14/15	0.96	0.11	-1.14	47,53,62,66	0
11	NAG	D	505	14/15	0.97	0.09	-1.85	49,53,63,68	0
11	NAG	D	502	14/15	0.84	0.34	-	80,90,96,98	0
11	FUC	B	507	10/11	0.95	0.18	-	49,56,58,59	0
11	NAG	C	504	14/15	0.88	0.34	-	58,64,67,69	0
11	FUC	A	519	10/11	0.94	0.20	-	35,46,52,57	0
9	FUC	A	514	10/11	0.87	0.27	-	56,67,73,78	0
11	NAG	D	506	14/15	0.88	0.30	-	54,65,74,75	0
11	NAG	A	521	14/15	0.86	0.28	-	51,59,64,65	0
11	NAG	B	506	14/15	0.94	0.17	-	46,53,55,56	0
11	FUC	D	507	10/11	0.91	0.17	-	57,66,71,71	0
11	NAG	C	510	14/15	0.85	0.34	-	50,68,78,81	0
11	FUC	C	505	10/11	0.92	0.29	-	68,70,79,81	0
11	FUC	C	511	10/11	0.92	0.23	-	61,70,74,78	0
11	FUC	D	503	10/11	0.95	0.26	-	70,79,86,88	0
12	FUC	B	513	10/11	0.91	0.34	-	69,75,76,78	0
9	NAG	A	515	14/15	0.93	0.24	-	53,61,68,68	0
11	NAG	A	517	14/15	0.96	0.11	-	34,37,44,47	0
11	NAG	B	505	14/15	0.95	0.10	-	38,46,52,58	0
12	NAG	B	512	14/15	0.93	0.20	-	52,64,69,69	0
11	NAG	D	501	14/15	0.93	0.20	-	50,70,79,79	0
11	NAG	A	518	14/15	0.96	0.20	-	32,40,43,47	0
9	NAG	A	513	14/15	0.96	0.15	-	47,53,62,62	0
11	NAG	C	503	14/15	0.95	0.15	-	48,59,64,68	0
11	FUC	A	522	10/11	0.94	0.33	-	58,62,69,69	0

## 6.4 Ligands ⓘ

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
5	OLV	B	504	13/13	0.79	0.36	13.62	46,62,75,76	0
5	OLV	C	512	13/13	0.81	0.43	10.92	48,64,72,75	0
5	OLV	A	504	13/13	0.72	0.41	9.69	35,56,71,72	0
5	OLV	D	511	13/13	0.78	0.39	7.91	38,60,72,74	0
6	SO4	C	515	5/5	0.92	0.40	7.31	71,76,79,97	0
4	GOL	A	503	6/6	0.94	0.21	6.67	45,48,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	A	505	5/5	0.95	0.42	6.54	59,66,86,90	0
4	GOL	C	508	6/6	0.92	0.24	6.52	49,49,57,58	0
10	NAG	D	504	14/15	0.94	0.18	5.97	57,66,69,74	0
6	SO4	D	515	5/5	0.95	0.35	4.89	67,72,88,96	0
6	SO4	D	514	5/5	0.93	0.34	4.84	57,62,62,77	0
10	NAG	C	507	14/15	0.92	0.26	3.76	57,64,68,69	0
6	SO4	A	510	5/5	0.94	0.26	2.49	54,58,76,91	0
10	NAG	B	503	14/15	0.89	0.20	1.84	54,60,64,65	0
10	NAG	D	516	14/15	0.96	0.17	1.25	40,48,54,58	0
10	NAG	C	501	14/15	0.97	0.14	0.65	46,51,55,55	0
10	NAG	B	511	14/15	0.96	0.17	0.51	47,51,55,58	0
10	NAG	A	516	14/15	0.97	0.13	0.32	38,44,51,54	0
6	SO4	A	508	5/5	0.99	0.06	-1.63	43,46,51,57	0
3	FE	A	502	1/1	0.96	0.07	-1.87	45,45,45,45	1
2	ZN	D	508	1/1	1.00	0.05	-2.31	41,41,41,41	0
2	ZN	A	501	1/1	0.99	0.05	-2.39	44,44,44,44	0
3	FE	D	509	1/1	0.98	0.06	-2.50	48,48,48,48	1
3	FE	C	506	1/1	0.99	0.07	-2.62	56,56,56,56	0
3	FE	B	502	1/1	1.00	0.07	-2.67	48,48,48,48	1
2	ZN	C	502	1/1	0.99	0.05	-3.11	42,42,42,42	0
2	ZN	B	501	1/1	1.00	0.06	-3.42	51,51,51,51	0
6	SO4	C	513	5/5	0.96	0.38	-	52,63,81,84	0
6	SO4	A	509	5/5	0.95	0.45	-	57,63,84,90	0
8	EDO	A	512	4/4	0.96	0.19	-	44,45,47,47	0
6	SO4	C	514	5/5	0.97	0.41	-	61,72,78,90	0
6	SO4	B	510	5/5	0.91	0.30	-	66,70,93,98	0
6	SO4	B	509	5/5	0.96	0.33	-	63,67,83,95	0
7	ACT	A	511	4/4	0.92	0.33	-	41,46,47,52	0
6	SO4	D	513	5/5	0.98	0.35	-	52,52,58,77	0
6	SO4	A	506	5/5	0.92	0.33	-	51,53,69,90	0
6	SO4	B	508	5/5	0.98	0.46	-	67,74,86,93	0
6	SO4	D	512	5/5	0.97	0.35	-	59,62,75,83	0
6	SO4	A	507	5/5	0.97	0.42	-	60,69,78,86	0
4	GOL	D	510	6/6	0.86	0.17	-	53,55,61,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.