Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:07 PM GMT

PDB ID	:	4KKZ
Title	:	The crystal structure of red kidney bean purple acid phosphatase in complex with diethylene glycol monovanadate
Authors	:	Feder, D.; Guddat, L.W.; Schenk, G.
Deposited on	:	2013-05-06
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

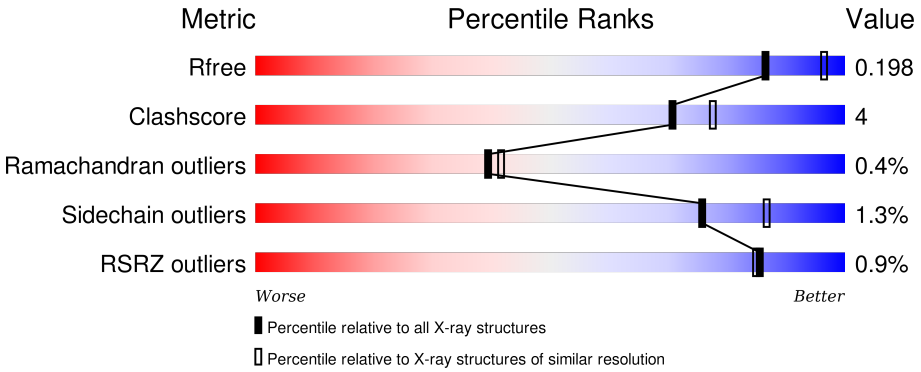
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 >=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 <=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	92% 7%
1	B	426	92% 6%
1	C	426	91% 8%
1	D	426	91% 9%

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	ACT	A	521	-	-	-	X
10	ACT	B	522	-	-	-	X
10	ACT	C	533	-	-	-	X
11	NA	A	530	-	-	-	X
11	NA	B	524	-	-	-	X
11	NA	C	529	-	-	-	X
11	NA	D	528	-	-	-	X
12	1RF	A	531	-	-	-	X
12	1RF	B	529	-	-	X	X
12	1RF	C	534	-	-	-	X
13	PGE	C	527	-	-	X	X
4	NAG	B	504	-	-	-	X
4	NAG	C	503	-	-	-	X
4	NAG	C	505	-	-	-	X
4	NAG	D	505	-	-	-	X
5	NAG	A	504	-	-	-	X
6	SO4	A	507	-	-	-	X
6	SO4	A	514	-	-	-	X
6	SO4	B	506	-	-	-	X
6	SO4	B	507	-	-	-	X
6	SO4	B	530	-	-	X	-
6	SO4	C	512	-	-	-	X
6	SO4	C	513	-	-	-	X
6	SO4	C	532	-	-	-	X
6	SO4	D	509	-	-	-	X
6	SO4	D	510	-	-	-	X
6	SO4	D	511	-	-	-	X
6	SO4	D	530	-	-	-	X
7	EDO	A	529	-	-	-	X
7	EDO	B	514	-	-	-	X
7	EDO	B	515	-	-	-	X
7	EDO	B	527	-	-	X	-
7	EDO	C	530	-	-	-	X
7	EDO	C	531	-	-	X	-
7	EDO	D	531	-	-	-	X
8	GOL	A	527	-	-	-	X
8	GOL	B	521	-	-	-	X
8	GOL	C	525	-	-	-	X
8	GOL	C	528	-	-	-	X
8	GOL	D	519	-	-	-	X
8	GOL	D	527	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 16671 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	424	Total	C	N	O	S	0	3	0
			3519	2256	614	639	10			
1	B	425	Total	C	N	O	S	0	3	0
			3507	2254	605	638	10			
1	C	423	Total	C	N	O	S	0	4	0
			3505	2248	608	639	10			
1	D	426	Total	C	N	O	S	0	3	0
			3514	2254	609	640	11			

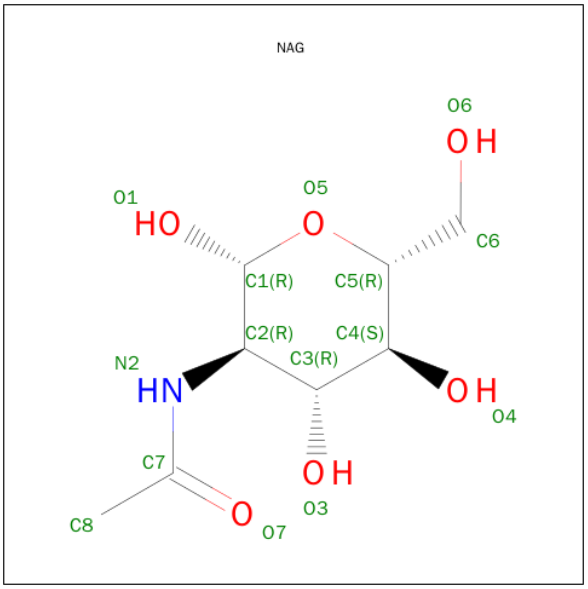
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

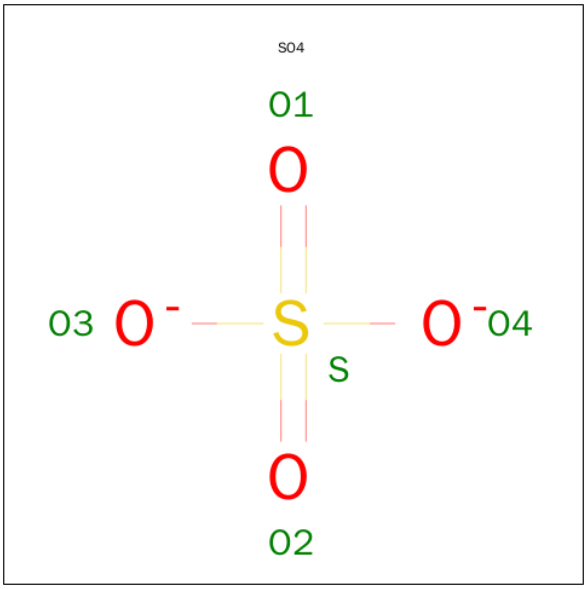


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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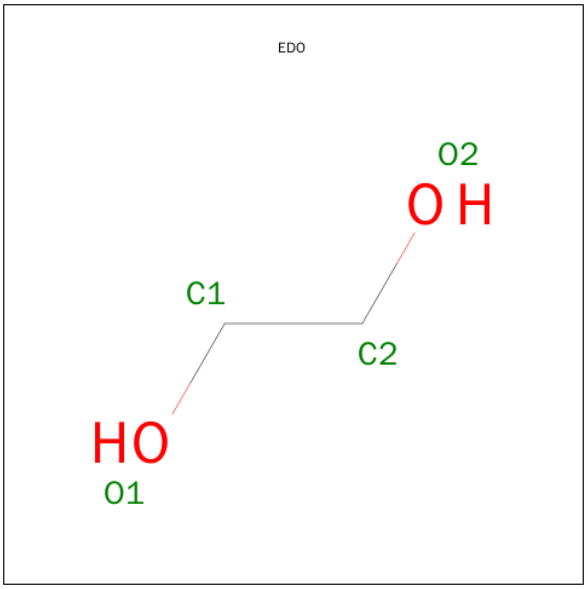
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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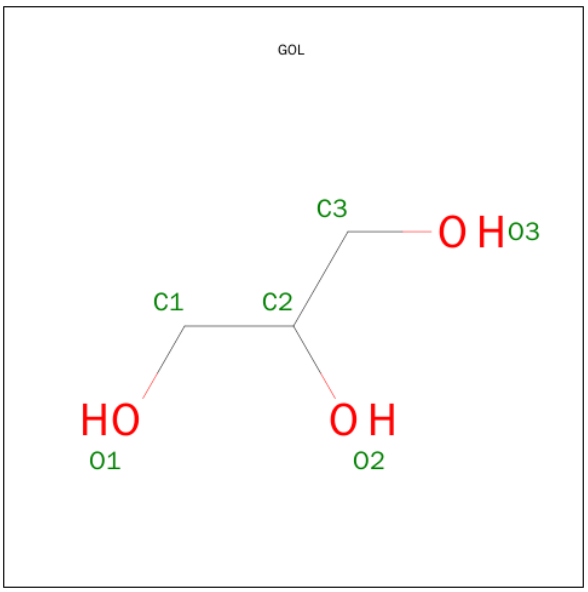
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

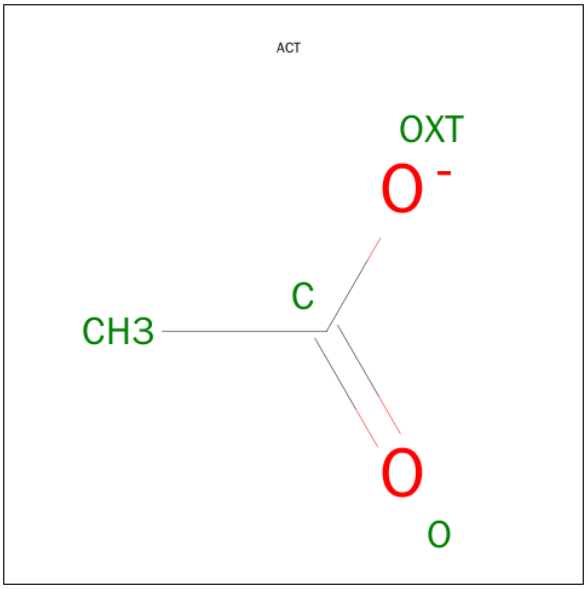


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0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

- 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 38 22 2 14	0	0
9	B	3	Total C N O 38 22 2 14	0	0
9	C	3	Total C N O 38 22 2 14	0	0
9	D	3	Total C N O 38 22 2 14	0	0

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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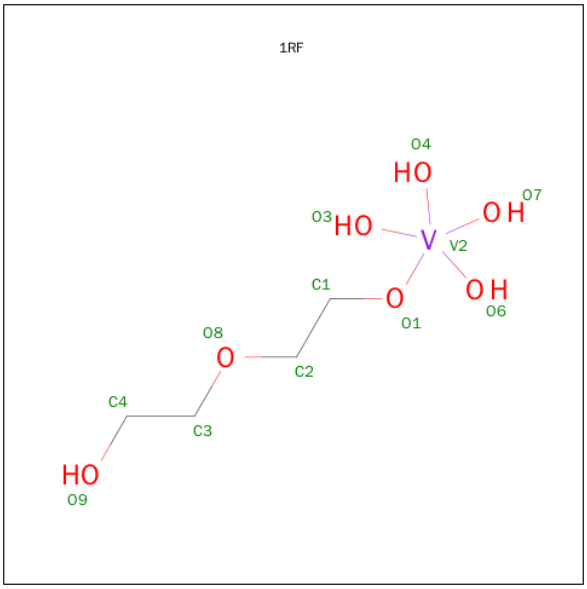
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	2	Total Na 2 2	0	0
11	A	2	Total Na 2 2	0	0
11	D	4	Total Na 4 4	0	0
11	C	2	Total Na 2 2	0	0

- Molecule 12 is VANADIUM(5+) HYDROXIDE 2-(2-HYDROXYETHOXY)ETHANOLATE (1:4:1) (three-letter code: 1RF) (formula: $C_4H_{13}O_7V$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O V 8 2 5 1	0	0
12	B	1	Total C O V 12 4 7 1	0	0

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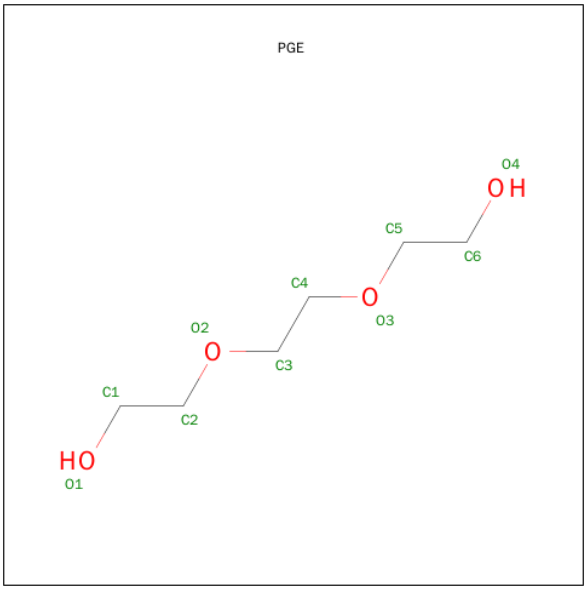
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C O V 8 2 5 1	0	0
12	D	1	Total O V 6 5 1	0	0

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 10 6 4	0	0
13	D	1	Total C O 7 4 3	0	0

- Molecule 14 is water.

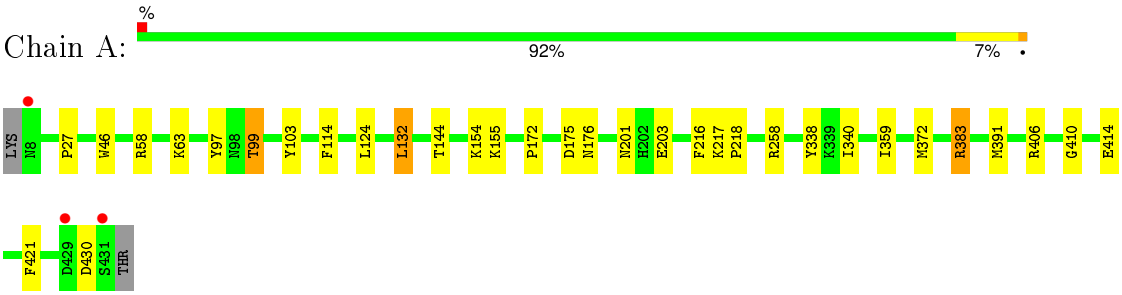
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	494	Total O 494 494	0	0
14	B	443	Total O 443 443	0	0
14	C	427	Total O 427 427	0	0
14	D	444	Total O 444 444	0	0

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.

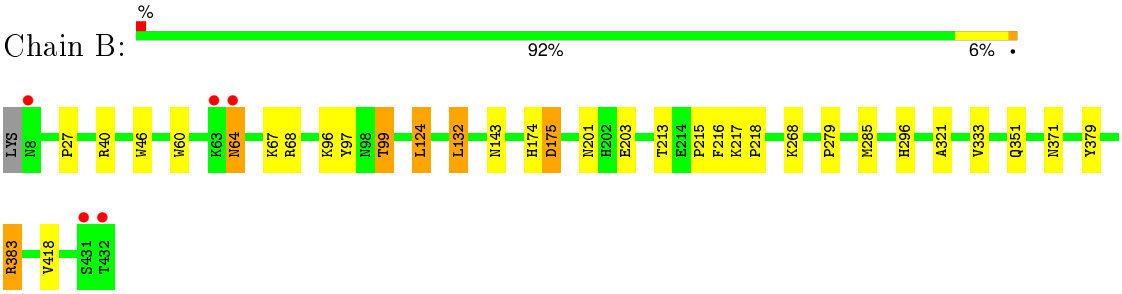
- Molecule 1: Purple acid phosphatase

Chain A:



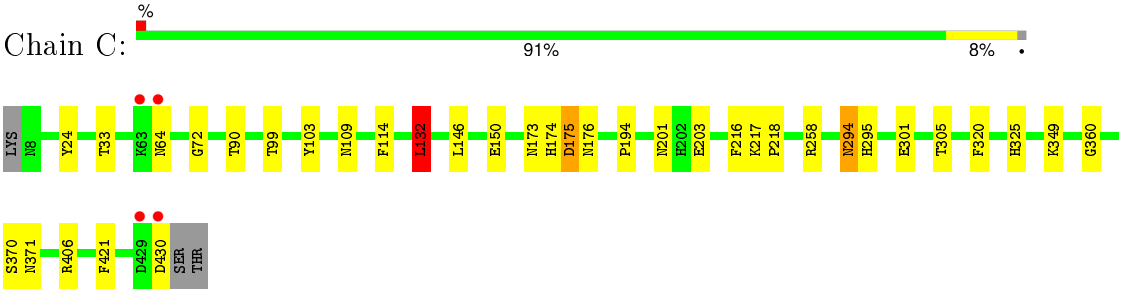
- Molecule 1: Purple acid phosphatase

Chain B:



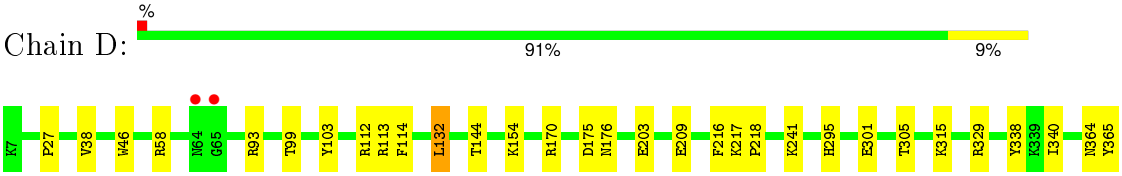
- Molecule 1: Purple acid phosphatase

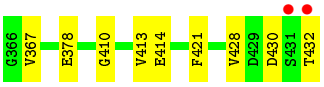
Chain C:



- Molecule 1: Purple acid phosphatase

Chain D:




G366
V367
E378
G410
V413
E414
F421
V428
D429
D430
S431
T432

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.24Å 126.24Å 296.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.20) 99.9 (19.97-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 2.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.151 , 0.197 0.155 , 0.198	Depositor DCC
R_{free} test set	7012 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.4	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 139307 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16671	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PGE, NAG, 1RF, NA, SO4, EDO, FUC, ACT, FE

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	0.41	0/3638	0.54	1/4946 (0.0%)
1	B	0.40	0/3632	0.52	1/4941 (0.0%)
1	C	0.40	0/3627	0.56	3/4936 (0.1%)
1	D	0.39	0/3633	0.52	1/4941 (0.0%)
All	All	0.40	0/14530	0.53	6/19764 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294[A]	ASN	N-CA-C	6.71	129.12	111.00
1	C	294[B]	ASN	N-CA-C	6.71	129.12	111.00
1	A	132	LEU	CA-CB-CG	-6.61	100.11	115.30
1	B	132	LEU	CA-CB-CG	-6.48	100.39	115.30
1	C	132	LEU	CA-CB-CG	-6.10	101.27	115.30
1	D	132	LEU	CA-CB-CG	-5.86	101.81	115.30

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	3519	0	3329	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3507	0	3316	29	0
1	C	3505	0	3291	29	0
1	D	3514	0	3305	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	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	28	0	26	0	0
4	B	42	0	39	1	0
4	C	42	0	39	0	0
4	D	42	0	39	0	0
5	A	28	0	25	3	0
6	A	30	0	0	2	0
6	B	45	0	0	5	0
6	C	55	0	0	0	0
6	D	55	0	0	0	0
7	A	32	0	48	4	0
7	B	24	0	36	5	0
7	C	16	0	24	6	0
7	D	40	0	60	9	0
8	A	18	0	24	1	0
8	B	12	0	16	3	0
8	C	30	0	40	3	0
8	D	18	0	24	1	0
9	A	38	0	34	0	0
9	B	38	0	34	0	0
9	C	38	0	34	0	0
9	D	38	0	34	0	0
10	A	12	0	9	1	0
10	B	12	0	9	1	0
10	C	8	0	6	1	0
10	D	8	0	6	2	0
11	A	2	0	0	0	0
11	B	2	0	0	0	0
11	C	2	0	0	0	0
11	D	4	0	0	0	0
12	A	8	0	2	2	0
12	B	12	0	9	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	8	0	2	4	0
12	D	6	0	0	0	0
13	C	10	0	14	6	0
13	D	7	0	9	1	0
14	A	494	0	0	1	0
14	B	443	0	0	9	0
14	C	427	0	0	2	0
14	D	444	0	0	2	0
All	All	16671	0	13883	125	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 4.

All (125) 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:D:364:ASN:HD22	1:D:365:TYR:H	1.12	0.95
7:B:527:EDO:C1	12:B:529:1RF:H5	1.97	0.94
12:B:529:1RF:O9	1:C:258:ARG:NE	2.09	0.85
1:D:295:HIS:NE2	7:D:529:EDO:H12	1.92	0.85
1:B:351:GLN:HB2	8:B:521:GOL:H2	1.59	0.85
1:D:93:ARG:NH1	14:D:1021:HOH:O	2.11	0.82
12:C:534:1RF:O6	12:C:534:1RF:H2	1.80	0.81
1:D:364:ASN:ND2	1:D:365:TYR:H	1.79	0.79
5:A:504:NAG:H61	1:C:24:TYR:OH	1.83	0.78
7:C:531:EDO:O1	12:C:534:1RF:H1	1.84	0.78
7:B:527:EDO:H12	12:B:529:1RF:H5	1.67	0.76
1:B:68:ARG:NH2	6:B:530:SO4:O2	2.19	0.75
1:B:64:ASN:ND2	6:B:530:SO4:O1	2.19	0.74
1:D:170[B]:ARG:NH1	7:D:524:EDO:O2	2.21	0.73
12:B:529:1RF:C4	1:C:258:ARG:HE	2.01	0.72
1:D:364:ASN:HD22	1:D:365:TYR:N	1.88	0.72
1:C:406:ARG:HH22	8:C:524:GOL:H2	1.54	0.72
7:B:527:EDO:O1	12:B:529:1RF:H5	1.90	0.71
1:C:173:ASN:H	10:C:533:ACT:H2	1.54	0.71
1:A:144:THR:HG23	7:A:512:EDO:H21	1.75	0.68
1:A:406:ARG:HH22	8:A:520:GOL:H2	1.59	0.67
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.30	0.67
1:B:351:GLN:CB	8:B:521:GOL:H2	2.24	0.66
1:B:418:VAL:HG21	7:B:520:EDO:H12	1.79	0.65
12:B:529:1RF:H8	14:C:1023:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ASN:ND2	1:D:365:TYR:N	2.44	0.63
14:B:1030:HOH:O	7:C:531:EDO:H22	1.99	0.62
1:D:364:ASN:HD21	1:D:367:VAL:H	1.48	0.62
1:C:370:SER:H	13:C:527:PGE:H42	1.64	0.61
1:D:329:ARG:HH12	1:D:432:THR:HB	1.65	0.61
1:B:296:HIS:HE1	12:B:529:1RF:H3	1.65	0.61
12:A:531:1RF:O6	12:A:531:1RF:H1	2.00	0.60
1:B:383:ARG:HD3	6:B:509:SO4:O3	2.02	0.60
1:D:113:ARG:HH12	7:D:516[B]:EDO:H11	1.67	0.60
1:B:40:ARG:NH1	14:B:928:HOH:O	2.35	0.60
1:B:143:ASN:HD22	4:B:505:NAG:H83	1.68	0.59
1:B:296:HIS:CE1	12:B:529:1RF:H3	2.38	0.58
12:B:529:1RF:O6	12:B:529:1RF:H1	2.04	0.58
1:C:371[A]:ASN:HB3	13:C:527:PGE:H32	1.86	0.57
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.40	0.57
1:A:58:ARG:NH2	14:A:959:HOH:O	2.37	0.57
1:D:410:GLY:H	7:D:517:EDO:H12	1.70	0.57
12:B:529:1RF:H7	14:B:1035:HOH:O	2.05	0.56
10:B:522:ACT:H1	14:B:914:HOH:O	2.05	0.56
1:C:201:ASN:ND2	12:C:534:1RF:O3	2.33	0.56
1:D:58:ARG:NH2	10:D:515:ACT:O	2.38	0.56
1:C:295:HIS:NE2	7:C:531:EDO:H21	2.20	0.56
1:B:201:ASN:ND2	12:B:529:1RF:O3	2.31	0.56
1:B:124:LEU:HD12	1:B:279:PRO:HG3	1.88	0.56
7:B:527:EDO:H12	12:B:529:1RF:C3	2.36	0.55
1:C:370:SER:N	13:C:527:PGE:H42	2.21	0.55
1:B:371:ASN:HB2	14:B:1033:HOH:O	2.06	0.54
1:A:410:GLY:HA3	7:A:522:EDO:H21	1.89	0.54
1:B:351:GLN:CG	8:B:521:GOL:H2	2.40	0.52
1:C:72:GLY:HA2	8:C:525:GOL:H32	1.92	0.51
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.91	0.51
12:B:529:1RF:O9	1:C:258:ARG:CZ	2.58	0.51
1:D:421:PHE:CD2	1:D:428:VAL:HG23	2.46	0.51
1:A:172:PRO:HB3	5:A:505:NAG:H81	1.93	0.51
1:A:383:ARG:HD2	6:A:508:SO4:O3	2.10	0.51
1:B:96:LYS:HB2	1:B:99:THR:HG21	1.94	0.50
1:D:112:ARG:HB3	8:D:521:GOL:H12	1.94	0.49
1:D:209:GLU:OE2	7:D:531:EDO:O2	2.30	0.49
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.95	0.49
1:A:201:ASN:ND2	12:A:531:1RF:O7	2.40	0.49
1:D:410:GLY:H	7:D:517:EDO:C1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TYR:O	1:A:99:THR:HG22	2.13	0.48
1:A:391:MET:HB2	7:A:529:EDO:H11	1.95	0.48
1:D:27:PRO:HB3	1:D:46:TRP:CD1	2.49	0.48
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.50	0.47
1:D:413:VAL:HG21	7:D:517:EDO:H12	1.97	0.47
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.50	0.47
1:A:414:GLU:OE2	7:A:529:EDO:H12	2.15	0.46
1:C:203:GLU:O	1:C:216:PHE:HA	2.15	0.46
1:D:103:TYR:CE1	1:D:114:PHE:HB2	2.50	0.46
1:C:33:THR:HA	1:C:194:PRO:HB3	1.98	0.46
7:C:531:EDO:HO1	12:C:534:1RF:H1	1.81	0.46
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.51	0.46
7:D:525:EDO:O1	10:D:526:ACT:O	2.29	0.46
1:B:97:TYR:O	1:B:99:THR:HG22	2.16	0.45
1:B:64:ASN:ND2	6:B:530:SO4:S	2.90	0.45
1:D:103:TYR:CZ	1:D:114:PHE:HB2	2.52	0.45
1:D:154:LYS:HE2	1:D:414:GLU:OE2	2.16	0.45
1:C:109:ASN:OD1	14:C:812:HOH:O	2.21	0.44
1:B:268[A]:LYS:HG3	14:B:824:HOH:O	2.17	0.44
1:C:406:ARG:NH2	8:C:524:GOL:H2	2.29	0.44
1:C:294[B]:ASN:HB3	13:C:527:PGE:H12	1.99	0.44
12:B:529:1RF:O9	1:C:258:ARG:NH2	2.50	0.44
1:B:285:MET:O	1:B:321:ALA:HA	2.17	0.44
1:B:217:LYS:HB3	1:B:218:PRO:HD3	2.00	0.44
1:B:203:GLU:O	1:B:216:PHE:HA	2.17	0.44
1:D:315:LYS:HE2	7:D:523:EDO:C2	2.48	0.44
1:A:258:ARG:HB2	6:A:514:SO4:O4	2.18	0.43
1:D:38:VAL:HG12	1:D:241:LYS:HE3	2.00	0.43
1:A:372:MET:SD	1:A:383:ARG:HD3	2.58	0.43
1:B:213:THR:O	1:B:215:PRO:HD3	2.18	0.43
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.53	0.43
1:B:174:HIS:O	1:B:175:ASP:C	2.56	0.43
1:A:338:TYR:CZ	1:A:340:ILE:HA	2.54	0.43
1:B:68:ARG:NH1	6:B:530:SO4:O2	2.52	0.43
13:C:527:PGE:H32	13:C:527:PGE:H12	1.80	0.43
1:B:124:LEU:HA	1:B:124:LEU:HD12	1.88	0.43
1:A:27:PRO:HB3	1:A:46:TRP:CD1	2.53	0.43
1:C:371[B]:ASN:HB2	13:C:527:PGE:H32	2.00	0.42
1:B:60:TRP:HB3	1:B:67:LYS:HA	2.01	0.42
1:A:154:LYS:HZ1	10:A:525:ACT:H3	1.83	0.42
1:C:146:LEU:O	1:C:150:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:OG1	13:D:518:PGE:H4	2.19	0.42
1:D:203:GLU:O	1:D:216:PHE:HA	2.18	0.42
1:B:268[B]:LYS:HG3	14:B:836:HOH:O	2.18	0.42
1:C:132:LEU:HD22	1:C:320:PHE:CD1	2.55	0.42
1:D:301:GLU:O	1:D:305:THR:HG23	2.20	0.42
14:B:1030:HOH:O	7:C:531:EDO:H11	2.19	0.42
5:A:504:NAG:H62	5:A:505:NAG:C1	2.50	0.41
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.56	0.41
1:C:174:HIS:O	1:C:175:ASP:C	2.59	0.41
1:D:315:LYS:HD3	14:D:883:HOH:O	2.21	0.41
1:A:203:GLU:O	1:A:216:PHE:HA	2.21	0.41
1:B:333:VAL:HG21	1:B:379:TYR:HB2	2.02	0.41
1:C:72:GLY:HA3	1:C:90:THR:OG1	2.21	0.40
1:C:325:HIS:HA	1:C:360:GLY:O	2.21	0.40
1:C:301:GLU:O	1:C:305:THR:HG23	2.21	0.40
14:B:1030:HOH:O	7:C:531:EDO:C1	2.70	0.40
1:A:103:TYR:CZ	1:A:114:PHE:HB2	2.56	0.40
1:C:217:LYS:HB3	1:C:218:PRO:HD3	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	425/426 (100%)	404 (95%)	19 (4%)	2 (0%)	34	35
1	B	426/426 (100%)	406 (95%)	18 (4%)	2 (0%)	34	35
1	C	425/426 (100%)	405 (95%)	18 (4%)	2 (0%)	34	35
1	D	427/426 (100%)	407 (95%)	19 (4%)	1 (0%)	52	59
All	All	1703/1704 (100%)	1622 (95%)	74 (4%)	7 (0%)	39	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASP
1	A	175	ASP
1	C	175	ASP
1	D	175	ASP
1	B	64	ASN
1	C	64	ASN
1	A	155	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	376/375 (100%)	369 (98%)	7 (2%)	65	77
1	B	374/375 (100%)	370 (99%)	4 (1%)	80	89
1	C	372/375 (99%)	368 (99%)	4 (1%)	80	89
1	D	373/375 (100%)	369 (99%)	4 (1%)	80	89
All	All	1495/1500 (100%)	1476 (99%)	19 (1%)	76	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	99	THR
1	A	124	LEU
1	A	132	LEU
1	A	176	ASN
1	A	359	ILE
1	A	383	ARG
1	B	99	THR
1	B	124	LEU
1	B	132	LEU
1	B	383	ARG
1	C	99	THR
1	C	132	LEU
1	C	176	ASN
1	C	349	LYS

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Mol	Chain	Res	Type
1	D	99	THR
1	D	132	LEU
1	D	176	ASN
1	D	378	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	364	ASN

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

14 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	$\#\|Z\| > 2$
5	NAG	A	504	1,5	14,14,15	0.35	0	15,19,21	1.29	2 (13%)
5	NAG	A	505	5	14,14,15	0.34	0	15,19,21	0.68	0
9	NAG	A	517	9,1	14,14,15	0.52	0	15,19,21	0.88	1 (6%)
9	NAG	A	518	9	14,14,15	0.48	0	15,19,21	0.72	0
9	FUC	A	519	9	10,10,11	0.68	0	14,14,16	0.91	1 (7%)
9	NAG	B	516	9,1	14,14,15	0.49	0	15,19,21	0.93	1 (6%)
9	NAG	B	517	9	14,14,15	0.43	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	FUC	B	518	9	10,10,11	0.66	0	14,14,16	1.02	1 (7%)
9	NAG	C	518	9,1	14,14,15	0.49	0	15,19,21	0.78	0
9	NAG	C	519	9	14,14,15	0.53	0	15,19,21	0.81	1 (6%)
9	FUC	C	520	9	10,10,11	0.80	0	14,14,16	0.90	0
9	NAG	D	534	9,1	14,14,15	0.52	0	15,19,21	0.71	0
9	NAG	D	535	9	14,14,15	0.60	0	15,19,21	0.76	1 (6%)
9	FUC	D	536	9	10,10,11	0.87	0	14,14,16	1.01	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	504	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	505	5	-	0/6/23/26	0/1/1/1
9	NAG	A	517	9,1	-	0/6/23/26	0/1/1/1
9	NAG	A	518	9	-	0/6/23/26	0/1/1/1
9	FUC	A	519	9	-	0/0/17/20	0/1/1/1
9	NAG	B	516	9,1	-	0/6/23/26	0/1/1/1
9	NAG	B	517	9	-	0/6/23/26	0/1/1/1
9	FUC	B	518	9	-	0/0/17/20	0/1/1/1
9	NAG	C	518	9,1	-	0/6/23/26	0/1/1/1
9	NAG	C	519	9	-	0/6/23/26	0/1/1/1
9	FUC	C	520	9	-	0/0/17/20	0/1/1/1
9	NAG	D	534	9,1	-	0/6/23/26	0/1/1/1
9	NAG	D	535	9	-	0/6/23/26	0/1/1/1
9	FUC	D	536	9	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	535	NAG	C2-N2-C7	-2.36	120.00	123.04
5	A	504	NAG	C2-N2-C7	-2.23	120.17	123.04
9	C	519	NAG	C2-N2-C7	-2.06	120.39	123.04
9	A	517	NAG	C1-O5-C5	2.27	115.13	112.25
9	B	517	NAG	C1-O5-C5	2.40	115.30	112.25
9	A	519	FUC	C1-O5-C5	2.49	116.23	112.38
9	B	516	NAG	C1-O5-C5	2.80	115.80	112.25
9	D	536	FUC	C1-O5-C5	2.84	116.77	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	518	FUC	C1-O5-C5	2.96	116.96	112.38
5	A	504	NAG	C1-O5-C5	3.55	116.76	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	NAG	2	0
5	A	505	NAG	2	0

5.6 Ligand geometry (i)

Of 123 ligands modelled in this entry, 18 are monoatomic - leaving 105 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	NAG	A	503	1	14,14,15	0.54	0	15,19,21	1.21	2 (13%)
6	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.22	0
6	SO4	A	507	-	4,4,4	0.08	0	6,6,6	0.09	0
6	SO4	A	508	-	4,4,4	0.13	0	6,6,6	0.09	0
6	SO4	A	509	-	4,4,4	0.17	0	6,6,6	0.18	0
6	SO4	A	510	-	4,4,4	0.19	0	6,6,6	0.10	0
7	EDO	A	511	-	3,3,3	0.52	0	2,2,2	0.34	0
7	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.42	0
7	EDO	A	513	-	3,3,3	0.50	0	2,2,2	0.55	0
6	SO4	A	514	-	4,4,4	0.32	0	6,6,6	0.25	0
4	NAG	A	515	1	14,14,15	0.44	0	15,19,21	1.06	1 (6%)
8	GOL	A	516	-	5,5,5	0.31	0	5,5,5	0.22	0
8	GOL	A	520	-	5,5,5	0.29	0	5,5,5	0.33	0
10	ACT	A	521	-	1,3,3	1.20	0	0,3,3	0.00	-
7	EDO	A	522	-	3,3,3	0.42	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	523	-	3,3,3	0.48	0	2,2,2	0.52	0
7	EDO	A	524	-	3,3,3	0.45	0	2,2,2	0.42	0
10	ACT	A	525	-	1,3,3	1.41	0	0,3,3	0.00	-
7	EDO	A	526	-	3,3,3	0.47	0	2,2,2	0.46	0
8	GOL	A	527	-	5,5,5	0.27	0	5,5,5	0.56	0
10	ACT	A	528	-	1,3,3	1.03	0	0,3,3	0.00	-
7	EDO	A	529	-	3,3,3	0.50	0	2,2,2	0.26	0
12	1RF	A	531	3,2	3,7,11	1.56	1 (33%)	1,12,16	1.20	0
4	NAG	B	503	1	14,14,15	0.45	0	15,19,21	0.98	2 (13%)
4	NAG	B	504	1	14,14,15	1.01	1 (7%)	15,19,21	1.79	5 (33%)
4	NAG	B	505	1	14,14,15	0.54	0	15,19,21	0.88	0
6	SO4	B	506	-	4,4,4	0.09	0	6,6,6	0.09	0
6	SO4	B	507	-	4,4,4	0.12	0	6,6,6	0.26	0
6	SO4	B	508	-	4,4,4	0.18	0	6,6,6	0.13	0
6	SO4	B	509	-	4,4,4	0.21	0	6,6,6	0.22	0
6	SO4	B	510	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	B	511	-	4,4,4	0.18	0	6,6,6	0.14	0
6	SO4	B	512	-	4,4,4	0.15	0	6,6,6	0.12	0
7	EDO	B	513	-	3,3,3	0.46	0	2,2,2	0.65	0
7	EDO	B	514	-	3,3,3	0.47	0	2,2,2	0.52	0
7	EDO	B	515	-	3,3,3	0.42	0	2,2,2	0.38	0
10	ACT	B	519	-	1,3,3	1.29	0	0,3,3	0.00	-
7	EDO	B	520	-	3,3,3	0.52	0	2,2,2	0.74	0
8	GOL	B	521	-	5,5,5	0.88	0	5,5,5	0.48	0
10	ACT	B	522	11	1,3,3	0.51	0	0,3,3	0.00	-
10	ACT	B	523	-	1,3,3	1.11	0	0,3,3	0.00	-
8	GOL	B	525	-	5,5,5	0.38	0	5,5,5	0.40	0
6	SO4	B	526	-	4,4,4	0.18	0	6,6,6	0.11	0
7	EDO	B	527	-	3,3,3	0.47	0	2,2,2	0.43	0
7	EDO	B	528	-	3,3,3	0.50	0	2,2,2	0.42	0
12	1RF	B	529	3,2	7,11,11	1.26	1 (14%)	4,16,16	1.42	0
6	SO4	B	530	11	4,4,4	0.54	0	6,6,6	0.49	0
4	NAG	C	503	1	14,14,15	0.52	0	15,19,21	0.65	0
4	NAG	C	504	1	14,14,15	0.69	0	15,19,21	1.27	2 (13%)
4	NAG	C	505	1	14,14,15	0.32	0	15,19,21	1.19	2 (13%)
6	SO4	C	506	-	4,4,4	0.21	0	6,6,6	0.11	0
6	SO4	C	507	-	4,4,4	0.17	0	6,6,6	0.29	0
6	SO4	C	508	-	4,4,4	0.15	0	6,6,6	0.14	0
6	SO4	C	509	-	4,4,4	0.17	0	6,6,6	0.27	0
6	SO4	C	510	-	4,4,4	0.18	0	6,6,6	0.08	0
6	SO4	C	511	-	4,4,4	0.12	0	6,6,6	0.12	0
6	SO4	C	512	-	4,4,4	0.14	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	C	513	-	4,4,4	0.17	0	6,6,6	0.37	0
6	SO4	C	514	-	4,4,4	0.16	0	6,6,6	0.14	0
6	SO4	C	515	-	4,4,4	0.15	0	6,6,6	0.12	0
7	EDO	C	516	-	3,3,3	0.48	0	2,2,2	0.47	0
8	GOL	C	517	-	5,5,5	0.35	0	5,5,5	0.44	0
7	EDO	C	521	-	3,3,3	0.41	0	2,2,2	0.51	0
8	GOL	C	522	-	5,5,5	0.29	0	5,5,5	0.25	0
10	ACT	C	523	-	1,3,3	0.92	0	0,3,3	0.00	-
8	GOL	C	524	-	5,5,5	0.32	0	5,5,5	0.31	0
8	GOL	C	525	-	5,5,5	0.34	0	5,5,5	0.30	0
13	PGE	C	527	-	9,9,9	0.49	0	8,8,8	1.45	0
8	GOL	C	528	-	5,5,5	0.37	0	5,5,5	0.89	0
7	EDO	C	530	-	3,3,3	0.40	0	2,2,2	0.54	0
7	EDO	C	531	-	3,3,3	0.47	0	2,2,2	0.43	0
6	SO4	C	532	-	4,4,4	0.19	0	6,6,6	0.18	0
10	ACT	C	533	-	1,3,3	1.63	0	0,3,3	0.00	-
12	1RF	C	534	3,2	3,7,11	1.89	1 (33%)	1,12,16	1.16	0
4	NAG	D	503	1	14,14,15	0.52	0	15,19,21	0.70	0
4	NAG	D	504	1	14,14,15	0.57	0	15,19,21	0.86	0
4	NAG	D	505	1	14,14,15	0.42	0	15,19,21	0.97	1 (6%)
6	SO4	D	506	-	4,4,4	0.19	0	6,6,6	0.18	0
6	SO4	D	507	-	4,4,4	0.18	0	6,6,6	0.19	0
6	SO4	D	508	-	4,4,4	0.13	0	6,6,6	0.15	0
6	SO4	D	509	-	4,4,4	0.15	0	6,6,6	0.20	0
6	SO4	D	510	11	4,4,4	0.09	0	6,6,6	0.34	0
6	SO4	D	511	11	4,4,4	0.34	0	6,6,6	0.08	0
6	SO4	D	512	-	4,4,4	0.15	0	6,6,6	0.09	0
6	SO4	D	513	-	4,4,4	0.18	0	6,6,6	0.18	0
6	SO4	D	514	-	4,4,4	0.19	0	6,6,6	0.27	0
10	ACT	D	515	-	1,3,3	1.28	0	0,3,3	0.00	-
7	EDO	D	516[A]	-	3,3,3	0.46	0	2,2,2	0.48	0
7	EDO	D	516[B]	-	3,3,3	0.48	0	2,2,2	0.44	0
7	EDO	D	517	-	3,3,3	0.54	0	2,2,2	0.15	0
13	PGE	D	518	-	6,6,9	0.43	0	5,5,8	1.40	0
8	GOL	D	519	-	5,5,5	0.31	0	5,5,5	0.35	0
7	EDO	D	520	-	3,3,3	0.53	0	2,2,2	0.40	0
8	GOL	D	521	-	5,5,5	0.25	0	5,5,5	0.47	0
7	EDO	D	522	-	3,3,3	0.47	0	2,2,2	0.55	0
7	EDO	D	523	-	3,3,3	0.42	0	2,2,2	0.45	0
7	EDO	D	524	-	3,3,3	0.46	0	2,2,2	0.48	0
7	EDO	D	525	-	3,3,3	0.47	0	2,2,2	0.54	0
10	ACT	D	526	-	1,3,3	1.19	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GOL	D	527	-	5,5,5	0.26	0	5,5,5	0.20	0
7	EDO	D	529	-	3,3,3	0.16	0	2,2,2	0.26	0
6	SO4	D	530	-	4,4,4	0.18	0	6,6,6	0.16	0
7	EDO	D	531	-	3,3,3	0.46	0	2,2,2	0.56	0
6	SO4	D	532	-	4,4,4	0.17	0	6,6,6	0.46	0
12	1RF	D	538	11,3,2	0,5,11	0.00	-	0,10,16	0.00	-

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	NAG	A	503	1	-	0/6/23/26	0/1/1/1
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	EDO	A	511	-	-	0/1/1/1	0/0/0/0
7	EDO	A	512	-	-	0/1/1/1	0/0/0/0
7	EDO	A	513	-	-	0/1/1/1	0/0/0/0
6	SO4	A	514	-	-	0/0/0/0	0/0/0/0
4	NAG	A	515	1	-	0/6/23/26	0/1/1/1
8	GOL	A	516	-	-	0/4/4/4	0/0/0/0
8	GOL	A	520	-	-	0/4/4/4	0/0/0/0
10	ACT	A	521	-	-	0/0/0/0	0/0/0/0
7	EDO	A	522	-	-	0/1/1/1	0/0/0/0
7	EDO	A	523	-	-	0/1/1/1	0/0/0/0
7	EDO	A	524	-	-	0/1/1/1	0/0/0/0
10	ACT	A	525	-	-	0/0/0/0	0/0/0/0
7	EDO	A	526	-	-	0/1/1/1	0/0/0/0
8	GOL	A	527	-	-	0/4/4/4	0/0/0/0
10	ACT	A	528	-	-	0/0/0/0	0/0/0/0
7	EDO	A	529	-	-	0/1/1/1	0/0/0/0
12	1RF	A	531	3,2	-	0/0/5/9	0/0/0/0
4	NAG	B	503	1	-	0/6/23/26	0/1/1/1
4	NAG	B	504	1	-	0/6/23/26	0/1/1/1
4	NAG	B	505	1	-	0/6/23/26	0/1/1/1
6	SO4	B	506	-	-	0/0/0/0	0/0/0/0
6	SO4	B	507	-	-	0/0/0/0	0/0/0/0
6	SO4	B	508	-	-	0/0/0/0	0/0/0/0
6	SO4	B	509	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	510	-	-	0/0/0/0	0/0/0/0
6	SO4	B	511	-	-	0/0/0/0	0/0/0/0
6	SO4	B	512	-	-	0/0/0/0	0/0/0/0
7	EDO	B	513	-	-	0/1/1/1	0/0/0/0
7	EDO	B	514	-	-	0/1/1/1	0/0/0/0
7	EDO	B	515	-	-	0/1/1/1	0/0/0/0
10	ACT	B	519	-	-	0/0/0/0	0/0/0/0
7	EDO	B	520	-	-	0/1/1/1	0/0/0/0
8	GOL	B	521	-	-	0/4/4/4	0/0/0/0
10	ACT	B	522	11	-	0/0/0/0	0/0/0/0
10	ACT	B	523	-	-	0/0/0/0	0/0/0/0
8	GOL	B	525	-	-	0/4/4/4	0/0/0/0
6	SO4	B	526	-	-	0/0/0/0	0/0/0/0
7	EDO	B	527	-	-	0/1/1/1	0/0/0/0
7	EDO	B	528	-	-	0/1/1/1	0/0/0/0
12	1RF	B	529	3,2	-	0/4/9/9	0/0/0/0
6	SO4	B	530	11	-	0/0/0/0	0/0/0/0
4	NAG	C	503	1	-	0/6/23/26	0/1/1/1
4	NAG	C	504	1	-	0/6/23/26	0/1/1/1
4	NAG	C	505	1	-	0/6/23/26	0/1/1/1
6	SO4	C	506	-	-	0/0/0/0	0/0/0/0
6	SO4	C	507	-	-	0/0/0/0	0/0/0/0
6	SO4	C	508	-	-	0/0/0/0	0/0/0/0
6	SO4	C	509	-	-	0/0/0/0	0/0/0/0
6	SO4	C	510	-	-	0/0/0/0	0/0/0/0
6	SO4	C	511	-	-	0/0/0/0	0/0/0/0
6	SO4	C	512	-	-	0/0/0/0	0/0/0/0
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
7	EDO	C	516	-	-	0/1/1/1	0/0/0/0
8	GOL	C	517	-	-	0/4/4/4	0/0/0/0
7	EDO	C	521	-	-	0/1/1/1	0/0/0/0
8	GOL	C	522	-	-	0/4/4/4	0/0/0/0
10	ACT	C	523	-	-	0/0/0/0	0/0/0/0
8	GOL	C	524	-	-	0/4/4/4	0/0/0/0
8	GOL	C	525	-	-	0/4/4/4	0/0/0/0
13	PGE	C	527	-	-	0/7/7/7	0/0/0/0
8	GOL	C	528	-	-	0/4/4/4	0/0/0/0
7	EDO	C	530	-	-	0/1/1/1	0/0/0/0
7	EDO	C	531	-	-	0/1/1/1	0/0/0/0
6	SO4	C	532	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ACT	C	533	-	-	0/0/0/0	0/0/0/0
12	1RF	C	534	3,2	-	0/0/5/9	0/0/0/0
4	NAG	D	503	1	-	0/6/23/26	0/1/1/1
4	NAG	D	504	1	-	0/6/23/26	0/1/1/1
4	NAG	D	505	1	-	0/6/23/26	0/1/1/1
6	SO4	D	506	-	-	0/0/0/0	0/0/0/0
6	SO4	D	507	-	-	0/0/0/0	0/0/0/0
6	SO4	D	508	-	-	0/0/0/0	0/0/0/0
6	SO4	D	509	-	-	0/0/0/0	0/0/0/0
6	SO4	D	510	11	-	0/0/0/0	0/0/0/0
6	SO4	D	511	11	-	0/0/0/0	0/0/0/0
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
10	ACT	D	515	-	-	0/0/0/0	0/0/0/0
7	EDO	D	516[A]	-	-	0/1/1/1	0/0/0/0
7	EDO	D	516[B]	-	-	0/1/1/1	0/0/0/0
7	EDO	D	517	-	-	0/1/1/1	0/0/0/0
13	PGE	D	518	-	-	0/4/4/7	0/0/0/0
8	GOL	D	519	-	-	0/4/4/4	0/0/0/0
7	EDO	D	520	-	-	0/1/1/1	0/0/0/0
8	GOL	D	521	-	-	0/4/4/4	0/0/0/0
7	EDO	D	522	-	-	0/1/1/1	0/0/0/0
7	EDO	D	523	-	-	0/1/1/1	0/0/0/0
7	EDO	D	524	-	-	0/1/1/1	0/0/0/0
7	EDO	D	525	-	-	0/1/1/1	0/0/0/0
10	ACT	D	526	-	-	0/0/0/0	0/0/0/0
8	GOL	D	527	-	-	0/4/4/4	0/0/0/0
7	EDO	D	529	-	-	0/1/1/1	0/0/0/0
6	SO4	D	530	-	-	0/0/0/0	0/0/0/0
7	EDO	D	531	-	-	0/1/1/1	0/0/0/0
6	SO4	D	532	-	-	0/0/0/0	0/0/0/0
12	1RF	D	538	11,3,2	-	0/0/0/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	534	1RF	O1-V2	-2.82	1.69	1.80
12	B	529	1RF	O1-V2	-2.57	1.70	1.80
4	B	504	NAG	C2-N2	-2.23	1.42	1.46
12	A	531	1RF	O1-V2	-2.16	1.72	1.80

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	NAG	C2-N2-C7	-3.50	118.55	123.04
4	D	505	NAG	C2-N2-C7	-2.88	119.34	123.04
4	C	505	NAG	C6-C5-C4	-2.46	106.94	113.02
4	B	504	NAG	C4-C3-C2	-2.22	107.78	111.23
4	B	503	NAG	C2-N2-C7	-2.20	120.21	123.04
4	B	504	NAG	O4-C4-C3	-2.19	105.41	110.34
4	B	504	NAG	C6-C5-C4	-2.17	107.67	113.02
4	B	504	NAG	C3-C4-C5	2.06	113.79	110.20
4	A	503	NAG	C1-O5-C5	2.13	114.96	112.25
4	C	504	NAG	C3-C4-C5	2.57	114.68	110.20
4	B	503	NAG	C1-O5-C5	2.58	115.52	112.25
4	C	505	NAG	C1-O5-C5	2.68	115.65	112.25
4	A	515	NAG	C1-O5-C5	2.85	115.86	112.25
4	C	504	NAG	C4-C3-C2	2.87	115.68	111.23
4	B	504	NAG	C1-O5-C5	4.62	118.11	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	508	SO4	1	0
7	A	512	EDO	1	0
6	A	514	SO4	1	0
8	A	520	GOL	1	0
7	A	522	EDO	1	0
10	A	525	ACT	1	0
7	A	529	EDO	2	0
12	A	531	1RF	2	0
4	B	505	NAG	1	0
6	B	509	SO4	1	0
7	B	520	EDO	1	0
8	B	521	GOL	3	0
10	B	522	ACT	1	0
7	B	527	EDO	4	0
12	B	529	1RF	14	0
6	B	530	SO4	4	0
8	C	524	GOL	2	0
8	C	525	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	527	PGE	6	0
7	C	531	EDO	6	0
10	C	533	ACT	1	0
12	C	534	1RF	4	0
10	D	515	ACT	1	0
7	D	516[B]	EDO	1	0
7	D	517	EDO	3	0
13	D	518	PGE	1	0
8	D	521	GOL	1	0
7	D	523	EDO	1	0
7	D	524	EDO	1	0
7	D	525	EDO	1	0
10	D	526	ACT	1	0
7	D	529	EDO	1	0
7	D	531	EDO	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	424/426 (99%)	-0.82	3 (0%)	89	88	4, 11, 24, 55	0
1	B	425/426 (99%)	-0.74	5 (1%)	81	80	6, 13, 29, 66	0
1	C	423/426 (99%)	-0.78	4 (0%)	85	85	4, 12, 26, 62	0
1	D	426/426 (100%)	-0.78	4 (0%)	85	85	5, 12, 28, 58	0
All	All	1698/1704 (99%)	-0.78	16 (0%)	85	85	4, 12, 28, 66	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	ASN	6.8
1	A	431	SER	6.0
1	D	431	SER	5.7
1	C	64	ASN	4.8
1	A	8	ASN	4.5
1	D	64	ASN	4.3
1	A	429	ASP	3.9
1	D	432	THR	3.7
1	C	63	LYS	3.4
1	B	432	THR	2.9
1	B	8	ASN	2.9
1	C	430	ASP	2.3
1	D	65	GLY	2.1
1	B	63	LYS	2.1
1	C	429	ASP	2.1
1	B	431	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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^2)	Q<0.9
5	NAG	A	504	14/15	0.90	0.16	4.28	27,33,40,46	0
9	NAG	D	534	14/15	0.95	0.12	1.23	17,23,31,38	0
9	NAG	C	518	14/15	0.95	0.12	0.85	12,24,34,39	0
9	NAG	A	518	14/15	0.92	0.18	-	14,21,30,34	0
9	FUC	A	519	10/11	0.94	0.23	-	19,24,30,37	0
9	NAG	D	535	14/15	0.89	0.29	-	18,33,53,53	0
9	NAG	B	517	14/15	0.93	0.15	-	14,22,27,33	0
9	FUC	D	536	10/11	0.86	0.27	-	28,37,42,47	0
5	NAG	A	505	14/15	0.73	0.39	-	37,50,55,62	1
9	FUC	B	518	10/11	0.93	0.13	-	14,22,31,34	0
9	NAG	B	516	14/15	0.96	0.09	-	10,15,19,20	0
9	NAG	A	517	14/15	0.95	0.11	-	13,18,23,24	0
9	NAG	C	519	14/15	0.89	0.28	-	19,41,50,51	0
9	FUC	C	520	10/11	0.77	0.28	-	34,46,50,53	0

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^{th} 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^2)	Q<0.9
6	SO4	A	514	5/5	0.96	0.38	21.07	41,44,49,56	0
6	SO4	D	510	5/5	0.99	0.26	20.60	24,33,35,40	0
11	NA	D	528	1/1	0.97	0.20	15.08	6,6,6,6	0
7	EDO	B	515	4/4	0.96	0.23	13.44	16,23,25,40	0
8	GOL	D	527	6/6	0.92	0.15	12.23	8,17,25,43	0
6	SO4	D	530	5/5	0.92	0.17	12.21	25,28,34,40	5
7	EDO	B	514	4/4	0.88	0.20	11.26	25,26,31,38	0
8	GOL	B	521	6/6	0.77	0.27	10.84	34,36,45,48	0
4	NAG	C	505	14/15	0.86	0.21	9.97	27,37,42,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	ACT	A	521	4/4	0.89	0.17	9.80	24,31,35,40	0
10	ACT	B	522	4/4	0.95	0.14	9.12	20,25,26,36	0
6	SO4	B	506	5/5	0.97	0.22	8.33	17,26,38,42	0
4	NAG	B	504	14/15	0.92	0.18	8.20	24,30,37,43	0
6	SO4	C	532	5/5	0.79	0.34	7.76	41,45,59,74	0
8	GOL	C	528	6/6	0.92	0.14	7.70	10,16,22,40	0
6	SO4	C	512	5/5	0.92	0.31	6.79	46,49,58,72	0
6	SO4	B	507	5/5	0.96	0.29	6.57	33,36,44,51	0
12	1RF	A	531	8/12	0.94	0.16	6.09	10,19,27,28	8
10	ACT	C	533	4/4	0.84	0.32	5.53	30,36,39,45	0
12	1RF	C	534	8/12	0.94	0.19	5.13	14,19,27,28	8
4	NAG	D	505	14/15	0.91	0.15	4.80	28,34,47,52	0
8	GOL	D	519	6/6	0.95	0.11	4.45	18,23,27,27	0
11	NA	A	530	1/1	0.99	0.13	4.19	5,5,5,5	0
13	PGE	C	527	10/10	0.90	0.23	4.01	17,29,42,48	0
11	NA	B	524	1/1	1.00	0.15	3.94	1,1,1,1	0
6	SO4	A	507	5/5	0.98	0.24	3.67	32,33,36,50	0
7	EDO	D	531	4/4	0.76	0.22	3.27	34,39,40,44	0
12	1RF	B	529	12/12	0.95	0.15	3.04	13,27,31,39	12
6	SO4	D	511	5/5	0.93	0.20	2.93	30,43,46,46	0
6	SO4	C	513	5/5	0.82	0.25	2.85	27,42,43,56	0
7	EDO	A	529	4/4	0.90	0.14	2.73	13,19,25,27	0
6	SO4	D	509	5/5	0.94	0.21	2.47	24,32,38,41	0
8	GOL	A	527	6/6	0.89	0.21	2.42	29,34,38,41	0
7	EDO	C	530	4/4	0.95	0.13	2.38	12,21,29,30	0
11	NA	C	529	1/1	1.00	0.13	2.31	2,2,2,2	0
4	NAG	C	503	14/15	0.95	0.14	2.26	14,23,29,41	0
8	GOL	C	525	6/6	0.90	0.27	2.10	22,32,45,49	0
7	EDO	B	528	4/4	0.88	0.29	1.96	20,25,32,54	0
4	NAG	D	503	14/15	0.94	0.14	1.77	15,22,31,40	0
8	GOL	C	517	6/6	0.97	0.09	1.69	13,14,18,25	0
10	ACT	D	515	4/4	0.97	0.18	1.67	25,31,35,38	0
12	1RF	D	538	6/12	0.96	0.11	1.60	14,19,29,29	6
4	NAG	B	505	14/15	0.93	0.13	1.52	13,21,30,32	0
4	NAG	A	503	14/15	0.95	0.11	1.04	14,18,26,28	0
8	GOL	B	525	6/6	0.94	0.13	0.99	21,25,29,31	0
8	GOL	A	516	6/6	0.98	0.08	0.89	12,14,15,17	0
7	EDO	A	523	4/4	0.95	0.09	-0.19	16,18,25,30	0
7	EDO	B	520	4/4	0.93	0.12	-0.21	27,31,31,33	0
7	EDO	D	524	4/4	0.94	0.10	-0.22	33,35,36,39	0
11	NA	C	526	1/1	0.94	0.07	-0.28	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	SO4	A	506	5/5	0.99	0.06	-1.52	17,17,23,24	0
3	FE	B	502	1/1	0.98	0.04	-2.34	9,9,9,9	1
3	FE	C	502	1/1	1.00	0.02	-2.91	14,14,14,14	1
3	FE	D	502	1/1	1.00	0.02	-3.09	13,13,13,13	1
3	FE	A	502	1/1	0.98	0.03	-3.55	8,8,8,8	1
2	ZN	B	501	1/1	1.00	0.02	-4.40	12,12,12,12	1
2	ZN	A	501	1/1	1.00	0.02	-5.15	12,12,12,12	1
2	ZN	C	501	1/1	1.00	0.02	-5.42	12,12,12,12	1
2	ZN	D	501	1/1	1.00	0.03	-5.59	8,8,8,8	1
6	SO4	C	507	5/5	0.92	0.23	-	28,32,54,55	0
7	EDO	C	521	4/4	0.97	0.10	-	23,27,30,46	0
6	SO4	D	506	5/5	0.93	0.35	-	53,64,77,84	0
7	EDO	D	523	4/4	0.89	0.12	-	38,47,51,52	0
6	SO4	D	514	5/5	0.94	0.46	-	44,51,63,65	0
10	ACT	D	526	4/4	0.91	0.11	-	23,37,40,45	0
4	NAG	D	504	14/15	0.69	0.32	-	41,50,68,69	0
6	SO4	C	515	5/5	0.91	0.34	-	55,56,71,76	0
7	EDO	B	527	4/4	0.87	0.25	-	34,39,47,52	0
7	EDO	B	513	4/4	0.94	0.30	-	30,35,42,43	0
8	GOL	C	524	6/6	0.96	0.26	-	26,34,42,51	0
6	SO4	B	509	5/5	0.97	0.28	-	37,39,45,48	0
6	SO4	D	512	5/5	0.96	0.33	-	44,50,55,58	0
8	GOL	C	522	6/6	0.95	0.27	-	30,34,43,45	0
7	EDO	A	524	4/4	0.91	0.12	-	20,35,37,44	0
6	SO4	C	510	5/5	0.95	0.37	-	50,53,59,71	0
7	EDO	A	522	4/4	0.94	0.21	-	21,28,33,40	0
7	EDO	A	526	4/4	0.85	0.12	-	30,37,38,44	0
6	SO4	B	510	5/5	0.97	0.33	-	37,52,63,66	0
6	SO4	B	512	5/5	0.98	0.21	-	21,28,34,35	0
7	EDO	C	531	4/4	0.92	0.25	-	25,34,38,45	0
11	NA	A	532	1/1	0.94	0.16	-	35,35,35,35	0
10	ACT	A	525	4/4	0.89	0.13	-	35,41,46,48	0
6	SO4	C	506	5/5	0.82	0.39	-	68,69,80,82	0
11	NA	D	539	1/1	0.94	0.27	-	42,42,42,42	0
7	EDO	D	525	4/4	0.92	0.21	-	21,22,31,46	0
7	EDO	D	516[A]	4/4	0.85	0.21	-	28,30,32,32	4
6	SO4	C	514	5/5	0.91	0.32	-	53,58,74,86	0
6	SO4	D	532	5/5	0.90	0.19	-	36,37,52,54	0
7	EDO	D	522	4/4	0.89	0.22	-	34,45,48,60	0
6	SO4	D	513	5/5	0.93	0.32	-	42,61,66,70	0
6	SO4	A	510	5/5	0.96	0.41	-	49,56,66,76	0
11	NA	D	537	1/1	0.94	0.21	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	C	504	14/15	0.75	0.36	-	35,45,58,58	0
7	EDO	A	511	4/4	0.65	0.35	-	40,42,44,47	0
6	SO4	B	508	5/5	0.96	0.25	-	31,44,48,58	0
4	NAG	A	515	14/15	0.85	0.29	-	27,44,53,56	0
6	SO4	D	507	5/5	0.94	0.29	-	29,40,45,46	0
7	EDO	D	516[B]	4/4	0.85	0.21	-	28,30,31,32	4
7	EDO	A	513	4/4	0.85	0.29	-	31,34,41,45	0
4	NAG	B	503	14/15	0.89	0.34	-	29,48,58,62	0
7	EDO	C	516	4/4	0.94	0.32	-	32,35,39,44	0
11	NA	B	531	1/1	0.80	0.16	-	54,54,54,54	0
11	NA	D	533	1/1	0.89	0.34	-	57,57,57,57	0
6	SO4	D	508	5/5	0.93	0.37	-	44,45,66,75	0
6	SO4	B	526	5/5	0.94	0.29	-	40,66,68,70	0
6	SO4	C	508	5/5	0.88	0.36	-	44,52,78,82	0
6	SO4	B	511	5/5	0.96	0.27	-	43,53,57,64	0
10	ACT	B	523	4/4	0.80	0.21	-	32,35,46,48	0
13	PGE	D	518	7/10	0.86	0.37	-	26,35,45,64	0
6	SO4	A	508	5/5	0.96	0.31	-	34,36,47,48	0
8	GOL	A	520	6/6	0.80	0.25	-	31,35,43,47	0
6	SO4	A	509	5/5	0.96	0.28	-	34,41,46,48	0
6	SO4	C	511	5/5	0.98	0.38	-	43,44,52,54	0
7	EDO	D	520	4/4	0.88	0.13	-	34,42,42,56	0
7	EDO	A	512	4/4	0.93	0.29	-	33,33,37,39	0
8	GOL	D	521	6/6	0.90	0.25	-	34,36,39,42	0
7	EDO	D	517	4/4	0.85	0.30	-	25,37,42,48	0
7	EDO	D	529	4/4	0.91	0.27	-	27,28,28,32	0
10	ACT	C	523	4/4	0.94	0.32	-	36,38,39,41	0
6	SO4	C	509	5/5	0.95	0.39	-	52,55,60,67	0
10	ACT	A	528	4/4	0.95	0.08	-	20,36,38,45	0
10	ACT	B	519	4/4	0.86	0.21	-	42,47,50,55	0
6	SO4	B	530	5/5	0.88	0.32	-	62,64,81,97	0

6.5 Other polymers (i)

There are no such residues in this entry.