Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:54 PM GMT

PDB ID	:	4DSY
Title	:	Crystal structure of red kidney bean purple acid phosphatase in complex with Maybridge fragment CC24201
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	:	2.30 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:

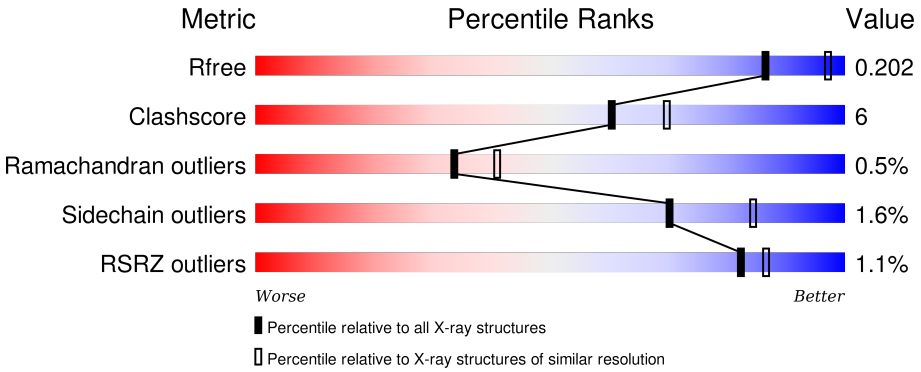
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	89% 10%
1	B	426	2% 88% 11%
1	C	426	86% 13%
1	D	426	2% 88% 11%

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	EDO	A	521	-	-	X	-
10	EDO	B	519	-	-	-	X
10	EDO	C	514	-	-	-	X
10	EDO	D	516	-	-	-	X
10	EDO	D	518	-	-	-	X
4	0LO	A	503	-	-	-	X
5	GOL	C	512	-	-	X	-
5	GOL	D	512	-	-	X	X
6	NAG	B	505	-	-	-	X
6	NAG	C	506	-	-	-	X
6	NAG	D	508	-	-	-	X
8	SO4	A	513	-	-	-	X
8	SO4	A	518	-	-	-	X
8	SO4	D	515	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16004 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	425	Total	C	N	O	S	0	2	0
			3524	2261	616	637	10			
1	B	426	Total	C	N	O	S	9	1	0
			3519	2258	612	639	10			
1	C	423	Total	C	N	O	S	1	1	0
			3496	2245	609	632	10			
1	D	426	Total	C	N	O	S	5	1	0
			3515	2257	610	637	11			

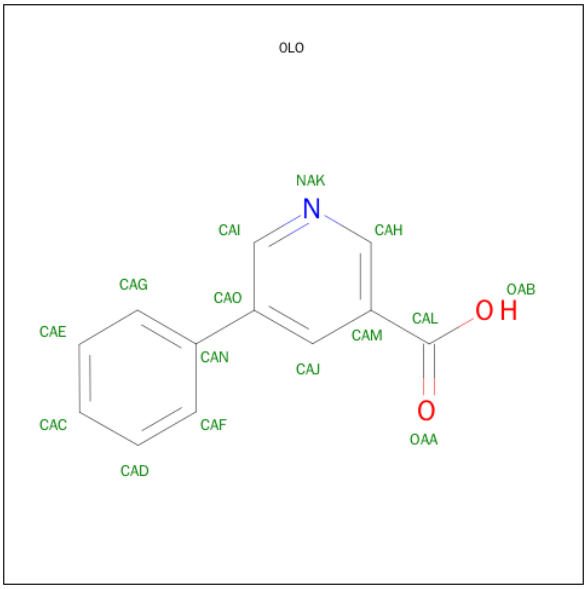
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

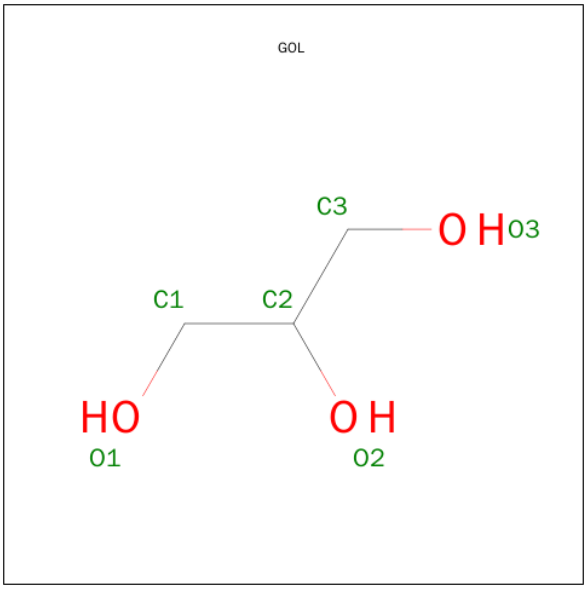
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 5-PHENYLPYRIDINE-3-CARBOXYLIC ACID (three-letter code: 0LO) (formula: $C_{12}H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	12	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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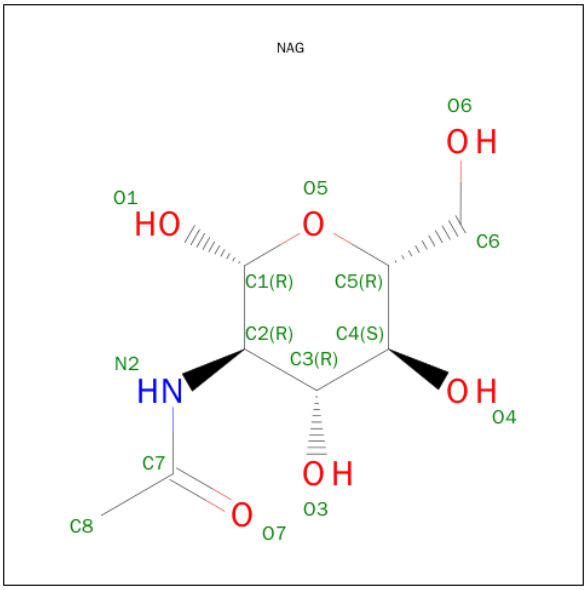
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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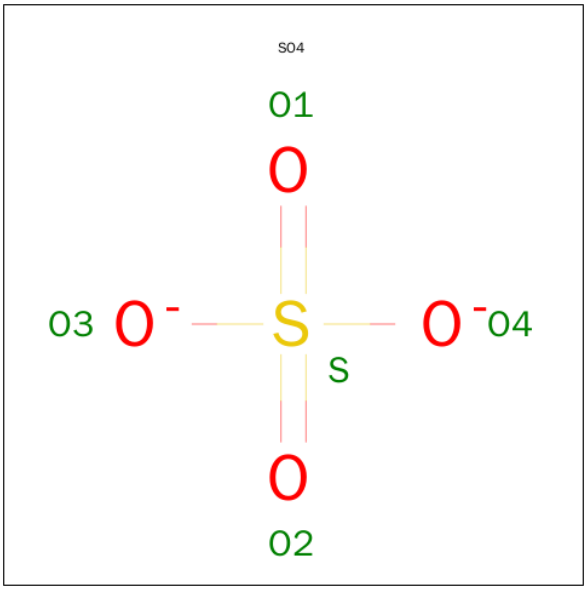
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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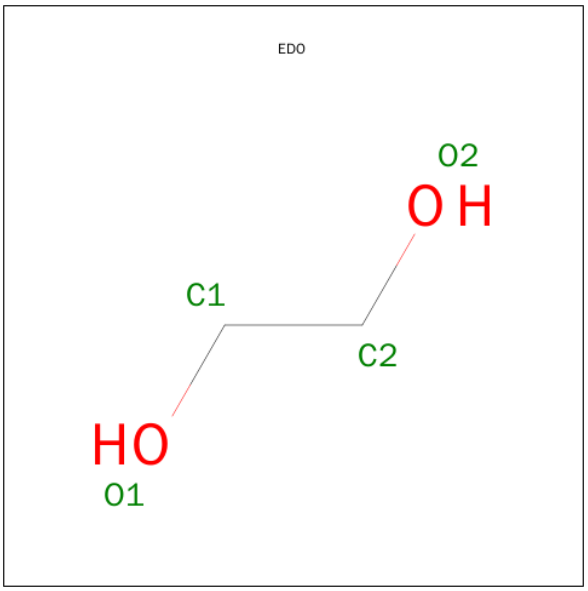
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0

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

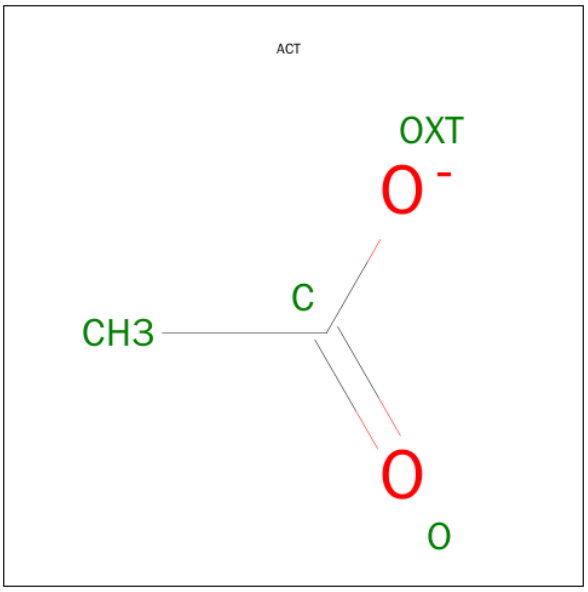
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total C N O 38 22 2 14	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	C	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	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
10	D	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 ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- 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 24 14 1 9	0	0
12	C	2	Total C N O 24 14 1 9	0	0

- Molecule 13 is water.

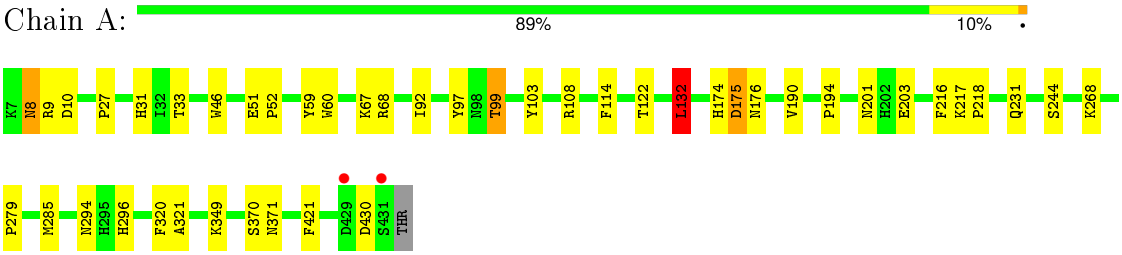
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	377	Total O 377 377	0	0
13	B	322	Total O 322 322	0	0
13	C	305	Total O 305 305	0	0
13	D	354	Total O 354 354	0	0

3 Residue-property plots (i)

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

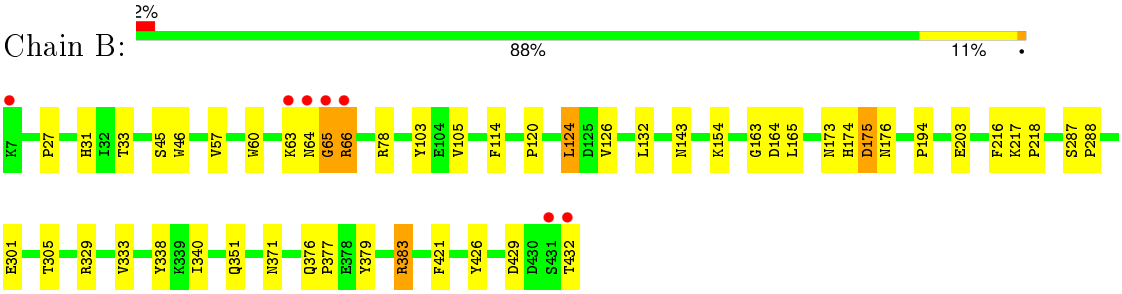
- Molecule 1: Purple acid phosphatase

Chain A:



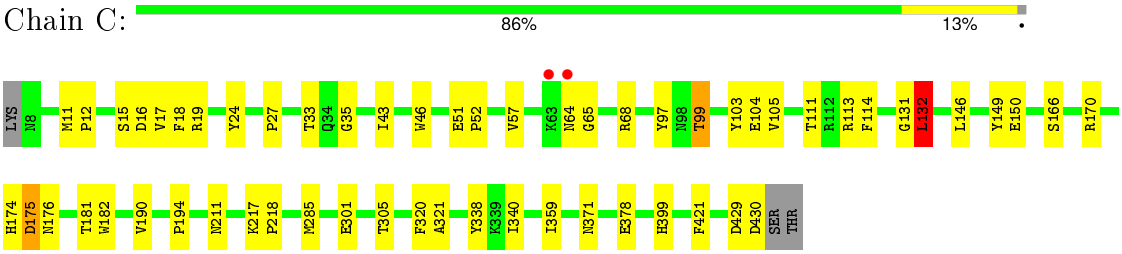
- Molecule 1: Purple acid phosphatase

Chain B:



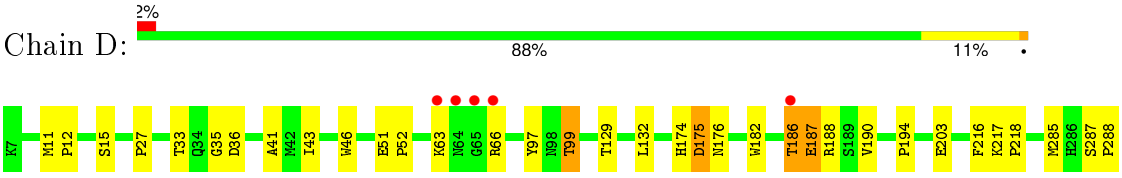
- Molecule 1: Purple acid phosphatase

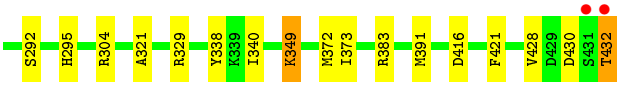
Chain C:



- Molecule 1: Purple acid phosphatase

Chain D:




S292
H295
R304
A321
R329
Y338
K339
I340
K349
M372
I373
R383
M391
D416
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	127.70Å 127.70Å 299.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.86 – 2.30 19.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.86-2.30) 99.9 (19.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.161 , 0.207 0.160 , 0.202	Depositor DCC
R_{free} test set	6316 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.2	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 125962 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, NAG, EDO, FUC, FE, ACT, 0LO, SO4

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	0.40	0/3644	0.54	1/4953 (0.0%)
1	B	0.38	0/3638	0.53	1/4946 (0.0%)
1	C	0.38	0/3618	0.52	1/4919 (0.0%)
1	D	0.39	0/3637	0.54	0/4944
All	All	0.39	0/14537	0.53	3/19762 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	132	LEU	CA-CB-CG	-6.63	100.06	115.30
1	A	132	LEU	CA-CB-CG	-5.28	103.16	115.30
1	B	78	ARG	NE-CZ-NH2	-5.06	117.77	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	3524	0	3339	42	0
1	B	3519	0	3334	35	0
1	C	3496	0	3316	42	0
1	D	3515	0	3336	36	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	15	0	8	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	4	0
5	D	24	0	32	6	0
6	A	14	0	13	0	0
6	B	28	0	26	1	0
6	C	28	0	26	2	0
6	D	28	0	26	0	0
7	A	76	0	68	0	0
7	B	38	0	34	0	0
7	C	38	0	34	1	0
7	D	76	0	68	3	0
8	A	20	0	0	0	0
8	B	20	0	0	1	0
8	C	10	0	0	0	0
8	D	5	0	0	0	0
9	A	38	0	34	1	0
10	A	12	0	18	10	0
10	B	20	0	30	1	0
10	C	8	0	12	1	0
10	D	12	0	18	1	0
11	A	4	0	3	0	0
11	D	4	0	3	0	0
12	B	24	0	22	0	0
12	C	24	0	22	1	0
13	A	377	0	0	3	0
13	B	322	0	0	2	0
13	C	305	0	0	2	0
13	D	354	0	0	1	0
All	All	16004	0	13846	160	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 6.

All (160) 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:304:ARG:HH22	5:D:512:GOL:H12	1.17	1.04
1:A:370:SER:H	10:A:521:EDO:H22	1.26	1.00
1:D:304:ARG:NH2	5:D:512:GOL:H12	1.91	0.84
1:D:349:LYS:H	1:D:349:LYS:HD3	1.47	0.80
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.65	0.78
1:C:68:ARG:HH12	5:C:512:GOL:H2	1.49	0.77
1:C:146:LEU:O	1:C:150:GLU:HG2	1.86	0.75
1:D:329:ARG:NH1	1:D:416:ASP:OD2	2.19	0.74
1:C:64:ASN:ND2	1:C:65:GLY:H	1.87	0.72
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.25	0.72
1:D:349:LYS:H	1:D:349:LYS:CD	2.03	0.70
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.74	0.70
1:B:383:ARG:HD3	8:B:514:SO4:O3	1.92	0.69
1:B:65:GLY:CA	1:B:66:ARG:HB2	2.24	0.68
1:D:421:PHE:CD2	1:D:428:VAL:HG22	2.29	0.67
1:B:143:ASN:HD22	6:B:506:NAG:H83	1.60	0.67
1:A:371:ASN:H	10:A:521:EDO:H12	1.59	0.67
1:A:231:GLN:HG2	13:A:926:HOH:O	1.95	0.67
1:A:97:TYR:O	1:A:99:THR:HG22	1.95	0.66
1:C:170[A]:ARG:HD3	13:C:788:HOH:O	1.94	0.66
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.78	0.66
1:B:65:GLY:N	1:B:66:ARG:HB2	2.11	0.65
1:D:186:THR:O	1:D:188:ARG:N	2.30	0.65
1:D:186:THR:O	1:D:187:GLU:C	2.35	0.64
1:C:64:ASN:HD22	1:C:65:GLY:H	1.43	0.63
1:A:370:SER:H	10:A:521:EDO:C2	2.05	0.63
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.80	0.63
1:D:304:ARG:HH22	5:D:512:GOL:C1	2.04	0.62
1:A:371:ASN:H	10:A:521:EDO:C1	2.13	0.62
1:A:132:LEU:HD22	1:A:320:PHE:CD1	2.35	0.62
1:B:351:GLN:OE1	1:B:429:ASP:HA	2.00	0.61
1:A:8:ASN:ND2	1:A:10:ASP:H	1.99	0.61
1:A:8:ASN:HD21	1:A:10:ASP:HB2	1.66	0.61
7:D:506:NAG:H2	7:D:507:FUC:H5	1.83	0.61
1:D:329:ARG:HH22	1:D:432:THR:HG21	1.64	0.60
1:A:370:SER:N	10:A:521:EDO:H22	2.09	0.60
1:D:349:LYS:N	1:D:349:LYS:HD3	2.15	0.60
1:B:173:ASN:OD1	10:B:519:EDO:H11	2.01	0.60
1:C:97:TYR:O	1:C:99:THR:HG22	2.03	0.59
1:B:66:ARG:HE	1:B:66:ARG:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:HA	1:B:194:PRO:HB3	1.85	0.58
1:D:174:HIS:O	1:D:175:ASP:C	2.42	0.57
1:C:132:LEU:HD22	1:C:320:PHE:CD1	2.39	0.57
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.68	0.56
1:A:27:PRO:HB3	1:A:46:TRP:CD1	2.41	0.56
1:B:203:GLU:O	1:B:216:PHE:HA	2.05	0.55
1:C:174:HIS:O	1:C:175:ASP:C	2.44	0.55
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.41	0.55
1:D:329:ARG:NH2	1:D:432:THR:HG21	2.22	0.55
1:A:349:LYS:H	10:A:520:EDO:H11	1.72	0.55
1:D:97:TYR:O	1:D:99:THR:HG22	2.07	0.55
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.42	0.54
1:B:65:GLY:HA2	1:B:66:ARG:CB	2.36	0.54
1:D:33:THR:HA	1:D:194:PRO:HB3	1.89	0.54
1:B:65:GLY:H	1:B:66:ARG:HB2	1.73	0.54
1:C:113:ARG:HH12	10:C:501:EDO:H12	1.73	0.54
1:C:11:MET:HE3	6:C:503:NAG:C8	2.38	0.54
1:C:33:THR:HA	1:C:194:PRO:HB3	1.89	0.53
1:A:8:ASN:HD22	1:A:10:ASP:H	1.58	0.51
1:B:57:VAL:HG22	1:B:105:VAL:HG12	1.92	0.51
1:C:27:PRO:HB3	1:C:46:TRP:CD1	2.45	0.51
1:A:174:HIS:O	1:A:175:ASP:C	2.49	0.51
1:B:174:HIS:O	1:B:175:ASP:C	2.48	0.51
1:C:64:ASN:HD21	5:C:512:GOL:C3	2.24	0.51
1:A:8:ASN:HD22	1:A:9:ARG:N	2.07	0.51
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.45	0.50
1:A:349:LYS:HG3	10:A:520:EDO:H21	1.94	0.50
1:B:120:PRO:HG2	1:B:126:VAL:HG11	1.94	0.50
1:D:292:SER:O	1:D:373:ILE:HG12	2.12	0.50
1:B:65:GLY:CA	1:B:66:ARG:CB	2.88	0.49
1:B:65:GLY:HA2	1:B:66:ARG:HB2	1.94	0.49
1:A:97:TYR:O	1:A:99:THR:CG2	2.59	0.49
1:A:8:ASN:HD22	1:A:8:ASN:C	2.16	0.49
1:D:27:PRO:HB3	1:D:46:TRP:CD1	2.48	0.49
1:D:421:PHE:HD2	1:D:428:VAL:HG22	1.75	0.49
1:C:57:VAL:HG22	1:C:105:VAL:HG12	1.94	0.49
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.48	0.49
1:C:211:ASN:ND2	13:C:878:HOH:O	2.36	0.49
1:A:370:SER:OG	10:A:521:EDO:H22	2.12	0.49
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.48	0.49
1:B:288:PRO:HD2	13:B:715:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:PRO:HD2	1:D:15:SER:OG	2.13	0.48
1:C:301:GLU:O	1:C:305:THR:HG23	2.13	0.48
1:C:285:MET:O	1:C:321:ALA:HA	2.12	0.48
1:A:244:SER:HB2	1:A:279:PRO:HD2	1.94	0.48
1:D:190:VAL:O	1:D:190:VAL:HG22	2.13	0.48
1:B:31:HIS:CD2	1:B:45:SER:HB2	2.49	0.48
9:A:511:FUC:H61	9:A:512:NAG:H83	1.96	0.47
1:B:103:TYR:CE2	1:B:114:PHE:HB2	2.49	0.47
1:D:182:TRP:O	1:D:186:THR:OG1	2.29	0.46
1:C:132:LEU:CD2	1:C:320:PHE:CG	2.99	0.46
1:B:338:TYR:CZ	1:B:340:ILE:HA	2.50	0.46
1:A:371:ASN:HB2	10:A:521:EDO:H12	1.98	0.46
1:D:35:GLY:HA2	1:D:43:ILE:HG13	1.97	0.45
1:B:154:LYS:HE2	13:B:744:HOH:O	2.16	0.45
5:D:512:GOL:H11	13:D:764:HOH:O	2.16	0.45
1:C:190:VAL:O	1:C:190:VAL:HG22	2.16	0.45
1:B:60:TRP:HB2	1:B:65:GLY:HA3	1.99	0.44
1:A:201:ASN:ND2	4:A:503:0LO:OAA	2.44	0.44
1:D:372:MET:SD	5:D:503:GOL:H32	2.57	0.44
1:B:301:GLU:O	1:B:305:THR:HG23	2.17	0.44
1:B:421:PHE:HB3	1:B:426:TYR:O	2.18	0.44
7:D:506:NAG:HN2	7:D:507:FUC:H61	1.81	0.44
1:C:11:MET:CE	1:C:17:VAL:HG21	2.47	0.44
1:B:163:GLY:O	1:B:164:ASP:HB2	2.18	0.44
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.53	0.44
1:A:296:HIS:CE1	4:A:503:0LO:H6	2.52	0.44
1:D:129:THR:HG22	1:D:391[A]:MET:CE	2.47	0.44
1:A:203:GLU:O	1:A:216:PHE:HA	2.16	0.44
1:D:329:ARG:HH21	1:D:432:THR:HB	1.82	0.44
1:C:11:MET:HE3	6:C:503:NAG:H82	2.00	0.44
1:C:12:PRO:HD2	1:C:15:SER:OG	2.18	0.44
1:B:120:PRO:HG2	1:B:126:VAL:CG1	2.48	0.44
1:A:122:THR:HG23	13:A:767:HOH:O	2.17	0.43
1:A:371:ASN:CB	10:A:521:EDO:H12	2.48	0.43
1:A:132:LEU:HD22	1:A:320:PHE:CG	2.54	0.43
1:C:16:ASP:O	1:C:19:ARG:HB2	2.18	0.43
1:A:68:ARG:HG2	1:A:68:ARG:NH1	2.32	0.43
1:D:51:GLU:HB2	1:D:52:PRO:HD2	2.01	0.43
1:C:68:ARG:NH1	5:C:512:GOL:H2	2.27	0.43
1:C:399:HIS:CG	7:C:507:NAG:H5	2.54	0.43
1:A:60:TRP:HB3	1:A:67:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ASN:HD21	5:C:512:GOL:H31	1.83	0.42
1:C:359:ILE:O	1:C:359:ILE:HG13	2.19	0.42
1:A:103:TYR:CE1	1:A:114:PHE:HB2	2.54	0.42
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.54	0.42
1:B:329:ARG:NH2	1:B:432:THR:OG1	2.48	0.42
1:A:31:HIS:HD2	13:A:842:HOH:O	2.01	0.42
1:C:51:GLU:HB2	1:C:52:PRO:HD2	2.02	0.42
1:A:33:THR:HA	1:A:194:PRO:HB3	2.01	0.42
1:C:18:PHE:CD1	1:C:181:THR:HB	2.55	0.42
1:A:51:GLU:HB2	1:A:52:PRO:HD2	2.02	0.42
1:A:268:LYS:HB3	1:A:268:LYS:HE2	1.78	0.42
1:C:429:ASP:C	1:C:429:ASP:OD1	2.58	0.42
1:D:203:GLU:O	1:D:216:PHE:HA	2.19	0.42
1:B:165:LEU:HD13	1:B:203:GLU:CD	2.40	0.42
1:C:104:GLU:HB3	1:C:111:THR:CG2	2.50	0.42
7:D:506:NAG:C2	7:D:507:FUC:H5	2.49	0.41
1:A:59:TYR:CZ	1:A:92:ILE:HG23	2.55	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.82	0.41
1:B:376:GLN:HA	1:B:377:PRO:HD3	1.88	0.41
1:A:103:TYR:CZ	1:A:114:PHE:HB2	2.55	0.41
1:B:333:VAL:HG21	1:B:379:TYR:HB2	2.02	0.41
1:C:35:GLY:HA2	1:C:43:ILE:HG13	2.02	0.41
1:A:190:VAL:O	1:A:190:VAL:HG22	2.20	0.41
1:C:132:LEU:HD21	1:C:320:PHE:CD2	2.56	0.41
1:D:11:MET:HA	1:D:12:PRO:HD3	1.92	0.41
1:A:285:MET:O	1:A:321:ALA:HA	2.21	0.41
1:D:285:MET:O	1:D:321:ALA:HA	2.21	0.41
1:C:24:TYR:CD2	12:C:504:NAG:H82	2.56	0.41
1:C:11:MET:HA	1:C:12:PRO:HD3	1.84	0.40
1:C:166:SER:HA	1:C:182:TRP:CD1	2.56	0.40
1:D:36:ASP:HB3	1:D:41:ALA:HB3	2.03	0.40
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.55	0.40
1:D:383:ARG:HH21	5:D:503:GOL:H31	1.86	0.40
1:D:295:HIS:HB2	10:D:516:EDO:H12	2.03	0.40
1:A:132:LEU:CD2	1:A:320:PHE:CG	3.04	0.40
1:D:287:SER:HA	1:D:288:PRO:HD3	1.84	0.40
1:B:287:SER:HA	1:B:288:PRO:HD3	1.97	0.40
1:C:131:GLY:HA3	1:C:149:TYR:CE1	2.56	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%)	403 (95%)	21 (5%)	1 (0%)	52	64
1	B	425/426 (100%)	400 (94%)	21 (5%)	4 (1%)	21	24
1	C	422/426 (99%)	400 (95%)	21 (5%)	1 (0%)	52	64
1	D	425/426 (100%)	405 (95%)	17 (4%)	3 (1%)	26	31
All	All	1697/1704 (100%)	1608 (95%)	80 (5%)	9 (0%)	34	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	LYS
1	D	187	GLU
1	B	64	ASN
1	B	175	ASP
1	C	175	ASP
1	D	175	ASP
1	A	175	ASP
1	D	63	LYS
1	B	65	GLY

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%)	370 (98%)	6 (2%)	70	84
1	B	376/375 (100%)	370 (98%)	6 (2%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	373/375 (100%)	368 (99%)	5 (1%)	76 87
1	D	376/375 (100%)	369 (98%)	7 (2%)	65 81
All	All	1501/1500 (100%)	1477 (98%)	24 (2%)	70 84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	99	THR
1	A	108	ARG
1	A	132	LEU
1	A	176	ASN
1	A	294	ASN
1	B	66	ARG
1	B	124	LEU
1	B	132	LEU
1	B	176	ASN
1	B	371	ASN
1	B	383	ARG
1	C	99	THR
1	C	132	LEU
1	C	176	ASN
1	C	371	ASN
1	C	378	GLU
1	D	66	ARG
1	D	99	THR
1	D	132	LEU
1	D	176	ASN
1	D	186	THR
1	D	349	LYS
1	D	432	THR

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	294	ASN
1	A	295	HIS
1	A	371	ASN
1	B	371	ASN

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Mol	Chain	Res	Type
1	B	401	HIS
1	C	64	ASN
1	C	211	ASN
1	C	224	HIS
1	C	295	HIS
1	C	371	ASN
1	D	401	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

25 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	$\#\|Z\| > 2$
7	NAG	A	506	1,7	14,14,15	0.55	0	15,19,21	1.00	0
7	NAG	A	507	7	14,14,15	0.51	0	15,19,21	0.75	0
7	FUC	A	508	7	10,10,11	0.58	0	14,14,16	0.71	1 (7%)
9	NAG	A	510	9,1	14,14,15	0.55	0	15,19,21	1.17	2 (13%)
9	FUC	A	511	9	10,10,11	0.59	0	14,14,16	0.81	1 (7%)
9	NAG	A	512	9	14,14,15	0.53	0	15,19,21	0.80	0
7	NAG	A	514	1,7	14,14,15	0.77	0	15,19,21	1.33	4 (26%)
7	NAG	A	515	7	14,14,15	0.45	0	15,19,21	0.76	0
7	FUC	A	516	7	10,10,11	0.57	0	14,14,16	0.58	0
12	NAG	B	503	1,12	14,14,15	0.46	0	15,19,21	0.91	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FUC	B	504	12	10,10,11	0.58	0	14,14,16	0.75	0
7	NAG	B	507	1,7	14,14,15	0.56	0	15,19,21	0.99	1 (6%)
7	NAG	B	508	7	14,14,15	0.54	0	15,19,21	1.09	2 (13%)
7	FUC	B	509	7	10,10,11	0.64	0	14,14,16	0.90	0
12	NAG	C	504	1,12	14,14,15	0.57	0	15,19,21	0.86	1 (6%)
12	FUC	C	505	12	10,10,11	0.55	0	14,14,16	0.76	1 (7%)
7	NAG	C	507	1,7	14,14,15	0.65	0	15,19,21	1.09	1 (6%)
7	NAG	C	508	7	14,14,15	0.58	0	15,19,21	1.02	1 (6%)
7	FUC	C	509	7	10,10,11	0.51	0	14,14,16	1.15	1 (7%)
7	NAG	D	505	1,7	14,14,15	0.53	0	15,19,21	0.84	0
7	NAG	D	506	7	14,14,15	0.46	0	15,19,21	1.18	2 (13%)
7	FUC	D	507	7	10,10,11	0.59	0	14,14,16	0.97	0
7	NAG	D	509	1,7	14,14,15	0.45	0	15,19,21	0.72	0
7	NAG	D	510	7	14,14,15	0.63	0	15,19,21	0.95	1 (6%)
7	FUC	D	511	7	10,10,11	0.59	0	14,14,16	0.79	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
7	NAG	A	506	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	507	7	-	0/6/23/26	0/1/1/1
7	FUC	A	508	7	-	0/0/17/20	0/1/1/1
9	NAG	A	510	9,1	-	0/6/23/26	0/1/1/1
9	FUC	A	511	9	-	0/0/17/20	0/1/1/1
9	NAG	A	512	9	-	0/6/23/26	0/1/1/1
7	NAG	A	514	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	515	7	-	0/6/23/26	0/1/1/1
7	FUC	A	516	7	-	0/0/17/20	0/1/1/1
12	NAG	B	503	1,12	-	0/6/23/26	0/1/1/1
12	FUC	B	504	12	-	0/0/17/20	0/1/1/1
7	NAG	B	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	508	7	-	0/6/23/26	0/1/1/1
7	FUC	B	509	7	-	0/0/17/20	0/1/1/1
12	NAG	C	504	1,12	-	0/6/23/26	0/1/1/1
12	FUC	C	505	12	-	0/0/17/20	0/1/1/1
7	NAG	C	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	508	7	-	0/6/23/26	0/1/1/1
7	FUC	C	509	7	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	505	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	506	7	-	0/6/23/26	0/1/1/1
7	FUC	D	507	7	-	0/0/17/20	0/1/1/1
7	NAG	D	509	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	510	7	-	0/6/23/26	0/1/1/1
7	FUC	D	511	7	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	507	NAG	C2-N2-C7	-3.39	118.68	123.04
7	C	508	NAG	C2-N2-C7	-3.21	118.91	123.04
9	A	510	NAG	C2-N2-C7	-2.90	119.32	123.04
7	A	514	NAG	C3-C4-C5	-2.87	105.19	110.20
7	D	510	NAG	C2-N2-C7	-2.81	119.43	123.04
7	B	507	NAG	C2-N2-C7	-2.54	119.78	123.04
7	A	514	NAG	C4-C3-C2	-2.42	107.46	111.23
7	B	508	NAG	C3-C4-C5	-2.18	106.40	110.20
7	D	506	NAG	C4-C3-C2	-2.11	107.95	111.23
7	A	514	NAG	C2-N2-C7	-2.05	120.41	123.04
12	C	504	NAG	C2-N2-C7	-2.02	120.44	123.04
7	A	514	NAG	C1-O5-C5	2.03	114.83	112.25
7	A	508	FUC	O5-C5-C6	2.11	109.61	106.13
12	C	505	FUC	O5-C5-C6	2.19	109.75	106.13
12	B	503	NAG	C1-O5-C5	2.20	115.04	112.25
9	A	511	FUC	O5-C5-C6	2.24	109.83	106.13
7	B	508	NAG	C1-O5-C5	2.48	115.39	112.25
9	A	510	NAG	C1-O5-C5	2.49	115.41	112.25
7	D	506	NAG	C1-O5-C5	2.65	115.61	112.25
7	C	509	FUC	O5-C5-C6	3.06	111.19	106.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	511	FUC	1	0
9	A	512	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	504	NAG	1	0
7	C	507	NAG	1	0
7	D	506	NAG	3	0
7	D	507	FUC	3	0

5.6 Ligand geometry

Of 49 ligands modelled in this entry, 8 are monoatomic - leaving 41 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	0LO	A	503	3,2	13,16,16	0.40	0	17,21,21	1.18	1 (5%)
5	GOL	A	504	-	5,5,5	0.29	0	5,5,5	0.41	0
6	NAG	A	505	1	14,14,15	0.59	0	15,19,21	0.66	0
8	SO4	A	509	-	4,4,4	0.22	0	6,6,6	0.16	0
8	SO4	A	513	-	4,4,4	0.20	0	6,6,6	0.22	0
8	SO4	A	517	-	4,4,4	0.09	0	6,6,6	0.08	0
8	SO4	A	518	-	4,4,4	0.26	0	6,6,6	0.28	0
10	EDO	A	519	-	3,3,3	0.53	0	2,2,2	0.50	0
10	EDO	A	520	-	3,3,3	0.49	0	2,2,2	0.45	0
10	EDO	A	521	-	3,3,3	0.48	0	2,2,2	0.42	0
11	ACT	A	522	-	1,3,3	1.58	0	0,3,3	0.00	-
6	NAG	B	505	1	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
6	NAG	B	506	1	14,14,15	0.49	0	15,19,21	0.65	0
5	GOL	B	510	-	5,5,5	0.31	0	5,5,5	0.68	0
8	SO4	B	511	-	4,4,4	0.09	0	6,6,6	0.19	0
8	SO4	B	512	-	4,4,4	0.11	0	6,6,6	0.09	0
8	SO4	B	513	-	4,4,4	0.10	0	6,6,6	0.10	0
8	SO4	B	514	-	4,4,4	0.12	0	6,6,6	0.20	0
10	EDO	B	515	-	3,3,3	0.50	0	2,2,2	0.36	0
10	EDO	B	516	-	3,3,3	0.50	0	2,2,2	0.38	0
10	EDO	B	517	-	3,3,3	0.42	0	2,2,2	0.64	0
10	EDO	B	518	-	3,3,3	0.44	0	2,2,2	0.51	0
10	EDO	B	519	-	3,3,3	0.59	0	2,2,2	0.24	0
10	EDO	C	501	-	3,3,3	0.48	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	C	502	-	4,4,4	0.17	0	6,6,6	0.15	0
6	NAG	C	503	1	14,14,15	0.48	0	15,19,21	1.19	1 (6%)
6	NAG	C	506	1	14,14,15	0.48	0	15,19,21	1.66	2 (13%)
5	GOL	C	512	-	5,5,5	0.30	0	5,5,5	0.25	0
8	SO4	C	513	-	4,4,4	0.10	0	6,6,6	0.23	0
10	EDO	C	514	-	3,3,3	0.55	0	2,2,2	0.36	0
5	GOL	D	503	-	5,5,5	0.28	0	5,5,5	0.50	0
6	NAG	D	504	1	14,14,15	0.57	0	15,19,21	1.02	1 (6%)
6	NAG	D	508	1	14,14,15	0.54	0	15,19,21	1.45	3 (20%)
5	GOL	D	512	-	5,5,5	0.24	0	5,5,5	0.56	0
5	GOL	D	513	-	5,5,5	0.54	0	5,5,5	0.32	0
5	GOL	D	514	-	5,5,5	0.34	0	5,5,5	0.62	0
8	SO4	D	515	-	4,4,4	0.19	0	6,6,6	0.20	0
10	EDO	D	516	-	3,3,3	0.51	0	2,2,2	0.29	0
10	EDO	D	517	-	3,3,3	0.53	0	2,2,2	0.25	0
10	EDO	D	518	-	3,3,3	0.60	0	2,2,2	0.32	0
11	ACT	D	519	-	1,3,3	1.10	0	0,3,3	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	0LO	A	503	3,2	-	0/4/8/8	0/2/2/2
5	GOL	A	504	-	-	0/4/4/4	0/0/0/0
6	NAG	A	505	1	-	0/6/23/26	0/1/1/1
8	SO4	A	509	-	-	0/0/0/0	0/0/0/0
8	SO4	A	513	-	-	0/0/0/0	0/0/0/0
8	SO4	A	517	-	-	0/0/0/0	0/0/0/0
8	SO4	A	518	-	-	0/0/0/0	0/0/0/0
10	EDO	A	519	-	-	0/1/1/1	0/0/0/0
10	EDO	A	520	-	-	0/1/1/1	0/0/0/0
10	EDO	A	521	-	-	0/1/1/1	0/0/0/0
11	ACT	A	522	-	-	0/0/0/0	0/0/0/0
6	NAG	B	505	1	-	0/6/23/26	0/1/1/1
6	NAG	B	506	1	-	0/6/23/26	0/1/1/1
5	GOL	B	510	-	-	0/4/4/4	0/0/0/0
8	SO4	B	511	-	-	0/0/0/0	0/0/0/0
8	SO4	B	512	-	-	0/0/0/0	0/0/0/0
8	SO4	B	513	-	-	0/0/0/0	0/0/0/0
8	SO4	B	514	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	B	515	-	-	0/1/1/1	0/0/0/0
10	EDO	B	516	-	-	0/1/1/1	0/0/0/0
10	EDO	B	517	-	-	0/1/1/1	0/0/0/0
10	EDO	B	518	-	-	0/1/1/1	0/0/0/0
10	EDO	B	519	-	-	0/1/1/1	0/0/0/0
10	EDO	C	501	-	-	0/1/1/1	0/0/0/0
8	SO4	C	502	-	-	0/0/0/0	0/0/0/0
6	NAG	C	503	1	-	0/6/23/26	0/1/1/1
6	NAG	C	506	1	-	0/6/23/26	0/1/1/1
5	GOL	C	512	-	-	0/4/4/4	0/0/0/0
8	SO4	C	513	-	-	0/0/0/0	0/0/0/0
10	EDO	C	514	-	-	0/1/1/1	0/0/0/0
5	GOL	D	503	-	-	0/4/4/4	0/0/0/0
6	NAG	D	504	1	-	0/6/23/26	0/1/1/1
6	NAG	D	508	1	-	0/6/23/26	0/1/1/1
5	GOL	D	512	-	-	0/4/4/4	0/0/0/0
5	GOL	D	513	-	-	0/4/4/4	0/0/0/0
5	GOL	D	514	-	-	0/4/4/4	0/0/0/0
8	SO4	D	515	-	-	0/0/0/0	0/0/0/0
10	EDO	D	516	-	-	0/1/1/1	0/0/0/0
10	EDO	D	517	-	-	0/1/1/1	0/0/0/0
10	EDO	D	518	-	-	0/1/1/1	0/0/0/0
11	ACT	D	519	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	505	NAG	C2-N2-C7	-3.48	118.57	123.04
6	D	508	NAG	C2-N2-C7	-3.35	118.74	123.04
6	C	506	NAG	C4-C3-C2	-3.28	106.14	111.23
6	D	504	NAG	C2-N2-C7	-3.17	118.96	123.04
6	D	508	NAG	C4-C3-C2	-3.12	106.38	111.23
6	B	505	NAG	C4-C3-C2	-2.97	106.62	111.23
6	D	508	NAG	O3-C3-C2	2.01	113.09	109.11
6	B	505	NAG	C1-O5-C5	2.37	115.25	112.25
4	A	503	0LO	CAH-NAK-CAI	3.12	122.20	117.50
6	C	503	NAG	C1-O5-C5	3.30	116.44	112.25
6	C	506	NAG	C1-O5-C5	4.24	117.63	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	0LO	2	0
10	A	520	EDO	2	0
10	A	521	EDO	8	0
6	B	506	NAG	1	0
8	B	514	SO4	1	0
10	B	519	EDO	1	0
10	C	501	EDO	1	0
6	C	503	NAG	2	0
5	C	512	GOL	4	0
5	D	503	GOL	2	0
5	D	512	GOL	4	0
10	D	516	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	425/426 (99%)	-0.76	2 (0%)	91	94	15, 22, 38, 63	0
1	B	426/426 (100%)	-0.67	7 (1%)	74	80	16, 27, 45, 83	0
1	C	423/426 (99%)	-0.66	2 (0%)	91	94	18, 27, 43, 75	1 (0%)
1	D	426/426 (100%)	-0.67	7 (1%)	74	80	15, 25, 42, 76	1 (0%)
All	All	1700/1704 (99%)	-0.69	18 (1%)	82	86	15, 25, 42, 83	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	SER	4.8
1	C	64	ASN	4.1
1	B	63	LYS	4.0
1	D	64	ASN	4.0
1	B	432	THR	3.9
1	B	64	ASN	3.8
1	D	432	THR	3.8
1	D	431	SER	3.2
1	D	63	LYS	3.2
1	B	66	ARG	2.9
1	A	429	ASP	2.7
1	C	63	LYS	2.7
1	D	65	GLY	2.6
1	B	65	GLY	2.6
1	B	7	LYS	2.4
1	D	186	THR	2.2
1	B	431	SER	2.2
1	D	66	ARG	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)

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
7	NAG	A	506	14/15	0.93	0.12	0.96	35,44,53,53	0
7	NAG	C	507	14/15	0.97	0.11	0.70	29,36,43,47	0
7	NAG	D	509	14/15	0.96	0.10	-0.24	28,37,42,44	0
7	FUC	D	507	10/11	0.81	0.37	-	63,74,80,81	0
9	NAG	A	510	14/15	0.93	0.12	-	36,46,57,62	0
12	NAG	B	503	14/15	0.89	0.20	-	37,53,63,72	0
7	NAG	A	514	14/15	0.96	0.09	-	24,29,35,37	0
7	NAG	B	507	14/15	0.96	0.09	-	24,31,36,39	0
7	FUC	D	511	10/11	0.89	0.26	-	38,53,60,60	0
9	NAG	A	512	14/15	0.89	0.35	-	60,66,74,76	0
9	FUC	A	511	10/11	0.91	0.23	-	54,59,64,64	0
7	NAG	D	506	14/15	0.77	0.39	-	73,82,90,90	0
12	FUC	C	505	10/11	0.89	0.34	-	64,72,78,78	0
7	NAG	A	515	14/15	0.95	0.17	-	29,34,38,38	0
7	NAG	D	510	14/15	0.91	0.27	-	37,52,62,66	0
7	FUC	B	509	10/11	0.96	0.19	-	30,37,42,51	0
12	FUC	B	504	10/11	0.76	0.35	-	67,73,80,80	0
7	NAG	A	507	14/15	0.89	0.30	-	47,60,65,70	0
7	FUC	A	516	10/11	0.96	0.23	-	33,37,39,40	0
7	NAG	D	505	14/15	0.91	0.20	-	44,57,70,75	0
7	NAG	B	508	14/15	0.92	0.17	-	31,41,47,48	0
7	NAG	C	508	14/15	0.82	0.36	-	37,55,71,74	0
12	NAG	C	504	14/15	0.88	0.19	-	41,57,68,70	0
7	FUC	C	509	10/11	0.84	0.21	-	49,57,62,63	0
7	FUC	A	508	10/11	0.94	0.36	-	61,63,67,68	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
8	SO4	D	515	5/5	0.94	0.38	17.75	34,49,62,67	0
4	0LO	A	503	15/15	0.83	0.26	11.18	30,43,64,65	0
6	NAG	D	508	14/15	0.93	0.18	8.12	43,52,60,66	0
6	NAG	C	506	14/15	0.93	0.18	8.02	39,43,49,54	0
10	EDO	C	514	4/4	0.90	0.30	7.60	41,43,48,49	0
10	EDO	D	516	4/4	0.91	0.20	5.41	34,40,43,44	0
5	GOL	D	512	6/6	0.91	0.20	5.31	33,38,39,41	0
6	NAG	B	505	14/15	0.87	0.17	4.45	45,50,60,64	0
10	EDO	D	518	4/4	0.95	0.17	3.07	31,35,36,38	0
10	EDO	B	519	4/4	0.86	0.19	2.80	45,46,52,53	0
8	SO4	A	513	5/5	0.93	0.24	2.75	29,37,55,74	0
8	SO4	A	518	5/5	0.84	0.22	2.13	35,47,64,74	0
6	NAG	C	503	14/15	0.93	0.14	1.89	33,38,46,46	0
6	NAG	B	506	14/15	0.94	0.14	1.51	31,39,49,51	0
5	GOL	D	513	6/6	0.88	0.17	1.32	29,37,50,54	0
6	NAG	A	505	14/15	0.96	0.13	1.29	23,29,37,42	0
10	EDO	B	516	4/4	0.93	0.12	0.99	28,39,40,41	0
5	GOL	B	510	6/6	0.93	0.14	0.66	37,43,48,50	0
6	NAG	D	504	14/15	0.95	0.10	-0.01	31,37,46,47	0
5	GOL	C	512	6/6	0.84	0.15	-0.48	56,56,61,64	0
10	EDO	A	519	4/4	0.95	0.08	-0.87	29,32,32,42	0
5	GOL	A	504	6/6	0.98	0.06	-0.99	22,25,27,28	0
3	FE	D	502	1/1	0.99	0.06	-1.11	28,28,28,28	1
2	ZN	D	501	1/1	0.99	0.04	-1.26	24,24,24,24	1
8	SO4	A	509	5/5	0.99	0.06	-1.44	30,35,36,40	0
3	FE	B	502	1/1	1.00	0.05	-1.72	29,29,29,29	1
3	FE	A	502	1/1	0.99	0.05	-1.79	23,23,23,23	1
2	ZN	C	510	1/1	1.00	0.04	-2.64	25,25,25,25	1
3	FE	C	511	1/1	0.98	0.04	-2.82	32,32,32,32	1
2	ZN	A	501	1/1	1.00	0.03	-2.88	28,28,28,28	0
2	ZN	B	501	1/1	1.00	0.03	-4.76	27,27,27,27	0
8	SO4	B	512	5/5	0.96	0.36	-	62,68,82,86	0
10	EDO	B	515	4/4	0.92	0.18	-	52,56,59,61	0
11	ACT	D	519	4/4	0.93	0.17	-	34,50,51,52	0
8	SO4	B	511	5/5	0.95	0.28	-	55,58,71,75	0
5	GOL	D	503	6/6	0.93	0.12	-	36,39,41,44	0
8	SO4	C	502	5/5	0.95	0.34	-	81,86,91,99	0
11	ACT	A	522	4/4	0.84	0.21	-	51,56,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	SO4	C	513	5/5	0.97	0.28	-	48,58,71,79	0
8	SO4	B	514	5/5	0.95	0.35	-	51,52,62,71	0
10	EDO	C	501	4/4	0.88	0.18	-	44,45,47,53	0
10	EDO	D	517	4/4	0.88	0.22	-	49,51,52,54	0
10	EDO	A	520	4/4	0.94	0.24	-	36,48,51,55	0
10	EDO	A	521	4/4	0.96	0.21	-	30,30,39,49	0
10	EDO	B	517	4/4	0.92	0.25	-	54,55,57,68	0
8	SO4	A	517	5/5	0.97	0.39	-	54,57,59,78	0
8	SO4	B	513	5/5	0.96	0.33	-	43,70,79,86	0
5	GOL	D	514	6/6	0.81	0.20	-	36,46,49,52	0
10	EDO	B	518	4/4	0.90	0.21	-	58,66,67,73	0

6.5 Other polymers

There are no such residues in this entry.