Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:59 PM GMT

PDB ID	:	1W21
Title	:	STRUCTURE OF NEURAMINIDASE FROM ENGLISH DUCK SUBTYPE N6 COMPLEXED WITH 30 MM SIALIC ACID (NANA, NEU5AC), CRYSTAL SOAKED FOR 43 HOURS AT 291 K.
Authors	:	Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on	:	2004-06-25
Resolution	:	2.08 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:

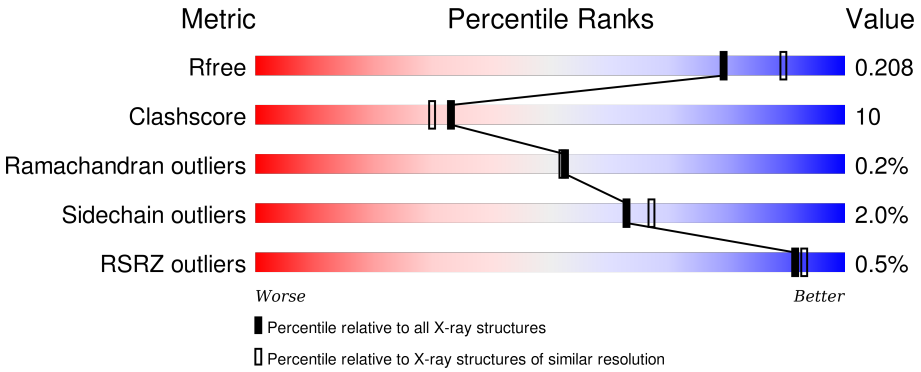
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.08 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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	389	86% 13%
1	B	389	% 86% 11%
1	C	389	% 85% 13%
1	D	389	85% 12%

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
2	SIA	A	1477	-	-	-	X
2	SIA	A	1478	-	-	-	X
2	SIA	B	2478	-	-	-	X
2	SIA	C	3477	-	-	-	X
2	SIA	C	3478	-	-	-	X
2	SIA	D	4478	-	-	-	X
3	GOL	A	1479	-	X	-	X
3	GOL	B	2479	-	X	-	X
3	GOL	C	3479	-	X	-	X
3	GOL	D	4479	-	X	-	X
4	NAG	A	1482	-	-	-	X
4	NAG	B	2481	-	-	-	X
4	NAG	B	2482	-	-	X	X
4	NAG	C	3480	-	-	-	X
4	NAG	C	3482	-	-	-	X
4	NAG	C	3483	-	-	X	X
5	BMA	A	1484	-	-	X	-
5	BMA	C	3484	-	-	X	-
6	MAN	A	1485	-	-	X	X
6	MAN	A	1486	-	-	-	X
6	MAN	A	1487	-	-	-	X
6	MAN	C	3487	-	-	-	X
6	MAN	C	3488	-	-	-	X
6	MAN	C	3489	-	-	-	X
7	CA	A	1488	-	-	-	X
7	CA	B	2487	-	-	-	X
7	CA	C	3491	-	-	-	X
7	CA	D	4481	-	-	-	X

2 Entry composition

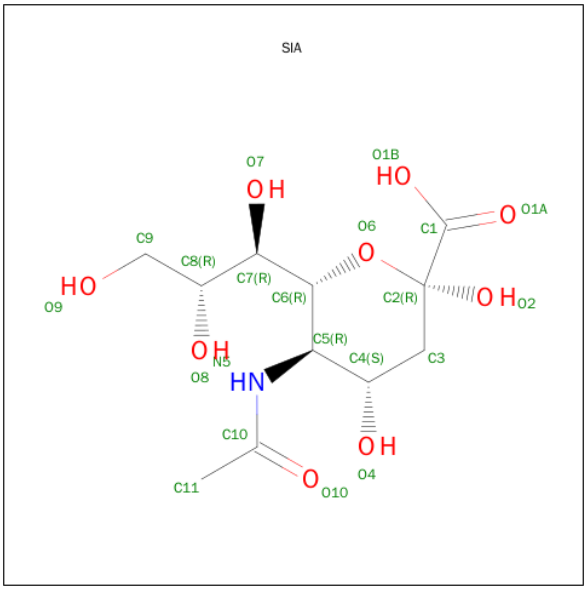
There are 8 unique types of molecules in this entry. The entry contains 14285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	B	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	C	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

- Molecule 2 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	A	1	Total	C	N	O	0	0
			21	11	1	9		

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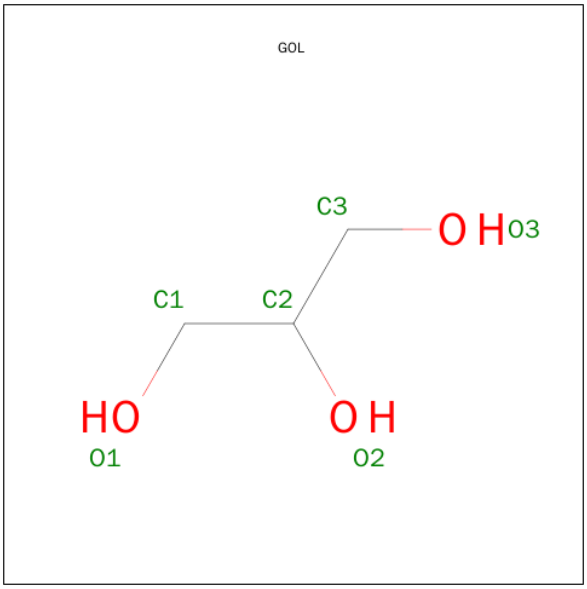
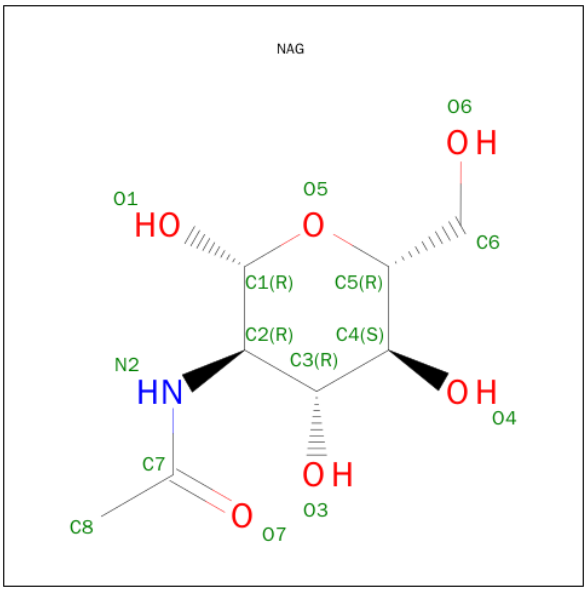
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 21 11 1 9	0	0
2	B	1	Total C N O 21 11 1 9	0	0
2	C	1	Total C N O 21 11 1 9	0	0
2	C	1	Total C N O 21 11 1 9	0	0
2	D	1	Total C N O 21 11 1 9	0	0
2	D	1	Total C N O 21 11 1 9	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



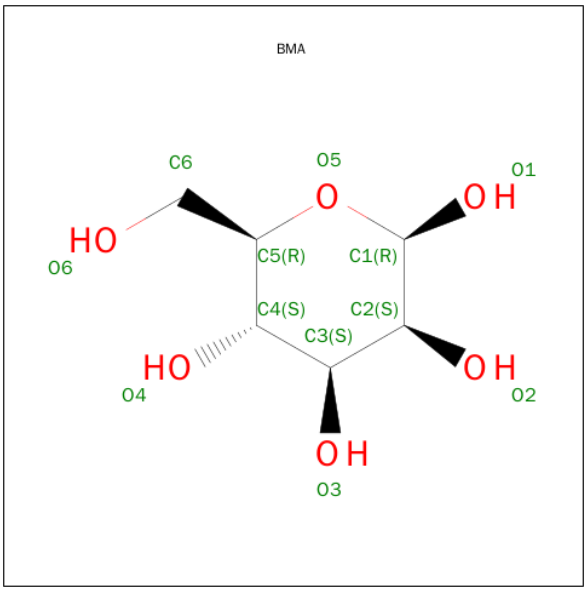
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



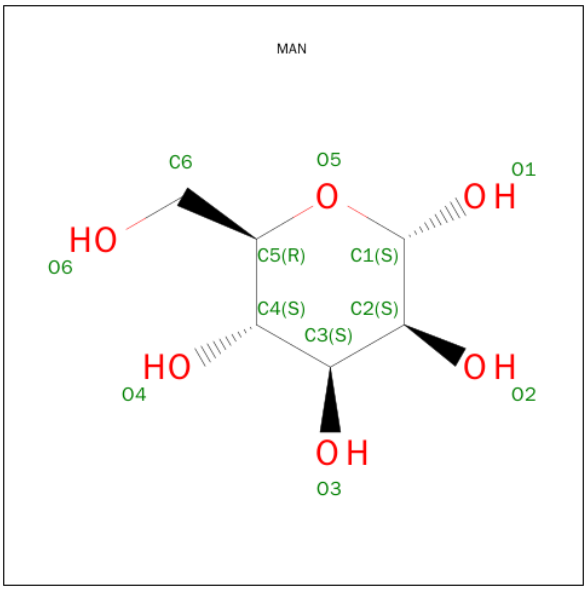
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total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

- Molecule 5 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	429	Total O 429 429	0	0
8	B	413	Total O 413 413	0	0
8	C	426	Total O 426 426	0	0

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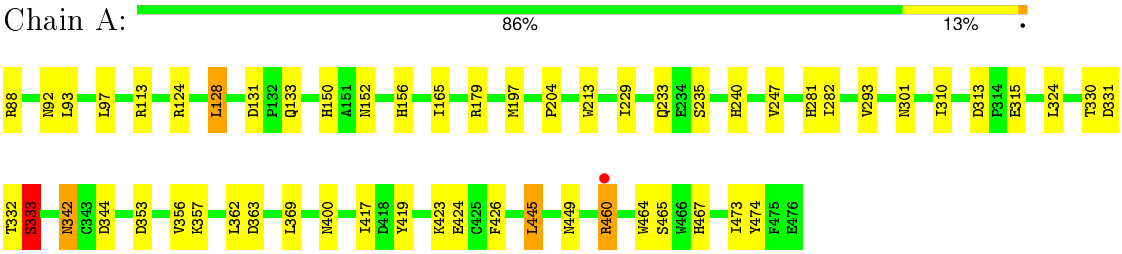
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	455	Total 455	O 455	0	0

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.

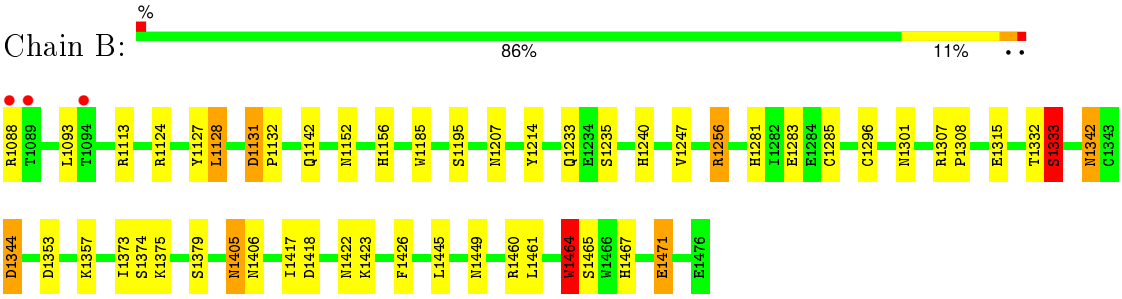
- Molecule 1: NEURAMINIDASE

Chain A:



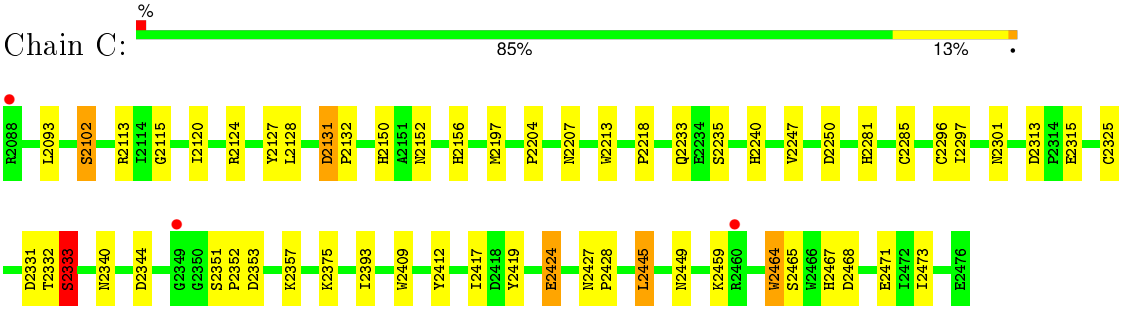
- Molecule 1: NEURAMINIDASE

Chain B:



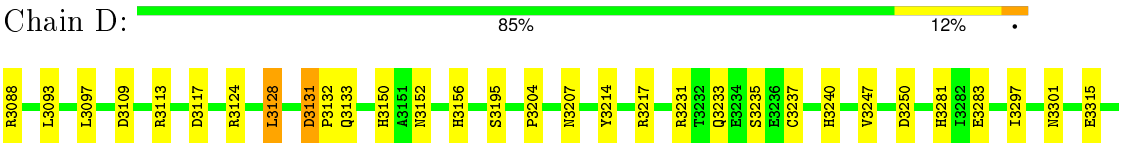
- Molecule 1: NEURAMINIDASE

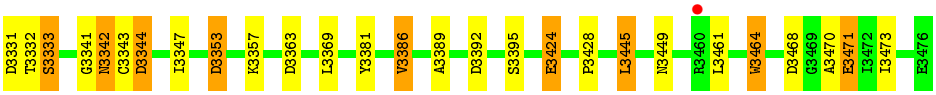
Chain C:



- Molecule 1: NEURAMINIDASE

Chain D:




D3331
T3332
S3333
G3341
N3342
C3343
D3344
I3347
D3353
K3357
D3363
L3369
Y3381
V3386
A3389
D3392
S3395
E3424
P3428
L3445
N3449
R3460
L3461
W3464
D3468
G3469
A3470
E3471
I3472
I3473
E3476

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.48Å 74.00Å 106.47Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	30.43 – 2.08 29.41 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.43-2.08) 98.0 (29.41-2.08)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.150 , 0.195 0.161 , 0.208	Depositor DCC
R_{free} test set	4913 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	1.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.2	EDS
Estimated twinning fraction	0.008 for -l,k,h 0.021 for -h,-k,l 0.015 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 98271 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14285	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, BMA, NAG, CA, SIA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.05	1/3083 (0.0%)	0.89	6/4185 (0.1%)
1	B	1.03	2/3083 (0.1%)	0.89	5/4185 (0.1%)
1	C	1.03	1/3083 (0.0%)	0.90	7/4185 (0.2%)
1	D	1.06	3/3084 (0.1%)	0.93	12/4185 (0.3%)
All	All	1.04	7/12333 (0.1%)	0.90	30/16740 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3471	GLU	CD-OE2	6.73	1.33	1.25
1	B	1471	GLU	CD-OE2	6.62	1.32	1.25
1	C	2102	SER	CB-OG	-5.53	1.35	1.42
1	A	474	TYR	CE1-CZ	5.38	1.45	1.38
1	D	3217	ARG	CZ-NH2	5.09	1.39	1.33
1	D	3381	TYR	CD1-CE1	5.03	1.46	1.39
1	B	1464	TRP	CE3-CZ3	5.00	1.47	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3250	ASP	CB-CG-OD2	9.23	126.61	118.30
1	B	1344	ASP	CB-CG-OD2	7.47	125.02	118.30
1	B	1333	SER	N-CA-C	-7.36	91.13	111.00
1	C	2131	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	2333	SER	N-CA-C	-7.28	91.34	111.00
1	C	2250	ASP	CB-CG-OD2	7.14	124.72	118.30
1	D	3131	ASP	CB-CG-OD2	7.13	124.71	118.30
1	A	313	ASP	CB-CG-OD2	6.75	124.37	118.30
1	D	3468	ASP	CB-CG-OD2	6.65	124.28	118.30
1	D	3344	ASP	CB-CG-OD2	6.37	124.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	333	SER	N-CA-C	-5.94	94.96	111.00
1	D	3333	SER	N-CA-C	-5.93	94.99	111.00
1	C	2313	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	2331	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	3353	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	2468	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	333	SER	CB-CA-C	5.56	120.67	110.10
1	C	2344	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	1131	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	1128	LEU	CB-CG-CD2	5.42	120.22	111.00
1	D	3128	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	131	ASP	CB-CG-OD2	5.36	123.13	118.30
1	D	3128	LEU	CB-CG-CD2	5.34	120.07	111.00
1	D	3363	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	331	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	3109	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	3392	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	1418	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	3331	ASP	CB-CG-OD1	5.04	122.84	118.30

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	3008	0	2888	50	0
1	B	3008	0	2888	54	0
1	C	3008	0	2888	51	0
1	D	3009	0	2888	55	0
2	A	42	0	36	4	0
2	B	42	0	36	4	0
2	C	42	0	36	4	0
2	D	42	0	36	4	0
3	A	6	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	4	1	0
3	C	6	0	4	1	0
3	D	6	0	4	1	0
4	A	56	0	51	15	0
4	B	42	0	39	13	0
4	C	56	0	52	15	0
4	D	14	0	13	3	0
5	A	11	0	10	6	0
5	B	11	0	10	3	0
5	C	22	0	20	10	0
6	A	33	0	30	6	0
6	B	33	0	30	2	0
6	C	55	0	50	10	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	429	0	0	5	0
8	B	413	0	0	13	0
8	C	426	0	0	8	0
8	D	455	0	0	7	0
All	All	14285	0	12017	247	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.

All (247) 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:A:92:ASN:HD21	4:A:1480:NAG:C1	1.16	1.52
1:B:1152:ASN:HD21	4:B:2480:NAG:C1	1.35	1.38
1:C:2152:ASN:HD21	4:C:3481:NAG:C1	1.37	1.37
1:A:152:ASN:HD21	4:A:1481:NAG:C1	1.46	1.26
1:D:3152:ASN:HD21	4:D:4480:NAG:C1	1.62	1.12
1:B:1152:ASN:ND2	4:B:2480:NAG:C1	2.19	1.05
1:C:2152:ASN:ND2	4:C:3481:NAG:C1	2.19	1.05
1:A:152:ASN:ND2	4:A:1481:NAG:C1	2.22	1.01
6:B:2484:MAN:O6	6:B:2485:MAN:C1	2.09	1.00
1:D:3152:ASN:ND2	4:D:4480:NAG:C1	2.30	0.94
4:C:3482:NAG:HO4	4:C:3483:NAG:C1	1.62	0.94
1:B:1373:ILE:HB	8:B:2328:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2093:LEU:H	1:C:2240:HIS:HD2	1.03	0.91
4:B:2481:NAG:O3	8:B:2405:HOH:O	1.72	0.90
1:D:3093:LEU:H	1:D:3240:HIS:HD2	1.21	0.88
1:B:1471:GLU:H	1:D:3150:HIS:HE1	1.17	0.88
1:C:2093:LEU:H	1:C:2240:HIS:CD2	1.90	0.88
1:A:150:HIS:HE1	1:C:2471:GLU:H	1.18	0.88
4:A:1483:NAG:H2	1:B:1207:ASN:HD21	1.39	0.87
1:B:1406:ASN:ND2	8:B:2328:HOH:O	2.06	0.87
1:A:93:LEU:H	1:A:240:HIS:HD2	1.23	0.87
4:A:1483:NAG:H2	1:B:1207:ASN:ND2	1.91	0.86
1:B:1093:LEU:H	1:B:1240:HIS:HD2	1.20	0.85
6:A:1485:MAN:O6	6:A:1486:MAN:C1	2.25	0.84
1:D:3386:VAL:HG22	1:D:3389:ALA:HB2	1.60	0.84
1:C:2150:HIS:HE1	1:D:3471:GLU:H	1.26	0.83
1:C:2281:HIS:HD2	1:C:2301:ASN:H	1.28	0.82
1:D:3233:GLN:HE21	1:D:3247:VAL:H	1.29	0.80
1:B:1233:GLN:HE21	1:B:1247:VAL:H	1.27	0.79
1:C:2233:GLN:HE21	1:C:2247:VAL:H	1.31	0.77
1:B:1281:HIS:HD2	1:B:1301:ASN:H	1.35	0.75
6:A:1485:MAN:O3	6:A:1487:MAN:C1	2.34	0.74
4:B:2481:NAG:O4	5:B:2483:BMA:C1	2.36	0.73
1:A:233:GLN:HE21	1:A:247:VAL:H	1.35	0.73
1:D:3281:HIS:HD2	1:D:3301:ASN:H	1.35	0.73
4:A:1483:NAG:C2	1:B:1207:ASN:HD21	2.02	0.73
4:C:3482:NAG:C4	4:C:3483:NAG:C1	2.67	0.71
1:B:1283:GLU:CG	8:B:2218:HOH:O	2.38	0.70
1:C:2207:ASN:ND2	4:C:3482:NAG:C1	2.55	0.69
1:A:281:HIS:HD2	1:A:301:ASN:H	1.36	0.69
1:D:3342:ASN:ND2	1:D:3344:ASP:H	1.91	0.69
6:C:3487:MAN:H3	6:C:3489:MAN:C1	2.23	0.69
6:C:3487:MAN:C3	6:C:3489:MAN:C1	2.71	0.69
4:B:2481:NAG:C1	4:B:2482:NAG:C4	2.72	0.68
1:B:1283:GLU:OE2	8:B:2218:HOH:O	2.11	0.68
1:C:2332:THR:O	1:C:2333:SER:HB2	1.94	0.68
1:A:93:LEU:H	1:A:240:HIS:CD2	2.11	0.68
1:B:1283:GLU:CD	8:B:2218:HOH:O	2.32	0.67
1:D:3093:LEU:H	1:D:3240:HIS:CD2	2.10	0.67
1:D:3471:GLU:HG3	1:D:3473:ILE:HG22	1.75	0.67
4:B:2481:NAG:O4	5:B:2483:BMA:O5	2.13	0.66
1:A:424:GLU:H	1:A:424:GLU:CD	1.98	0.66
1:D:3283:GLU:OE1	8:D:2256:HOH:O	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3483:NAG:O4	5:C:3490:BMA:C1	2.44	0.65
1:A:342:ASN:ND2	1:A:344:ASP:H	1.95	0.65
1:B:1379:SER:HB2	2:B:2478:SIA:H112	1.79	0.65
4:A:1482:NAG:O4	5:A:1484:BMA:C1	2.45	0.65
1:A:342:ASN:HD22	1:A:344:ASP:H	1.44	0.65
1:D:3342:ASN:HD22	1:D:3344:ASP:H	1.45	0.64
6:C:3487:MAN:O6	6:C:3488:MAN:C1	2.45	0.64
1:A:423:LYS:HE3	8:A:2347:HOH:O	1.98	0.64
1:C:2233:GLN:NE2	1:C:2247:VAL:H	1.95	0.64
1:B:1405:ASN:C	1:B:1405:ASN:HD22	2.02	0.64
1:D:3424:GLU:H	1:D:3424:GLU:CD	2.00	0.63
1:D:3333:SER:CB	1:D:3353:ASP:O	2.46	0.63
1:B:1093:LEU:H	1:B:1240:HIS:CD2	2.10	0.63
1:D:3333:SER:HB2	1:D:3353:ASP:O	1.98	0.63
5:B:2483:BMA:O6	6:B:2484:MAN:C1	2.46	0.63
1:C:2093:LEU:N	1:C:2240:HIS:HD2	1.87	0.63
1:A:150:HIS:CE1	1:C:2471:GLU:H	2.09	0.62
1:A:460:ARG:HD2	8:A:2419:HOH:O	1.98	0.62
4:A:1483:NAG:C1	1:B:1207:ASN:HD21	2.14	0.61
1:D:3283:GLU:CD	8:D:2256:HOH:O	2.39	0.61
1:C:2204:PRO:HD3	1:D:3464:TRP:HB3	1.81	0.61
1:A:124:ARG:HA	1:A:449:ASN:ND2	2.15	0.61
1:B:1375:LYS:NZ	8:B:2300:HOH:O	2.32	0.61
1:A:473:ILE:HG12	8:A:2389:HOH:O	2.00	0.61
4:B:2482:NAG:C1	1:D:3207:ASN:OD1	2.49	0.61
1:D:3332:THR:O	1:D:3333:SER:HB2	2.00	0.61
3:A:1479:GOL:H32	1:C:2113:ARG:NH2	2.16	0.61
1:C:2424:GLU:CD	1:C:2424:GLU:H	2.03	0.60
6:C:3487:MAN:O3	6:C:3489:MAN:C1	2.49	0.60
1:B:1342:ASN:HD22	1:B:1344:ASP:H	1.48	0.60
1:A:293:VAL:HG22	8:A:2224:HOH:O	2.02	0.60
2:A:1478:SIA:H6	2:A:1478:SIA:O1A	2.00	0.59
1:B:1127:TYR:CG	1:B:1235:SER:HA	2.37	0.59
1:B:1342:ASN:ND2	1:B:1344:ASP:H	2.01	0.59
1:A:467:HIS:H	1:A:467:HIS:CD2	2.20	0.58
1:C:2150:HIS:CE1	1:D:3471:GLU:H	2.15	0.58
1:C:2465:SER:OG	1:C:2467:HIS:HD2	1.86	0.58
1:D:3283:GLU:CG	8:D:2256:HOH:O	2.51	0.58
1:A:445:LEU:HD21	4:A:1481:NAG:H82	1.86	0.58
1:B:1333:SER:CB	1:B:1353:ASP:O	2.51	0.58
1:B:1131:ASP:HB2	1:B:1132:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1484:BMA:O6	6:A:1485:MAN:C1	2.52	0.57
1:D:3281:HIS:CD2	1:D:3301:ASN:H	2.17	0.57
1:B:1379:SER:OG	1:B:1406:ASN:ND2	2.38	0.56
1:B:1379:SER:HB2	2:B:2478:SIA:C11	2.36	0.56
1:B:1465:SER:OG	1:B:1467:HIS:HD2	1.88	0.56
4:A:1482:NAG:O4	5:A:1484:BMA:O5	2.22	0.56
1:C:2409:TRP:CZ3	2:C:3478:SIA:H112	2.41	0.56
4:C:3483:NAG:HO4	5:C:3490:BMA:C1	2.18	0.56
1:C:2281:HIS:CD2	1:C:2301:ASN:H	2.17	0.55
3:C:3479:GOL:H32	1:D:3113:ARG:NH2	2.21	0.55
5:C:3484:BMA:O3	6:C:3485:MAN:C1	2.54	0.55
1:B:1113:ARG:NH2	3:D:4479:GOL:H32	2.21	0.55
1:B:1461:LEU:O	4:B:2482:NAG:H62	2.07	0.55
1:B:1156:HIS:HB2	8:B:2083:HOH:O	2.06	0.55
4:B:2482:NAG:C1	1:D:3207:ASN:CG	2.76	0.55
1:B:1283:GLU:HG3	8:B:2218:HOH:O	2.05	0.54
1:B:1460:ARG:NH1	8:B:2368:HOH:O	2.37	0.54
1:C:2409:TRP:CE3	2:C:3478:SIA:H112	2.43	0.54
1:A:332:THR:O	1:A:333:SER:HB2	2.08	0.54
1:C:2150:HIS:HE1	1:D:3471:GLU:N	2.03	0.54
1:D:3088:ARG:NH2	1:D:3133:GLN:OE1	2.39	0.54
2:A:1477:SIA:H5	2:A:1477:SIA:O2	2.09	0.53
4:C:3483:NAG:C4	5:C:3490:BMA:C1	2.87	0.53
1:D:3369:LEU:HG	1:D:3386:VAL:HG13	1.89	0.53
2:B:2477:SIA:O2	2:B:2477:SIA:H5	2.09	0.53
4:A:1483:NAG:C2	1:B:1207:ASN:ND2	2.67	0.53
1:B:1256:ARG:HD3	8:B:2191:HOH:O	2.08	0.53
4:B:2482:NAG:C7	1:D:3207:ASN:HD21	2.21	0.53
2:D:4477:SIA:O2	2:D:4477:SIA:H5	2.09	0.53
1:A:156:HIS:HB2	8:A:2068:HOH:O	2.07	0.53
2:C:3477:SIA:O2	2:C:3477:SIA:H5	2.09	0.53
1:B:1471:GLU:H	1:D:3150:HIS:CE1	2.10	0.52
1:D:3342:ASN:HD22	1:D:3342:ASN:C	2.12	0.52
1:A:92:ASN:CG	4:A:1480:NAG:C1	2.74	0.52
1:A:424:GLU:N	1:A:424:GLU:CD	2.63	0.52
1:C:2297:ILE:HD12	1:C:2297:ILE:N	2.25	0.52
4:A:1482:NAG:C4	5:A:1484:BMA:C1	2.88	0.52
1:A:342:ASN:C	1:A:342:ASN:HD22	2.14	0.51
1:C:2235:SER:HB3	1:C:2357:LYS:HE2	1.92	0.51
1:B:1333:SER:HB3	1:B:1353:ASP:O	2.10	0.51
1:B:1423:LYS:HE2	8:D:2190:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3204:PRO:HG2	1:D:3207:ASN:HB2	1.93	0.51
1:D:3233:GLN:NE2	1:D:3247:VAL:H	2.02	0.51
1:B:1332:THR:O	1:B:1333:SER:HB2	2.10	0.51
2:D:4478:SIA:O1A	2:D:4478:SIA:H6	2.09	0.51
5:C:3484:BMA:C3	6:C:3485:MAN:C1	2.89	0.50
1:A:333:SER:CB	1:A:353:ASP:O	2.59	0.50
1:B:1195:SER:HB2	1:B:1214:TYR:CZ	2.47	0.50
4:A:1482:NAG:H4	5:A:1484:BMA:C1	2.42	0.50
1:A:235:SER:HB3	1:A:357:LYS:HE2	1.93	0.50
1:D:3231:ARG:NE	1:D:3283:GLU:OE2	2.42	0.49
1:A:333:SER:HB2	1:A:353:ASP:O	2.11	0.49
1:C:2124:ARG:HA	1:C:2449:ASN:ND2	2.27	0.49
6:A:1485:MAN:O3	6:A:1487:MAN:H5	2.11	0.49
6:C:3486:MAN:H62	8:C:3417:HOH:O	2.11	0.49
1:D:3471:GLU:OE2	1:D:3473:ILE:HG22	2.12	0.49
1:A:465:SER:OG	1:A:467:HIS:HD2	1.94	0.49
1:B:1333:SER:HB2	1:B:1353:ASP:O	2.12	0.49
1:D:3471:GLU:CG	1:D:3473:ILE:HG22	2.42	0.49
1:C:2333:SER:CB	1:C:2353:ASP:O	2.61	0.49
1:C:2240:HIS:HE1	1:C:2315:GLU:OE1	1.95	0.49
2:D:4477:SIA:O2	2:D:4477:SIA:C5	2.59	0.49
4:C:3480:NAG:C4	5:C:3484:BMA:C1	2.91	0.48
1:D:3333:SER:HB3	1:D:3353:ASP:O	2.13	0.48
2:A:1477:SIA:C5	2:A:1477:SIA:O2	2.59	0.48
1:C:2375:LYS:HG2	8:C:3306:HOH:O	2.13	0.48
1:D:3235:SER:HB3	1:D:3357:LYS:HE2	1.95	0.48
1:A:324:LEU:HD21	1:A:362:LEU:HD21	1.96	0.48
1:A:93:LEU:N	1:A:240:HIS:HD2	2.03	0.48
1:A:240:HIS:HE1	1:A:315:GLU:OE2	1.96	0.48
1:A:417:ILE:HG21	1:A:426:PHE:HB3	1.95	0.48
1:C:2127:TYR:CG	1:C:2235:SER:HA	2.49	0.47
1:B:1156:HIS:CE1	8:B:2082:HOH:O	2.66	0.47
1:D:3097:LEU:HD22	1:D:3428:PRO:HG3	1.96	0.47
1:A:460:ARG:O	1:A:460:ARG:HG3	2.14	0.47
1:D:3283:GLU:HG3	8:D:2256:HOH:O	2.14	0.47
1:B:1285:CYS:HB3	1:B:1296:CYS:HB3	1.97	0.47
1:B:1445:LEU:HD11	4:B:2480:NAG:H82	1.96	0.47
1:D:3131:ASP:HB2	1:D:3132:PRO:CD	2.44	0.47
1:C:2473:ILE:HG12	8:C:3386:HOH:O	2.13	0.47
1:D:3341:GLY:HA2	1:D:3347:ILE:HD11	1.96	0.47
2:B:2478:SIA:O1A	2:B:2478:SIA:H6	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1374:SER:N	8:B:2328:HOH:O	2.44	0.46
1:B:1281:HIS:CD2	1:B:1301:ASN:H	2.23	0.46
1:B:1342:ASN:C	1:B:1342:ASN:HD22	2.18	0.46
1:C:2333:SER:HB2	1:C:2353:ASP:O	2.15	0.46
1:A:417:ILE:HB	1:A:419:TYR:CZ	2.51	0.46
1:D:3445:LEU:HD21	4:D:4480:NAG:H82	1.98	0.46
4:B:2481:NAG:H83	4:B:2482:NAG:O4	2.15	0.46
1:D:3240:HIS:HE1	1:D:3315:GLU:OE1	1.99	0.45
4:C:3482:NAG:H62	1:D:3461:LEU:O	2.15	0.45
1:D:3131:ASP:HB2	1:D:3132:PRO:HD2	1.96	0.45
1:C:2207:ASN:CG	4:C:3482:NAG:C1	2.84	0.45
1:C:2417:ILE:HB	1:C:2419:TYR:CZ	2.52	0.45
5:C:3484:BMA:H3	6:C:3485:MAN:C1	2.47	0.45
1:A:330:THR:HG21	1:A:369:LEU:HB3	1.99	0.45
4:A:1482:NAG:HO4	5:A:1484:BMA:C1	2.25	0.44
1:C:2115:GLY:HA2	1:C:2120:ILE:HG12	1.99	0.44
1:D:3117:ASP:O	1:D:3117:ASP:CG	2.55	0.44
1:B:1235:SER:HB3	1:B:1357:LYS:HE2	1.98	0.44
1:C:2102:SER:HB2	1:C:2459:LYS:O	2.18	0.44
1:A:400:ASN:HB3	6:A:1485:MAN:C1	2.48	0.44
2:D:4477:SIA:O2	2:D:4477:SIA:O7	2.30	0.44
1:C:2427:ASN:HA	1:C:2428:PRO:HD3	1.88	0.44
1:B:1417:ILE:HG21	1:B:1426:PHE:HB3	1.99	0.44
1:A:97:LEU:HD12	1:A:363:ASP:HB2	1.99	0.44
1:C:2150:HIS:CE1	1:D:3470:ALA:HA	2.52	0.43
1:C:2285:CYS:HB3	1:C:2296:CYS:HB3	1.99	0.43
1:A:229:ILE:O	1:A:229:ILE:HG22	2.18	0.43
4:B:2481:NAG:C1	4:B:2482:NAG:H4	2.48	0.43
1:D:3297:ILE:HD12	1:D:3297:ILE:N	2.32	0.43
1:D:3124:ARG:HA	1:D:3449:ASN:ND2	2.33	0.43
1:B:1124:ARG:HA	1:B:1449:ASN:ND2	2.34	0.43
1:B:1240:HIS:HE1	1:B:1315:GLU:OE2	2.02	0.43
1:C:2150:HIS:HD2	8:D:2089:HOH:O	2.01	0.43
1:C:2156:HIS:CE1	8:C:3097:HOH:O	2.71	0.43
1:C:2445:LEU:HD21	4:C:3481:NAG:H82	2.01	0.43
1:C:2357:LYS:HB3	1:C:2412:TYR:CG	2.54	0.43
1:B:1467:HIS:CD2	1:B:1467:HIS:H	2.36	0.42
4:C:3480:NAG:HO4	5:C:3484:BMA:C1	2.24	0.42
1:A:150:HIS:HE1	1:C:2471:GLU:N	2.00	0.42
1:A:233:GLN:NE2	1:A:247:VAL:H	2.11	0.42
1:D:3342:ASN:HD22	1:D:3343:CYS:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2131:ASP:HB2	1:C:2132:PRO:CD	2.50	0.42
2:C:3477:SIA:C5	2:C:3477:SIA:O2	2.59	0.42
6:A:1485:MAN:C3	6:A:1487:MAN:C1	2.97	0.42
6:C:3485:MAN:O2	6:C:3486:MAN:C1	2.68	0.42
1:A:235:SER:HB3	1:A:357:LYS:CE	2.50	0.42
4:C:3483:NAG:O3	8:C:3412:HOH:O	2.21	0.42
1:D:3386:VAL:HG23	1:D:3395:SER:HB2	2.01	0.42
1:C:2325:CYS:O	1:C:2393:ILE:HA	2.19	0.41
1:C:2351:SER:HA	1:C:2352:PRO:HA	1.78	0.41
3:A:1479:GOL:H32	1:C:2113:ARG:HH22	1.82	0.41
1:B:1464:TRP:HB3	1:D:3204:PRO:HD3	2.03	0.41
1:D:3156:HIS:CE1	8:D:2134:HOH:O	2.74	0.41
1:A:204:PRO:HD3	1:C:2464:TRP:HB3	2.03	0.41
1:A:165:ILE:HA	1:A:179:ARG:O	2.20	0.41
1:B:1233:GLN:NE2	1:B:1247:VAL:H	2.05	0.41
1:C:2197:MET:HA	1:C:2213:TRP:O	2.21	0.41
4:C:3483:NAG:H4	5:C:3490:BMA:C1	2.51	0.41
1:A:150:HIS:HD2	8:C:3048:HOH:O	2.04	0.41
1:A:332:THR:HB	1:A:356:VAL:CG1	2.50	0.41
2:A:1477:SIA:O7	2:A:1477:SIA:O2	2.30	0.41
1:A:197:MET:HA	1:A:213:TRP:O	2.21	0.41
1:D:3195:SER:HB2	1:D:3214:TYR:CZ	2.56	0.41
1:C:2218:PRO:HB2	8:C:3166:HOH:O	2.21	0.41
1:A:282:ILE:HD12	1:A:310:ILE:HD11	2.02	0.41
1:A:88:ARG:HH12	1:A:133:GLN:HE22	1.69	0.41
1:A:124:ARG:HA	1:A:449:ASN:HD22	1.85	0.40
1:B:1307:ARG:HA	1:B:1308:PRO:HD3	1.94	0.40
5:C:3484:BMA:H2	6:C:3485:MAN:H5	2.04	0.40
1:C:2340:ASN:ND2	8:C:3268:HOH:O	2.53	0.40
1:A:113:ARG:NH2	3:B:2479:GOL:H32	2.36	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	387/389 (100%)	368 (95%)	18 (5%)	1 (0%)	46	44
1	B	387/389 (100%)	372 (96%)	14 (4%)	1 (0%)	46	44
1	C	387/389 (100%)	367 (95%)	19 (5%)	1 (0%)	46	44
1	D	387/389 (100%)	372 (96%)	15 (4%)	0	100	100
All	All	1548/1556 (100%)	1479 (96%)	66 (4%)	3 (0%)	52	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	B	1333	SER
1	C	2333	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	326 (98%)	5 (2%)	72	77
1	B	331/331 (100%)	321 (97%)	10 (3%)	48	50
1	C	331/331 (100%)	326 (98%)	5 (2%)	72	77
1	D	331/331 (100%)	324 (98%)	7 (2%)	61	65
All	All	1324/1324 (100%)	1297 (98%)	27 (2%)	63	67

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

Mol	Chain	Res	Type
1	A	128	LEU
1	A	342	ASN
1	A	445	LEU
1	A	460	ARG
1	A	464	TRP

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Mol	Chain	Res	Type
1	B	1088	ARG
1	B	1128	LEU
1	B	1142	GLN
1	B	1185	TRP
1	B	1256	ARG
1	B	1333	SER
1	B	1342	ASN
1	B	1405	ASN
1	B	1422	ASN
1	B	1464	TRP
1	C	2128	LEU
1	C	2333	SER
1	C	2424	GLU
1	C	2445	LEU
1	C	2464	TRP
1	D	3128	LEU
1	D	3237	CYS
1	D	3342	ASN
1	D	3386	VAL
1	D	3424	GLU
1	D	3445	LEU
1	D	3464	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	150	HIS
1	A	152	ASN
1	A	233	GLN
1	A	240	HIS
1	A	281	HIS
1	A	340	ASN
1	A	342	ASN
1	A	406	ASN
1	A	408	ASN
1	A	422	ASN
1	A	427	ASN
1	A	449	ASN
1	A	467	HIS
1	B	1142	GLN
1	B	1152	ASN

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Mol	Chain	Res	Type
1	B	1207	ASN
1	B	1233	GLN
1	B	1240	HIS
1	B	1281	HIS
1	B	1340	ASN
1	B	1342	ASN
1	B	1400	ASN
1	B	1405	ASN
1	B	1406	ASN
1	B	1408	ASN
1	B	1422	ASN
1	B	1427	ASN
1	B	1449	ASN
1	B	1467	HIS
1	C	2150	HIS
1	C	2152	ASN
1	C	2207	ASN
1	C	2233	GLN
1	C	2240	HIS
1	C	2270	GLN
1	C	2281	HIS
1	C	2340	ASN
1	C	2406	ASN
1	C	2408	ASN
1	C	2422	ASN
1	C	2427	ASN
1	C	2449	ASN
1	C	2467	HIS
1	D	3150	HIS
1	D	3152	ASN
1	D	3207	ASN
1	D	3233	GLN
1	D	3240	HIS
1	D	3281	HIS
1	D	3340	ASN
1	D	3342	ASN
1	D	3406	ASN
1	D	3422	ASN
1	D	3427	ASN
1	D	3449	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 43 ligands modelled in this entry, 4 are monoatomic - leaving 39 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SIA	A	1477	-	17,21,21	0.88	1 (5%)	19,31,31	1.22	3 (15%)
2	SIA	A	1478	-	17,21,21	0.91	1 (5%)	19,31,31	1.22	3 (15%)
3	GOL	A	1479	-	5,5,5	3.77	3 (60%)	5,5,5	6.27	4 (80%)
4	NAG	A	1480	1	14,14,15	0.24	0	15,19,21	0.85	1 (6%)
4	NAG	A	1481	-	14,14,15	0.25	0	15,19,21	0.82	1 (6%)
4	NAG	A	1482	4	14,14,15	0.26	0	15,19,21	0.84	1 (6%)
4	NAG	A	1483	4	14,14,15	0.26	0	15,19,21	0.85	1 (6%)
5	BMA	A	1484	-	11,11,12	0.25	0	14,15,17	0.60	0
6	MAN	A	1485	-	11,11,12	0.25	0	14,15,17	0.60	0
6	MAN	A	1486	-	11,11,12	0.26	0	14,15,17	0.60	0
6	MAN	A	1487	-	11,11,12	0.25	0	14,15,17	0.60	0
2	SIA	B	2477	-	17,21,21	0.88	1 (5%)	19,31,31	1.22	3 (15%)
2	SIA	B	2478	-	17,21,21	0.92	1 (5%)	19,31,31	1.23	3 (15%)
3	GOL	B	2479	-	5,5,5	3.34	3 (60%)	5,5,5	6.15	4 (80%)
4	NAG	B	2480	-	14,14,15	0.25	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	2481	4	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
4	NAG	B	2482	4	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
5	BMA	B	2483	-	11,11,12	0.26	0	14,15,17	0.60	0
6	MAN	B	2484	-	11,11,12	0.26	0	14,15,17	0.60	0
6	MAN	B	2485	-	11,11,12	0.25	0	14,15,17	0.60	0
6	MAN	B	2486	-	11,11,12	0.27	0	14,15,17	0.60	0
2	SIA	C	3477	-	17,21,21	0.90	1 (5%)	19,31,31	1.23	3 (15%)
2	SIA	C	3478	-	17,21,21	0.89	1 (5%)	19,31,31	1.22	3 (15%)
3	GOL	C	3479	-	5,5,5	3.52	3 (60%)	5,5,5	6.24	4 (80%)
4	NAG	C	3480	5	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
4	NAG	C	3481	-	14,14,15	0.26	0	15,19,21	0.84	1 (6%)
4	NAG	C	3482	4	14,14,15	0.26	0	15,19,21	0.84	1 (6%)
4	NAG	C	3483	4	14,14,15	0.25	0	15,19,21	0.84	1 (6%)
5	BMA	C	3484	4,6	11,11,12	0.26	0	14,15,17	0.60	0
6	MAN	C	3485	-	11,11,12	0.25	0	14,15,17	0.60	0
6	MAN	C	3486	-	11,11,12	0.25	0	14,15,17	0.60	0
6	MAN	C	3487	5	11,11,12	0.26	0	14,15,17	0.60	0
6	MAN	C	3488	-	11,11,12	0.25	0	14,15,17	0.61	0
6	MAN	C	3489	-	11,11,12	0.25	0	14,15,17	0.60	0
5	BMA	C	3490	-	11,11,12	0.25	0	14,15,17	0.60	0
2	SIA	D	4477	-	17,21,21	0.89	1 (5%)	19,31,31	1.22	3 (15%)
2	SIA	D	4478	-	17,21,21	0.89	1 (5%)	19,31,31	1.22	3 (15%)
3	GOL	D	4479	-	5,5,5	3.67	3 (60%)	5,5,5	6.43	4 (80%)
4	NAG	D	4480	-	14,14,15	0.24	0	15,19,21	0.85	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
2	SIA	A	1477	-	-	0/14/38/38	0/1/1/1
2	SIA	A	1478	-	-	0/14/38/38	0/1/1/1
3	GOL	A	1479	-	-	0/4/4/4	0/0/0/0
4	NAG	A	1480	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1481	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1482	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1483	4	-	0/6/23/26	0/1/1/1
5	BMA	A	1484	-	-	0/2/19/22	0/1/1/1
6	MAN	A	1485	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	1486	-	-	0/2/19/22	0/1/1/1
6	MAN	A	1487	-	-	0/2/19/22	0/1/1/1
2	SIA	B	2477	-	-	0/14/38/38	0/1/1/1
2	SIA	B	2478	-	-	0/14/38/38	0/1/1/1
3	GOL	B	2479	-	-	0/4/4/4	0/0/0/0
4	NAG	B	2480	-	-	0/6/23/26	0/1/1/1
4	NAG	B	2481	4	-	0/6/23/26	0/1/1/1
4	NAG	B	2482	4	-	0/6/23/26	0/1/1/1
5	BMA	B	2483	-	-	0/2/19/22	0/1/1/1
6	MAN	B	2484	-	-	0/2/19/22	0/1/1/1
6	MAN	B	2485	-	-	0/2/19/22	0/1/1/1
6	MAN	B	2486	-	-	0/2/19/22	0/1/1/1
2	SIA	C	3477	-	-	0/14/38/38	0/1/1/1
2	SIA	C	3478	-	-	0/14/38/38	0/1/1/1
3	GOL	C	3479	-	-	0/4/4/4	0/0/0/0
4	NAG	C	3480	5	-	0/6/23/26	0/1/1/1
4	NAG	C	3481	-	-	0/6/23/26	0/1/1/1
4	NAG	C	3482	4	-	0/6/23/26	0/1/1/1
4	NAG	C	3483	4	-	0/6/23/26	0/1/1/1
5	BMA	C	3484	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	3485	-	-	0/2/19/22	0/1/1/1
6	MAN	C	3486	-	-	0/2/19/22	0/1/1/1
6	MAN	C	3487	5	-	0/2/19/22	0/1/1/1
6	MAN	C	3488	-	-	0/2/19/22	0/1/1/1
6	MAN	C	3489	-	-	0/2/19/22	0/1/1/1
5	BMA	C	3490	-	-	0/2/19/22	0/1/1/1
2	SIA	D	4477	-	-	0/14/38/38	0/1/1/1
2	SIA	D	4478	-	-	0/14/38/38	0/1/1/1
3	GOL	D	4479	-	-	0/4/4/4	0/0/0/0
4	NAG	D	4480	-	-	0/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1479	GOL	C1-C2	-6.03	1.29	1.52
3	D	4479	GOL	C1-C2	-5.76	1.30	1.52
3	C	3479	GOL	C1-C2	-5.57	1.31	1.52
3	A	1479	GOL	O1-C1	-5.40	1.19	1.42
3	B	2479	GOL	C1-C2	-5.25	1.32	1.52
3	D	4479	GOL	O1-C1	-5.22	1.19	1.42
3	C	3479	GOL	O1-C1	-4.75	1.21	1.42
3	B	2479	GOL	O1-C1	-4.74	1.21	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3479	GOL	C3-C2	-2.77	1.41	1.52
3	D	4479	GOL	C3-C2	-2.24	1.43	1.52
3	B	2479	GOL	C3-C2	-2.10	1.44	1.52
3	A	1479	GOL	C3-C2	-2.03	1.44	1.52
2	B	2477	SIA	O2-C2	3.42	1.43	1.40
2	A	1477	SIA	O2-C2	3.43	1.43	1.40
2	D	4478	SIA	O2-C2	3.43	1.43	1.40
2	C	3478	SIA	O2-C2	3.46	1.43	1.40
2	D	4477	SIA	O2-C2	3.46	1.43	1.40
2	A	1478	SIA	O2-C2	3.50	1.43	1.40
2	C	3477	SIA	O2-C2	3.51	1.43	1.40
2	B	2478	SIA	O2-C2	3.56	1.43	1.40

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3477	SIA	C6-C5-N5	-3.50	104.97	111.07
2	B	2477	SIA	C6-C5-N5	-3.50	104.98	111.07
2	A	1477	SIA	C6-C5-N5	-3.50	104.98	111.07
2	C	3478	SIA	C6-C5-N5	-3.49	104.99	111.07
2	D	4478	SIA	C6-C5-N5	-3.49	104.99	111.07
2	B	2478	SIA	C6-C5-N5	-3.48	105.00	111.07
2	D	4477	SIA	C6-C5-N5	-3.48	105.00	111.07
2	A	1478	SIA	C6-C5-N5	-3.47	105.03	111.07
2	B	2478	SIA	C4-C5-N5	-2.50	104.98	110.41
2	C	3478	SIA	C4-C5-N5	-2.50	104.98	110.41
2	C	3477	SIA	C4-C5-N5	-2.49	104.99	110.41
2	B	2477	SIA	C4-C5-N5	-2.49	105.01	110.41
2	A	1478	SIA	C4-C5-N5	-2.49	105.01	110.41
2	D	4478	SIA	C4-C5-N5	-2.48	105.01	110.41
2	D	4477	SIA	C4-C5-N5	-2.48	105.03	110.41
2	A	1477	SIA	C4-C5-N5	-2.47	105.04	110.41
4	D	4480	NAG	C3-C2-N2	-2.34	104.96	110.56
4	B	2481	NAG	C3-C2-N2	-2.34	104.97	110.56
4	A	1480	NAG	C3-C2-N2	-2.33	104.98	110.56
4	A	1483	NAG	C3-C2-N2	-2.33	104.99	110.56
4	A	1482	NAG	C3-C2-N2	-2.33	104.99	110.56
4	C	3482	NAG	C3-C2-N2	-2.33	104.99	110.56
4	C	3480	NAG	C3-C2-N2	-2.32	105.01	110.56
4	B	2482	NAG	C3-C2-N2	-2.31	105.02	110.56
4	C	3483	NAG	C3-C2-N2	-2.31	105.02	110.56
4	B	2480	NAG	C3-C2-N2	-2.31	105.02	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3481	NAG	C3-C2-N2	-2.30	105.06	110.56
4	A	1481	NAG	C3-C2-N2	-2.28	105.09	110.56
2	B	2478	SIA	C7-C6-C5	-2.20	110.98	114.32
2	A	1478	SIA	C7-C6-C5	-2.20	110.99	114.32
2	D	4478	SIA	C7-C6-C5	-2.18	111.02	114.32
2	C	3478	SIA	C7-C6-C5	-2.17	111.03	114.32
2	D	4477	SIA	C7-C6-C5	-2.12	111.12	114.32
2	B	2477	SIA	C7-C6-C5	-2.11	111.13	114.32
2	C	3477	SIA	C7-C6-C5	-2.10	111.14	114.32
2	A	1477	SIA	C7-C6-C5	-2.09	111.15	114.32
3	A	1479	GOL	O2-C2-C1	3.09	122.82	108.65
3	B	2479	GOL	O2-C2-C3	3.20	123.32	108.65
3	C	3479	GOL	O2-C2-C3	3.36	124.06	108.65
3	D	4479	GOL	O2-C2-C1	3.50	124.69	108.65
3	D	4479	GOL	O2-C2-C3	3.51	124.75	108.65
3	B	2479	GOL	O2-C2-C1	3.65	125.38	108.65
3	C	3479	GOL	O2-C2-C1	3.96	126.79	108.65
3	A	1479	GOL	O2-C2-C3	3.96	126.81	108.65
3	C	3479	GOL	O3-C3-C2	5.49	136.83	110.18
3	A	1479	GOL	O3-C3-C2	5.78	138.21	110.18
3	D	4479	GOL	O3-C3-C2	6.22	140.36	110.18
3	B	2479	GOL	O3-C3-C2	6.24	140.44	110.18
3	B	2479	GOL	O1-C1-C2	11.25	164.73	110.18
3	C	3479	GOL	O1-C1-C2	11.72	167.04	110.18
3	A	1479	GOL	O1-C1-C2	11.75	167.15	110.18
3	D	4479	GOL	O1-C1-C2	11.97	168.22	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1477	SIA	3	0
2	A	1478	SIA	1	0
3	A	1479	GOL	2	0
4	A	1480	NAG	2	0
4	A	1481	NAG	3	0
4	A	1482	NAG	5	0
4	A	1483	NAG	5	0
5	A	1484	BMA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1485	MAN	6	0
6	A	1486	MAN	1	0
6	A	1487	MAN	3	0
2	B	2477	SIA	1	0
2	B	2478	SIA	3	0
3	B	2479	GOL	1	0
4	B	2480	NAG	3	0
4	B	2481	NAG	6	0
4	B	2482	NAG	7	0
5	B	2483	BMA	3	0
6	B	2484	MAN	2	0
6	B	2485	MAN	1	0
2	C	3477	SIA	2	0
2	C	3478	SIA	2	0
3	C	3479	GOL	1	0
4	C	3480	NAG	2	0
4	C	3481	NAG	3	0
4	C	3482	NAG	5	0
4	C	3483	NAG	7	0
5	C	3484	BMA	6	0
6	C	3485	MAN	5	0
6	C	3486	MAN	2	0
6	C	3487	MAN	4	0
6	C	3488	MAN	1	0
6	C	3489	MAN	3	0
5	C	3490	BMA	4	0
2	D	4477	SIA	3	0
2	D	4478	SIA	1	0
3	D	4479	GOL	1	0
4	D	4480	NAG	3	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	389/389 (100%)	-0.35	1 (0%)	94	95	11, 17, 26, 41	0
1	B	389/389 (100%)	-0.32	3 (0%)	87	89	11, 17, 25, 48	0
1	C	389/389 (100%)	-0.40	3 (0%)	87	89	11, 17, 26, 41	0
1	D	389/389 (100%)	-0.34	1 (0%)	94	95	11, 17, 25, 38	0
All	All	1556/1556 (100%)	-0.36	8 (0%)	91	93	11, 17, 26, 48	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1089	THR	3.0
1	A	460	ARG	2.7
1	B	1088	ARG	2.5
1	D	3460	ARG	2.5
1	C	2088	ARG	2.4
1	C	2349	GLY	2.4
1	B	1094	THR	2.2
1	C	2460	ARG	2.0

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

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	CA	C	3491	1/1	0.98	0.34	30.64	2,2,2,2	0
2	SIA	C	3478	21/21	0.47	0.72	22.38	28,32,34,36	21
7	CA	A	1488	1/1	0.98	0.27	21.52	8,8,8,8	0
7	CA	D	4481	1/1	0.99	0.28	17.33	4,4,4,4	0
2	SIA	A	1478	21/21	0.64	0.46	14.81	16,19,22,23	21
7	CA	B	2487	1/1	0.98	0.32	11.14	5,5,5,5	0
6	MAN	A	1487	11/12	0.75	0.22	11.10	41,52,54,60	0
6	MAN	C	3487	11/12	0.79	0.23	10.61	51,54,57,59	0
6	MAN	C	3489	11/12	0.81	0.20	9.51	39,41,47,51	0
6	MAN	A	1485	11/12	0.72	0.23	7.67	51,54,56,60	0
6	MAN	A	1486	11/12	0.64	0.27	7.62	55,59,64,66	0
4	NAG	C	3482	14/15	0.72	0.38	6.18	41,43,45,46	0
4	NAG	B	2481	14/15	0.73	0.35	5.01	29,40,42,43	0
3	GOL	C	3479	6/6	0.65	0.24	4.51	25,30,32,33	0
2	SIA	D	4478	21/21	0.73	0.23	4.27	22,33,35,39	21
4	NAG	B	2482	14/15	0.62	0.31	3.64	35,39,40,41	0
4	NAG	C	3480	14/15	0.49	0.33	3.31	35,40,42,43	0
4	NAG	A	1482	14/15	0.63	0.35	3.22	40,44,47,47	0
2	SIA	B	2478	21/21	0.79	0.21	3.16	24,32,37,37	21
2	SIA	C	3477	21/21	0.85	0.17	3.07	16,19,22,24	0
2	SIA	A	1477	21/21	0.84	0.16	2.94	17,19,23,24	0
3	GOL	A	1479	6/6	0.75	0.21	2.86	20,32,33,33	0
3	GOL	D	4479	6/6	0.78	0.21	2.73	24,34,36,37	0
6	MAN	C	3488	11/12	0.79	0.21	2.68	44,51,55,57	0
3	GOL	B	2479	6/6	0.69	0.20	2.51	27,30,34,35	0
4	NAG	C	3483	14/15	0.71	0.31	2.42	33,38,43,47	0
2	SIA	B	2477	21/21	0.87	0.15	1.75	17,19,21,24	0
2	SIA	D	4477	21/21	0.88	0.15	1.28	17,20,23,27	0
5	BMA	C	3490	11/12	0.75	0.28	-	58,64,65,66	0
6	MAN	B	2485	11/12	0.74	0.30	-	62,64,66,67	0
4	NAG	A	1480	14/15	0.80	0.23	-	36,42,44,45	0
5	BMA	A	1484	11/12	0.57	0.34	-	57,62,69,69	0
6	MAN	B	2486	11/12	0.72	0.35	-	67,73,75,76	0
6	MAN	C	3486	11/12	0.41	0.53	-	95,96,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BMA	B	2483	11/12	0.69	0.40	-	61,68,72,72	0
4	NAG	B	2480	14/15	0.85	0.21	-	21,33,39,43	0
5	BMA	C	3484	11/12	0.69	0.27	-	63,67,69,71	0
4	NAG	A	1483	14/15	0.58	0.35	-	54,62,63,64	0
4	NAG	C	3481	14/15	0.81	0.18	-	27,30,34,37	0
4	NAG	D	4480	14/15	0.77	0.22	-	25,33,37,38	0
6	MAN	C	3485	11/12	0.74	0.28	-	60,61,64,69	0
6	MAN	B	2484	11/12	0.64	0.29	-	71,72,74,75	0
4	NAG	A	1481	14/15	0.88	0.23	-	24,32,38,42	0

6.5 Other polymers (i)

There are no such residues in this entry.