Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:16 AM GMT

PDB ID	:	3OKW
Title	:	Mouse Semaphorin 6A, extracellular domains 1-2
Authors	:	Janssen, B.J.C.; Robinson, R.A.; Bell, C.H.; Siebold, C.; Jones, E.Y.
Deposited on	:	2010-08-25
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:

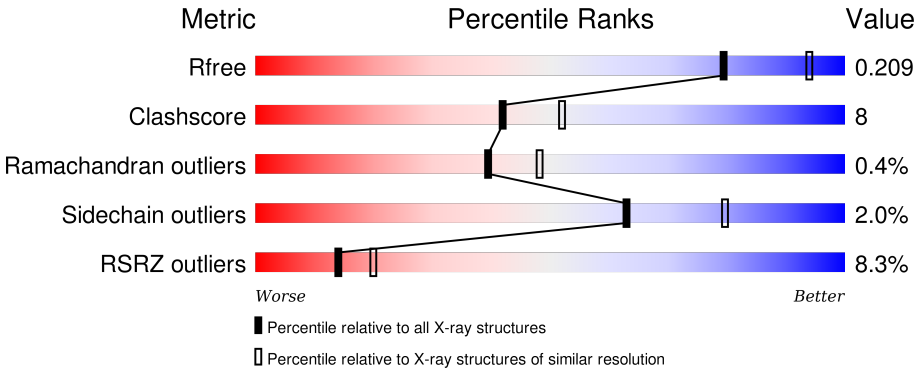
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	565	5% 81% 14%
1	B	565	10% 73% 19% 8%

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
3	NAG	B	1065	X	-	-	-
4	CIT	A	2001	-	-	-	X
5	GOL	A	2003	-	-	-	X
5	GOL	A	2004	-	-	-	X
5	GOL	A	2007	-	-	-	X
5	GOL	B	2017	-	-	-	X
5	GOL	B	2018	-	-	-	X
5	GOL	B	2019	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8995 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.

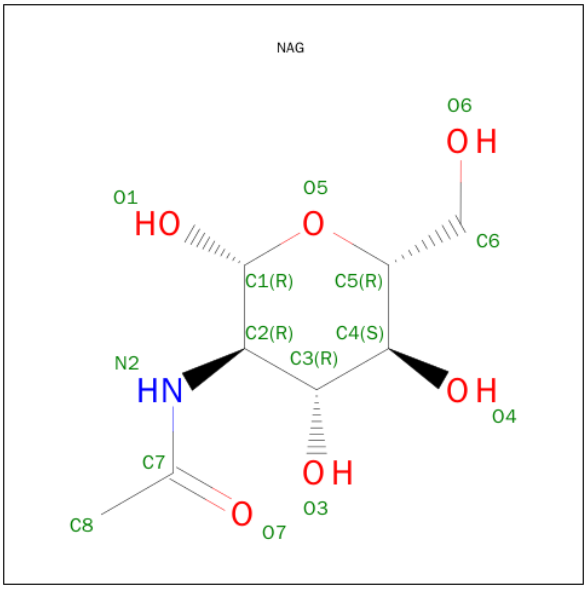
- Molecule 1 is a protein called Semaphorin-6A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4295	2718	747	799	31			
1	B	522	Total	C	N	O	S	0	0	0
			4148	2629	713	775	31			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLU	-	expression tag	UNP O35464
A	17	THR	-	expression tag	UNP O35464
A	18	GLY	-	expression tag	UNP O35464
A	572	GLY	-	expression tag	UNP O35464
A	573	THR	-	expression tag	UNP O35464
A	574	LYS	-	expression tag	UNP O35464
A	575	HIS	-	expression tag	UNP O35464
A	576	HIS	-	expression tag	UNP O35464
A	577	HIS	-	expression tag	UNP O35464
A	578	HIS	-	expression tag	UNP O35464
A	579	HIS	-	expression tag	UNP O35464
A	580	HIS	-	expression tag	UNP O35464
B	16	GLU	-	expression tag	UNP O35464
B	17	THR	-	expression tag	UNP O35464
B	18	GLY	-	expression tag	UNP O35464
B	572	GLY	-	expression tag	UNP O35464
B	573	THR	-	expression tag	UNP O35464
B	574	LYS	-	expression tag	UNP O35464
B	575	HIS	-	expression tag	UNP O35464
B	576	HIS	-	expression tag	UNP O35464
B	577	HIS	-	expression tag	UNP O35464
B	578	HIS	-	expression tag	UNP O35464
B	579	HIS	-	expression tag	UNP O35464
B	580	HIS	-	expression tag	UNP O35464

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

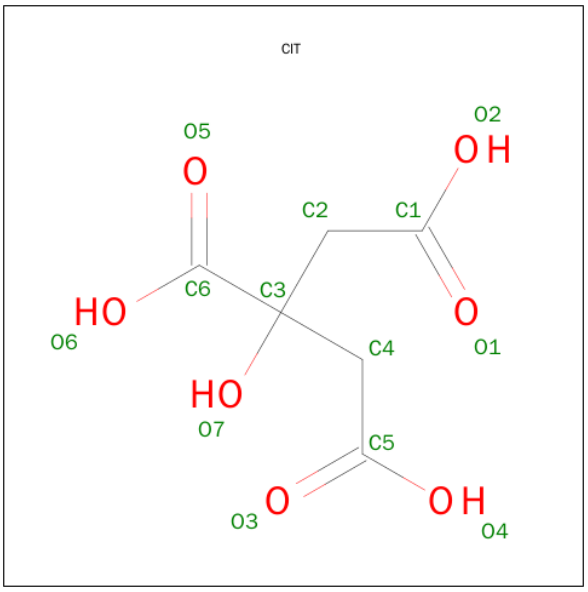


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

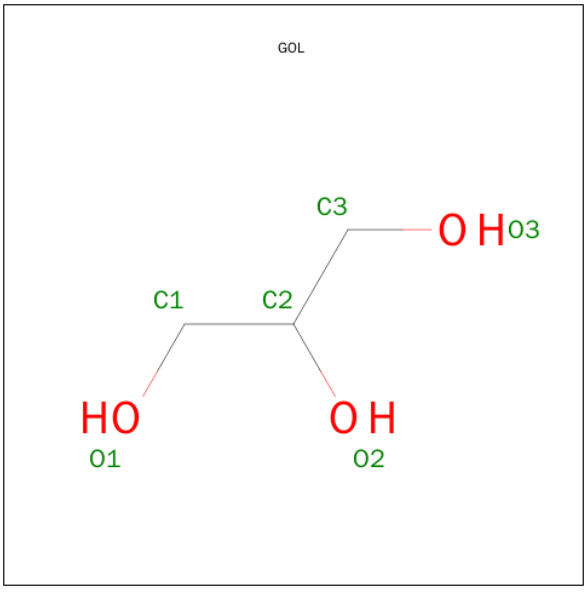
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0

- 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 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

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

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is water.

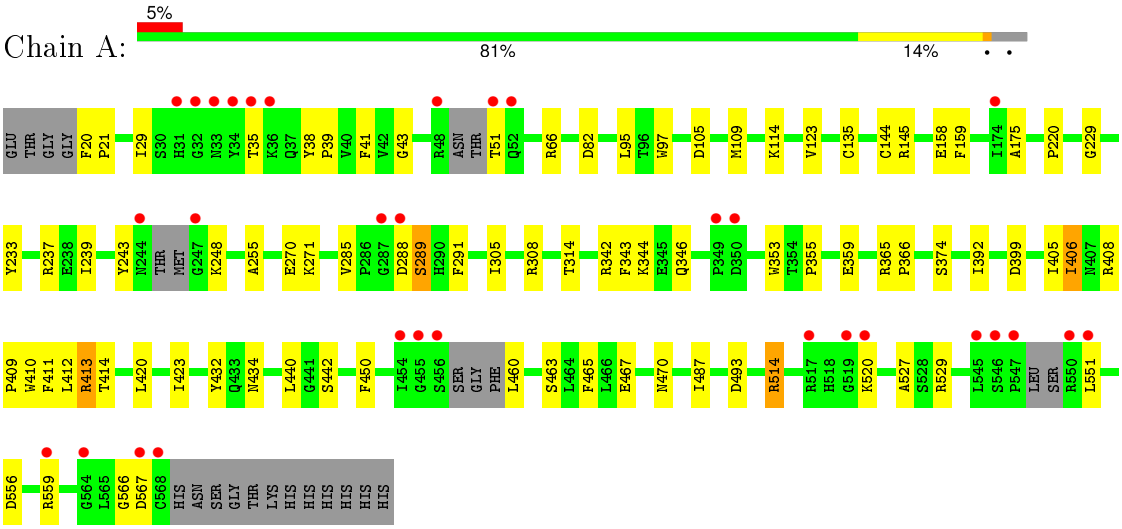
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	189	Total O 189 189	0	0
7	B	89	Total O 89 89	0	0

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.

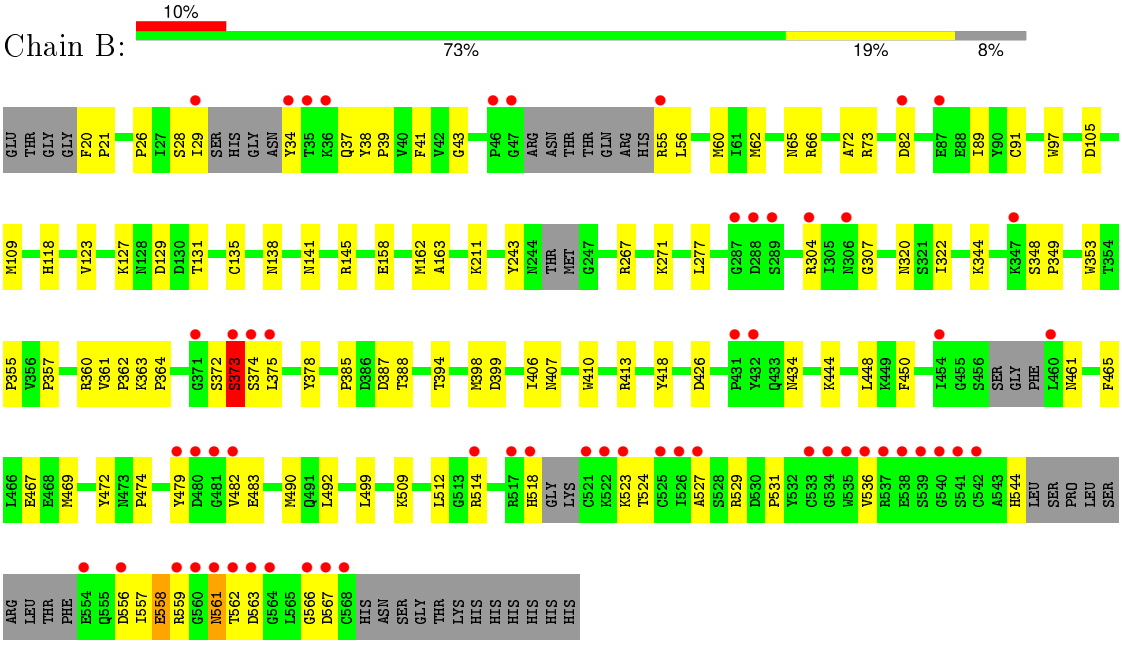
- Molecule 1: Semaphorin-6A

Chain A:



- Molecule 1: Semaphorin-6A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	97.04Å 97.04Å 153.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.43 – 2.30 32.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.43-2.30) 99.6 (32.43-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.184 , 0.219 0.169 , 0.209	Depositor DCC
R_{free} test set	3611 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.1	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.029 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 71390 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8995	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: MAN, GOL, BMA, NAG, CIT

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	0.43	0/4395	0.56	0/5944
1	B	0.38	0/4242	0.54	0/5736
All	All	0.40	0/8637	0.55	0/11680

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1065	NAG	C1

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	4295	0	4187	65	0
1	B	4148	0	4036	78	0
2	A	14	0	13	0	0
2	B	14	0	13	1	0
3	A	56	0	50	3	0
3	B	56	0	50	4	0
4	A	13	0	5	1	0
5	A	36	0	48	2	0
5	B	24	0	32	0	0
6	B	61	0	52	1	0
7	A	189	0	0	0	0
7	B	89	0	0	0	0
All	All	8995	0	8486	144	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 8.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASN:HA	3:B:1065:NAG:H83	1.56	0.87
1:A:229:GLY:H	5:A:2005:GOL:H11	1.36	0.86
1:B:277:LEU:HD22	1:B:398:MET:HE1	1.65	0.78
1:A:20:PHE:CE1	1:A:414:THR:HG21	2.19	0.77
1:A:20:PHE:HE1	1:A:414:THR:HG21	1.50	0.77
1:A:405:ILE:O	1:A:406:ILE:HB	1.84	0.77
1:A:410:TRP:CH2	1:A:460:LEU:HD22	2.21	0.76
1:B:129:ASP:OD1	1:B:131:THR:HG22	1.88	0.73
1:B:566:GLY:HA3	1:B:567:ASP:OD1	1.90	0.72
1:B:38:TYR:OH	1:B:514:ARG:HD3	1.91	0.71
1:B:490:MET:CE	1:B:499:LEU:HD21	2.21	0.70
1:B:406:ILE:O	1:B:406:ILE:HG22	1.91	0.70
1:B:55:ARG:HG2	1:B:55:ARG:HH11	1.55	0.70
1:A:450:PHE:CD1	1:A:463:SER:HB2	2.27	0.69
1:B:344:LYS:HE2	1:B:399:ASP:HA	1.73	0.69
1:A:410:TRP:HH2	1:A:460:LEU:HD22	1.55	0.69
1:B:490:MET:HE3	1:B:499:LEU:HD21	1.74	0.69
1:B:123:VAL:HB	1:B:135:CYS:HB2	1.76	0.68
1:B:127:LYS:HD3	1:B:131:THR:HG23	1.74	0.68
1:B:348:SER:HB2	1:B:349:PRO:HD2	1.77	0.67
1:A:66:ARG:HD3	1:A:82:ASP:OD2	1.95	0.67
1:B:362:PRO:HB2	1:B:388:THR:HG22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:VAL:CG2	1:A:291:PHE:HB3	2.26	0.66
1:A:566:GLY:HA3	1:A:567:ASP:OD1	1.97	0.65
1:A:434:ASN:HD22	3:A:1434:NAG:H83	1.61	0.65
1:B:364:PRO:HG3	1:B:378:TYR:CE2	2.32	0.64
1:B:145:ARG:HD3	1:B:158:GLU:HG2	1.80	0.64
1:A:123:VAL:HB	1:A:135:CYS:HB2	1.81	0.61
1:B:531:PRO:HA	1:B:557:ILE:HD11	1.82	0.61
1:A:114:LYS:HE3	4:A:2001:CIT:O2	2.01	0.61
1:B:523:LYS:HG3	1:B:562:THR:OG1	2.01	0.61
1:A:514:ARG:HH11	1:A:514:ARG:HB2	1.64	0.60
1:B:472:TYR:CE2	1:B:483:GLU:HG2	2.37	0.59
1:B:469:MET:HB3	1:B:514:ARG:HH22	1.65	0.59
1:B:66:ARG:HD3	1:B:82:ASP:OD2	2.02	0.59
1:B:105:ASP:O	1:B:109:MET:HG3	2.03	0.59
1:A:97:TRP:CH2	1:A:145:ARG:HG3	2.37	0.59
1:A:145:ARG:HD3	1:A:158:GLU:HG2	1.85	0.58
1:A:239:ILE:CD1	1:A:248:LYS:HE3	2.32	0.58
1:B:472:TYR:HE2	1:B:483:GLU:HG2	1.66	0.58
1:B:56:LEU:O	1:B:72:ALA:HB1	2.04	0.58
1:A:175:ALA:O	5:A:2003:GOL:H11	2.04	0.57
1:B:28:SER:O	1:B:467:GLU:HA	2.05	0.57
1:A:51:THR:O	1:A:51:THR:HG22	2.05	0.57
1:B:518:HIS:HB3	1:B:524:THR:HG22	1.87	0.56
3:B:1065:NAG:O3	3:B:1066:NAG:N2	2.39	0.56
1:A:288:ASP:O	1:A:289:SER:HB2	2.06	0.56
1:A:285:VAL:HG22	1:A:291:PHE:HB3	1.88	0.56
1:A:308:ARG:HH12	1:A:405:ILE:CG2	2.19	0.55
1:A:343:PHE:CZ	1:A:365:ARG:NH1	2.74	0.55
1:B:55:ARG:HG2	1:B:55:ARG:NH1	2.16	0.54
1:A:411:PHE:CE2	1:A:413:ARG:HG2	2.43	0.54
1:A:556:ASP:O	1:A:559:ARG:O	2.27	0.53
1:A:434:ASN:ND2	3:A:1434:NAG:H83	2.23	0.52
1:B:304:ARG:HH21	1:B:307:GLY:H	1.58	0.52
1:B:363:LYS:HA	1:B:364:PRO:C	2.29	0.52
1:B:41:PHE:HB2	1:B:89:ILE:HB	1.91	0.52
1:A:406:ILE:HG22	1:A:408:ARG:HG2	1.91	0.51
1:A:41:PHE:CZ	1:A:43:GLY:HA2	2.45	0.51
1:A:270:GLU:HG2	1:A:271:LYS:HG3	1.92	0.51
1:B:492:LEU:C	1:B:492:LEU:HD23	2.31	0.51
1:A:467:GLU:OE2	1:A:514:ARG:HD2	2.11	0.51
1:B:385:PRO:HB2	1:B:387:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PRO:HB2	1:B:509:LYS:HB3	1.93	0.50
1:A:20:PHE:CD2	1:A:21:PRO:HD2	2.47	0.50
1:A:288:ASP:O	1:A:289:SER:CB	2.59	0.50
1:B:355:PRO:HG3	1:B:399:ASP:OD2	2.12	0.50
1:A:305:ILE:CG2	1:A:460:LEU:HD21	2.43	0.49
1:A:420:LEU:HD13	1:A:440:LEU:HD13	1.94	0.49
1:A:239:ILE:HD12	1:A:248:LYS:HE3	1.92	0.49
1:B:406:ILE:CG2	1:B:406:ILE:O	2.59	0.49
1:A:467:GLU:OE1	1:A:514:ARG:NH1	2.45	0.48
1:A:20:PHE:HB2	1:B:320:ASN:HA	1.96	0.48
1:B:34:TYR:O	1:B:37:GLN:HG2	2.14	0.48
1:B:41:PHE:CZ	1:B:43:GLY:HA2	2.49	0.48
1:B:394:THR:HG22	1:B:394:THR:O	2.13	0.48
1:B:426:ASP:HB2	1:B:492:LEU:HD11	1.95	0.47
1:A:239:ILE:HD11	1:A:248:LYS:HE3	1.95	0.47
1:A:305:ILE:HG22	1:A:460:LEU:HD21	1.97	0.47
1:B:448:LEU:HB3	1:B:450:PHE:CE1	2.50	0.47
1:A:95:LEU:HD23	1:A:95:LEU:C	2.35	0.47
1:B:127:LYS:HD3	1:B:131:THR:CG2	2.44	0.47
1:B:26:PRO:HG2	1:B:29:ILE:HG13	1.96	0.47
1:A:344:LYS:HE2	1:A:399:ASP:HA	1.96	0.47
1:A:308:ARG:HH12	1:A:405:ILE:HG23	1.80	0.46
1:B:73:ARG:NH1	1:B:118:HIS:CE1	2.84	0.46
1:B:544:HIS:O	1:B:544:HIS:ND1	2.45	0.46
1:B:357:PRO:HD2	1:B:360:ARG:HD3	1.97	0.46
1:A:411:PHE:HE2	1:A:413:ARG:HG2	1.80	0.45
1:B:434:ASN:HD22	2:B:1434:NAG:H83	1.81	0.45
1:A:442:SER:H	1:A:487:ILE:HD12	1.81	0.45
1:A:414:THR:HG22	1:B:322:ILE:HD12	1.99	0.45
1:B:492:LEU:HG	1:B:512:LEU:HD21	1.99	0.45
1:A:344:LYS:HD3	1:A:353:TRP:HB3	1.98	0.45
1:B:55:ARG:HD3	1:B:479:TYR:CE1	2.51	0.45
1:B:556:ASP:HB3	1:B:561:ASN:OD1	2.17	0.45
1:B:418:TYR:HB3	1:B:444:LYS:HG3	1.99	0.45
1:B:472:TYR:O	1:B:474:PRO:HD3	2.16	0.44
1:B:344:LYS:HG2	1:B:353:TRP:HE3	1.82	0.44
1:B:361:VAL:HA	1:B:362:PRO:HD3	1.82	0.44
1:A:409:PRO:HG2	1:A:412:LEU:HD21	1.98	0.44
1:B:374:SER:C	1:B:375:LEU:HD12	2.38	0.44
1:B:304:ARG:NH2	1:B:307:GLY:H	2.15	0.44
1:B:407:ASN:HB3	3:B:1282:NAG:H62	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLY:HA2	1:A:567:ASP:HA	1.75	0.44
1:A:35:THR:HG21	1:A:470:ASN:O	2.18	0.44
1:A:342:ARG:HE	1:A:355:PRO:HB2	1.83	0.44
1:B:97:TRP:CH2	1:B:145:ARG:HG3	2.53	0.43
1:B:426:ASP:HB2	1:B:492:LEU:CD1	2.48	0.43
1:B:527:ALA:O	1:B:529:ARG:HG3	2.17	0.43
1:A:105:ASP:O	1:A:109:MET:HG3	2.19	0.43
1:A:527:ALA:O	1:A:529:ARG:HG3	2.19	0.43
1:B:558:GLU:C	1:B:559:ARG:HD2	2.39	0.42
1:B:479:TYR:O	1:B:482:VAL:HG12	2.18	0.42
1:A:285:VAL:HG23	1:A:285:VAL:O	2.19	0.42
1:B:512:LEU:HA	1:B:512:LEU:HD23	1.91	0.42
1:A:366:PRO:HB3	1:A:392:ILE:HB	2.01	0.42
1:B:490:MET:HE1	1:B:499:LEU:HD21	1.97	0.42
1:A:346:GLN:HG3	1:A:353:TRP:CE2	2.55	0.42
1:A:520:LYS:HB2	1:A:520:LYS:HE3	1.74	0.42
1:B:344:LYS:HD3	1:B:353:TRP:HB3	2.01	0.42
1:A:359:GLU:H	1:A:359:GLU:CD	2.23	0.42
1:B:145:ARG:HD3	1:B:158:GLU:CG	2.47	0.42
1:B:410:TRP:HH2	1:B:450:PHE:HB2	1.84	0.42
1:B:559:ARG:C	1:B:561:ASN:H	2.23	0.42
1:A:38:TYR:HA	1:A:39:PRO:HD3	1.91	0.42
1:B:461:ASN:CG	1:B:461:ASN:O	2.57	0.42
1:B:162:MET:O	1:B:163:ALA:HB3	2.20	0.41
1:B:344:LYS:HG2	1:B:353:TRP:HB3	2.01	0.41
1:A:233:TYR:HA	1:A:255:ALA:O	2.20	0.41
1:A:66:ARG:NH2	1:A:493:ASP:OD1	2.49	0.41
1:A:239:ILE:HD12	1:A:248:LYS:HG3	2.01	0.41
1:A:432:TYR:CE2	3:A:1435:NAG:H83	2.55	0.41
1:A:314:THR:HG23	1:A:423:ILE:HD11	2.03	0.41
1:B:518:HIS:HB3	1:B:524:THR:CG2	2.50	0.41
1:B:531:PRO:HA	1:B:557:ILE:CD1	2.51	0.41
1:A:144:CYS:HB2	1:A:159:PHE:HB2	2.02	0.41
1:A:220:PRO:HA	1:A:237:ARG:O	2.21	0.41
1:B:271:LYS:HE3	1:B:271:LYS:HB3	1.85	0.41
3:B:1282:NAG:O6	3:B:1283:NAG:H83	2.21	0.41
1:B:372:SER:O	1:B:373:SER:C	2.60	0.40
6:B:1461:NAG:H83	6:B:1461:NAG:H2	1.87	0.40
1:B:138:ASN:HB3	1:B:141:ASN:O	2.22	0.40
1:B:20:PHE:HA	1:B:21:PRO:HD3	1.88	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	530/565 (94%)	512 (97%)	16 (3%)	2 (0%)	39	48
1	B	508/565 (90%)	486 (96%)	20 (4%)	2 (0%)	39	48
All	All	1038/1130 (92%)	998 (96%)	36 (4%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	SER
1	A	406	ILE
1	B	373	SER
1	B	561	ASN

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	474/495 (96%)	467 (98%)	7 (2%)	72	85
1	B	458/495 (92%)	446 (97%)	12 (3%)	54	71
All	All	932/990 (94%)	913 (98%)	19 (2%)	63	79

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

Mol	Chain	Res	Type
1	A	29	ILE
1	A	243	TYR

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Mol	Chain	Res	Type
1	A	374	SER
1	A	413	ARG
1	A	465	PHE
1	A	514	ARG
1	A	551	LEU
1	B	60	MET
1	B	62	MET
1	B	91	CYS
1	B	211	LYS
1	B	243	TYR
1	B	267	ARG
1	B	373	SER
1	B	413	ARG
1	B	465	PHE
1	B	536	VAL
1	B	558	GLU
1	B	563	ASP

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

Mol	Chain	Res	Type
1	B	555	GLN

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

13 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	$\#\|Z\| > 2$
3	NAG	A	1282	1,3	14,14,15	0.48	0	15,19,21	0.92	0
3	NAG	A	1283	3	14,14,15	0.50	0	15,19,21	2.22	4 (26%)
3	NAG	A	1434	1,3	14,14,15	0.71	0	15,19,21	1.47	3 (20%)
3	NAG	A	1435	3	14,14,15	0.52	0	15,19,21	0.87	0
3	NAG	B	1065	1,3	14,14,15	0.41	0	15,19,21	1.34	2 (13%)
3	NAG	B	1066	3	14,14,15	0.61	0	15,19,21	1.48	1 (6%)
3	NAG	B	1282	1,3	14,14,15	0.53	0	15,19,21	1.04	1 (6%)
3	NAG	B	1283	3	14,14,15	0.49	0	15,19,21	1.59	1 (6%)
6	NAG	B	1461	1,6	14,14,15	0.38	0	15,19,21	1.28	1 (6%)
6	NAG	B	1462	6	14,14,15	0.46	0	15,19,21	0.82	1 (6%)
6	BMA	B	1463	6	11,11,12	0.62	0	14,15,17	1.53	2 (14%)
6	MAN	B	1464	6	11,11,12	0.57	0	14,15,17	1.05	1 (7%)
6	MAN	B	1465	6	11,11,12	0.52	0	14,15,17	0.69	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
3	NAG	A	1282	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1283	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1434	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1435	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1065	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	1066	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1282	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1283	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1461	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1462	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1463	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1464	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1465	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1283	NAG	C4-C3-C2	-3.97	105.06	111.23
3	A	1434	NAG	O4-C4-C3	-2.04	105.75	110.34
6	B	1462	NAG	C3-C4-C5	2.04	113.75	110.20
3	A	1434	NAG	C3-C4-C5	2.11	113.87	110.20
6	B	1463	BMA	C3-C4-C5	2.17	113.99	110.20
3	B	1282	NAG	C1-O5-C5	2.24	115.09	112.25
6	B	1464	MAN	C1-O5-C5	2.44	115.34	112.25
3	A	1283	NAG	C3-C2-N2	2.46	116.45	110.56
3	B	1065	NAG	O4-C4-C3	2.98	117.05	110.34
3	B	1065	NAG	C1-O5-C5	3.07	116.15	112.25
3	A	1283	NAG	C2-N2-C7	3.86	128.00	123.04
6	B	1461	NAG	C1-O5-C5	3.92	117.22	112.25
3	A	1434	NAG	C1-O5-C5	3.94	117.25	112.25
6	B	1463	BMA	C1-C2-C3	4.23	114.55	109.54
3	B	1283	NAG	C1-O5-C5	4.98	118.56	112.25
3	B	1066	NAG	C1-O5-C5	4.99	118.59	112.25
3	A	1283	NAG	C1-O5-C5	5.00	118.59	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1065	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1434	NAG	2	0
3	A	1435	NAG	1	0
3	B	1065	NAG	2	0
3	B	1066	NAG	1	0
3	B	1282	NAG	2	0
3	B	1283	NAG	1	0
6	B	1461	NAG	1	0

5.6 Ligand geometry (i)

13 ligands 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	$\#\|Z\| > 2$
2	NAG	A	1065	1	14,14,15	0.49	0	15,19,21	0.74	0
4	CIT	A	2001	-	3,12,12	1.17	0	3,17,17	2.05	1 (33%)
5	GOL	A	2002	-	5,5,5	0.31	0	5,5,5	0.29	0
5	GOL	A	2003	-	5,5,5	0.32	0	5,5,5	0.52	0
5	GOL	A	2004	-	5,5,5	0.34	0	5,5,5	0.49	0
5	GOL	A	2005	-	5,5,5	0.28	0	5,5,5	0.30	0
5	GOL	A	2006	-	5,5,5	0.35	0	5,5,5	0.26	0
5	GOL	A	2007	-	5,5,5	0.25	0	5,5,5	0.54	0
2	NAG	B	1434	1	14,14,15	0.45	0	15,19,21	1.05	1 (6%)
5	GOL	B	2016	-	5,5,5	0.48	0	5,5,5	0.26	0
5	GOL	B	2017	-	5,5,5	0.22	0	5,5,5	0.55	0
5	GOL	B	2018	-	5,5,5	0.41	0	5,5,5	0.38	0
5	GOL	B	2019	-	5,5,5	0.29	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1065	1	-	0/6/23/26	0/1/1/1
4	CIT	A	2001	-	-	0/6/16/16	0/0/0/0
5	GOL	A	2002	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2003	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2004	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2005	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2006	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2007	-	-	0/4/4/4	0/0/0/0
2	NAG	B	1434	1	-	0/6/23/26	0/1/1/1
5	GOL	B	2016	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2017	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2018	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2019	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	CIT	C3-C4-C5	-3.42	109.49	114.96
2	B	1434	NAG	C1-O5-C5	2.26	115.12	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	CIT	1	0
5	A	2003	GOL	1	0
5	A	2005	GOL	1	0
2	B	1434	NAG	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	540/565 (95%)	0.06	31 (5%)	27	36	24, 43, 88, 145	0
1	B	522/565 (92%)	0.44	57 (10%)	7	11	26, 60, 115, 150	0
All	All	1062/1130 (93%)	0.25	88 (8%)	14	20	24, 50, 107, 150	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	CYS	10.6
1	A	568	CYS	8.3
1	A	48	ARG	6.7
1	B	537	ARG	6.5
1	B	566	GLY	6.1
1	B	432	TYR	5.6
1	B	526	ILE	5.5
1	A	51	THR	5.5
1	B	536	VAL	5.3
1	A	287	GLY	5.0
1	B	541	SER	4.9
1	B	518	HIS	4.7
1	A	288	ASP	4.7
1	A	454	ILE	4.6
1	B	375	LEU	4.5
1	A	34	TYR	4.5
1	B	288	ASP	4.4
1	B	34	TYR	4.3
1	A	456	SER	4.3
1	B	534	GLY	4.3
1	B	562	THR	4.2
1	B	289	SER	4.1
1	B	564	GLY	4.0
1	B	567	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	33	ASN	4.0
1	B	481	GLY	4.0
1	A	550	ARG	4.0
1	B	479	TYR	4.0
1	B	371	GLY	3.9
1	B	482	VAL	3.9
1	A	31	HIS	3.8
1	B	514	ARG	3.8
1	B	559	ARG	3.8
1	B	306	ASN	3.7
1	B	480	ASP	3.6
1	B	554	GLU	3.6
1	B	431	PRO	3.5
1	B	527	ALA	3.4
1	B	36	LYS	3.3
1	A	32	GLY	3.2
1	B	29	ILE	3.2
1	B	540	GLY	3.2
1	A	551	LEU	3.2
1	B	523	LYS	3.2
1	B	82	ASP	3.1
1	B	287	GLY	3.1
1	B	561	ASN	3.1
1	A	349	PRO	3.1
1	B	539	SER	3.1
1	A	455	GLY	3.0
1	A	247	GLY	3.0
1	B	460	LEU	3.0
1	B	347	LYS	2.9
1	B	373	SER	2.9
1	B	560	GLY	2.9
1	B	556	ASP	2.9
1	A	520	LYS	2.7
1	B	304	ARG	2.6
1	B	374	SER	2.6
1	B	454	ILE	2.6
1	B	535	TRP	2.6
1	B	533	CYS	2.6
1	A	564	GLY	2.5
1	B	47	GLY	2.5
1	A	52	GLN	2.5
1	A	350	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	545	LEU	2.5
1	A	517	ARG	2.4
1	B	538	GLU	2.4
1	A	547	PRO	2.4
1	B	521	CYS	2.4
1	A	567	ASP	2.3
1	B	35	THR	2.3
1	A	36	LYS	2.3
1	B	525	CYS	2.3
1	B	542	CYS	2.3
1	A	546	SER	2.2
1	B	563	ASP	2.2
1	B	522	LYS	2.2
1	A	559	ARG	2.1
1	A	174	ILE	2.1
1	B	517	ARG	2.1
1	A	244	ASN	2.1
1	B	87	GLU	2.1
1	B	46	PRO	2.1
1	A	35	THR	2.0
1	B	55	ARG	2.0
1	A	519	GLY	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
3	NAG	B	1282	14/15	0.96	0.12	0.28	50,56,66,67	0
3	NAG	A	1282	14/15	0.93	0.10	-0.63	41,49,63,65	0
3	NAG	A	1435	14/15	0.74	0.37	-	98,112,114,116	0
3	NAG	B	1283	14/15	0.86	0.29	-	66,84,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	1434	14/15	0.92	0.18	-	57,70,93,97	0
6	BMA	B	1463	11/12	0.63	0.29	-	116,129,140,145	0
3	NAG	B	1066	14/15	0.72	0.39	-	123,131,133,135	0
6	MAN	B	1465	11/12	0.41	0.41	-	130,156,159,162	0
3	NAG	B	1065	14/15	0.82	0.24	-	132,136,149,151	0
6	NAG	B	1461	14/15	0.88	0.29	-	117,126,128,130	0
3	NAG	A	1283	14/15	0.86	0.27	-	72,84,96,101	0
6	NAG	B	1462	14/15	0.81	0.38	-	124,130,132,133	0
6	MAN	B	1464	11/12	0.48	0.42	-	147,151,160,160	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
4	CIT	A	2001	13/13	0.82	0.22	5.99	55,68,73,74	0
5	GOL	B	2018	6/6	0.75	0.34	5.19	51,62,73,73	0
5	GOL	B	2019	6/6	0.80	0.22	3.86	44,60,67,71	0
5	GOL	A	2004	6/6	0.86	0.21	2.66	57,66,67,67	0
5	GOL	A	2007	6/6	0.81	0.21	2.43	51,67,70,73	0
5	GOL	A	2003	6/6	0.94	0.27	2.32	40,56,62,65	0
5	GOL	B	2017	6/6	0.82	0.20	2.26	54,64,70,76	0
5	GOL	A	2002	6/6	0.94	0.11	-0.04	77,80,83,85	0
5	GOL	A	2005	6/6	0.64	0.26	-	75,78,82,84	0
5	GOL	A	2006	6/6	0.90	0.14	-	73,83,83,84	0
5	GOL	B	2016	6/6	0.80	0.22	-	43,58,60,64	0
2	NAG	B	1434	14/15	0.80	0.43	-	102,110,119,129	0
2	NAG	A	1065	14/15	0.84	0.43	-	93,100,110,112	0

6.5 Other polymers (i)

There are no such residues in this entry.