



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OKY  
Title : Plexin A2 in complex with Semaphorin 6A  
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Deposited on : 2010-08-25  
Resolution : 2.19 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

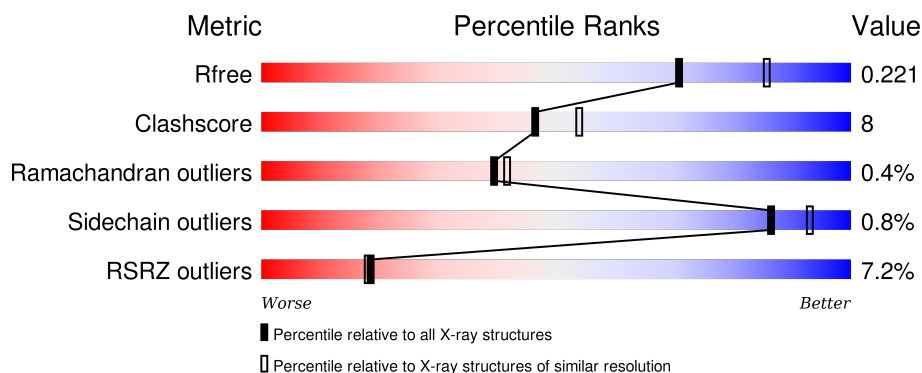
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	681	<div> <div>9%</div> <div>75%</div> <div>14%</div> <div>11%</div> </div>
2	B	565	<div> <div>4%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	2001	-	-	-	X
4	GOL	A	2003	-	-	-	X
4	GOL	A	2006	-	-	X	X
4	GOL	B	2004	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9600 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 Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4767	3028	808	903	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	33	THR	-	expression tag	UNP P70207
A	34	GLY	-	expression tag	UNP P70207
A	704	GLY	-	expression tag	UNP P70207
A	705	THR	-	expression tag	UNP P70207
A	706	LYS	-	expression tag	UNP P70207
A	707	HIS	-	expression tag	UNP P70207
A	708	HIS	-	expression tag	UNP P70207
A	709	HIS	-	expression tag	UNP P70207
A	710	HIS	-	expression tag	UNP P70207
A	711	HIS	-	expression tag	UNP P70207
A	712	HIS	-	expression tag	UNP P70207

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	540	Total	C	N	O	S	0	0	0
			4302	2723	747	800	32			

There are 12 discrepancies between the modelled and reference sequences:

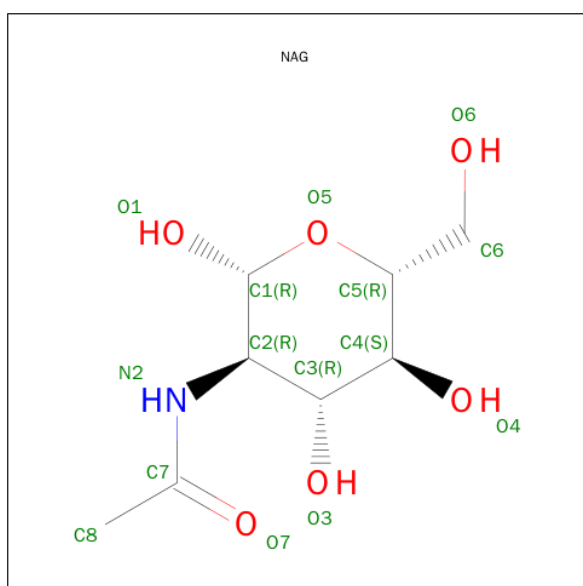
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	GLU	-	expression tag	UNP Q8BUT0
B	17	THR	-	expression tag	UNP Q8BUT0
B	18	GLY	-	expression tag	UNP Q8BUT0
B	572	GLY	-	expression tag	UNP Q8BUT0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	573	THR	-	expression tag	UNP Q8BUT0
B	574	LYS	-	expression tag	UNP Q8BUT0
B	575	HIS	-	expression tag	UNP Q8BUT0
B	576	HIS	-	expression tag	UNP Q8BUT0
B	577	HIS	-	expression tag	UNP Q8BUT0
B	578	HIS	-	expression tag	UNP Q8BUT0
B	579	HIS	-	expression tag	UNP Q8BUT0
B	580	HIS	-	expression tag	UNP Q8BUT0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	184	Total	O	0	0
			184	184		
6	B	205	Total	O	0	0
			205	205		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.54Å 159.60Å 139.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.19 39.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.6 (39.90-2.19) 93.6 (39.90-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.190 , 0.230 0.179 , 0.221	Depositor DCC
$R_{free}$ test set	4198 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.2	EDS
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 82680 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG

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	0.30	0/4879	0.48	0/6621
2	B	0.30	0/4403	0.49	0/5957
All	All	0.30	0/9282	0.48	0/12578

There are no bond length outliers.

There are no bond angle outliers.

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	4767	0	4654	69	0
2	B	4302	0	4198	70	0
3	A	56	0	52	0	0
3	B	28	0	26	1	0
4	A	18	0	24	8	0
4	B	12	0	16	5	0
5	B	28	0	25	0	0
6	A	184	0	0	3	0
6	B	205	0	0	0	0
All	All	9600	0	8995	138	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 (138) 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)
2:B:23:ASP:H	2:B:415:MET:HE1	1.28	0.96
1:A:576:ARG:H	1:A:615:SER:HB3	1.53	0.74
1:A:646:PHE:CD1	1:A:647:VAL:HG23	2.24	0.73
2:B:344:LYS:HE2	2:B:399:ASP:HA	1.71	0.72
1:A:121:TYR:HB2	4:A:2006:GOL:H32	1.72	0.72
2:B:453:ARG:HB2	2:B:461:ASN:O	1.91	0.71
1:A:57:ARG:HG3	1:A:121:TYR:OH	1.96	0.66
1:A:328:ILE:HG22	1:A:361:ARG:HE	1.60	0.66
2:B:514:ARG:O	2:B:517:ARG:HB3	1.96	0.66
1:A:41:PHE:HE1	1:A:79:ILE:HD11	1.60	0.66
1:A:294:VAL:HG22	4:A:2001:GOL:H2	1.79	0.65
1:A:605:GLN:HB3	1:A:612:ILE:HB	1.79	0.64
2:B:23:ASP:H	2:B:415:MET:CE	2.09	0.64
2:B:30:SER:HB2	2:B:469:MET:HB3	1.79	0.64
1:A:219:SER:HB2	1:A:222:VAL:O	1.99	0.63
1:A:326:PHE:CG	1:A:359:PRO:HG3	2.34	0.63
1:A:121:TYR:H	4:A:2006:GOL:H32	1.63	0.62
1:A:461:ASP:OD2	1:A:466:GLY:HA3	2.01	0.61
1:A:69:ARG:NH1	1:A:84:LYS:HG3	2.15	0.61
2:B:335:ILE:O	2:B:338:VAL:HG12	2.04	0.58
1:A:121:TYR:N	4:A:2006:GOL:H32	2.17	0.58
2:B:305:ILE:HG22	2:B:460:LEU:HD21	1.86	0.57
2:B:342:ARG:HE	2:B:355:PRO:HB3	1.70	0.57
2:B:66:ARG:HD3	2:B:82:ASP:OD2	2.04	0.56
1:A:482:ILE:HG23	1:A:497:VAL:HG13	1.86	0.56
1:A:57:ARG:HG3	1:A:121:TYR:CZ	2.40	0.55
1:A:482:ILE:HD13	1:A:497:VAL:HG11	1.89	0.55
1:A:444:SER:HB3	1:A:460:ALA:HB3	1.88	0.55
2:B:405:ILE:O	2:B:406:ILE:HB	2.07	0.54
1:A:137:CYS:SG	1:A:159:LEU:HD22	2.47	0.54
1:A:41:PHE:CE1	1:A:79:ILE:HD11	2.42	0.53
2:B:409:PRO:HG2	2:B:412:LEU:HD21	1.89	0.53
2:B:467:GLU:OE2	2:B:514:ARG:NH1	2.42	0.53
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.44	0.53
2:B:431:PRO:HG3	2:B:545:LEU:CD2	2.39	0.52
2:B:175:ALA:HB3	4:B:2002:GOL:H11	1.92	0.52
2:B:64:MET:HG2	2:B:69:TYR:CE2	2.44	0.52
1:A:121:TYR:HB2	4:A:2006:GOL:C3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ARG:HG2	2:B:158:GLU:HA	1.92	0.52
2:B:511:PRO:O	2:B:514:ARG:NH2	2.42	0.52
1:A:256:LEU:HD11	1:A:335:LEU:HD21	1.92	0.51
1:A:560:MET:HE1	1:A:582:VAL:HG11	1.92	0.51
2:B:22:GLU:HG3	2:B:415:MET:HE1	1.93	0.51
2:B:405:ILE:HG22	2:B:406:ILE:HG12	1.92	0.51
2:B:406:ILE:O	2:B:406:ILE:HG22	2.10	0.51
1:A:618:PRO:O	1:A:621:VAL:HG22	2.11	0.51
1:A:521:LEU:HD13	1:A:555:SER:C	2.31	0.51
2:B:556:ASP:O	2:B:559:ARG:O	2.29	0.50
2:B:545:LEU:N	2:B:545:LEU:HD12	2.26	0.50
1:A:106:VAL:HG12	6:A:3121:HOH:O	2.12	0.50
2:B:420:LEU:HD13	2:B:440:LEU:HD13	1.94	0.50
2:B:450:PHE:CD1	2:B:463:SER:HB2	2.47	0.50
2:B:175:ALA:O	4:B:2002:GOL:H32	2.11	0.50
2:B:123:VAL:HB	2:B:135:CYS:HB2	1.94	0.50
2:B:22:GLU:HG3	2:B:415:MET:CE	2.41	0.49
2:B:245:THR:O	2:B:246:MET:HB2	2.13	0.49
2:B:518:HIS:ND1	2:B:524:THR:HG22	2.28	0.49
1:A:318:PRO:HD3	1:A:332:GLU:O	2.13	0.49
2:B:301:ASP:HB2	4:B:2004:GOL:H32	1.93	0.49
2:B:60:MET:HE3	4:B:2002:GOL:H2	1.95	0.49
2:B:214:SER:HA	2:B:217:LEU:O	2.12	0.49
2:B:539:SER:HB2	2:B:541:SER:OG	2.13	0.49
1:A:539:ARG:HG3	6:A:3117:HOH:O	2.12	0.48
1:A:560:MET:HE3	1:A:586:PRO:HD2	1.95	0.48
1:A:123:GLU:O	1:A:125:ARG:HG3	2.12	0.48
1:A:326:PHE:CD1	1:A:359:PRO:HG3	2.49	0.48
1:A:576:ARG:N	1:A:615:SER:HB3	2.25	0.48
1:A:121:TYR:HD1	4:A:2006:GOL:H11	1.78	0.48
1:A:258:VAL:HG11	1:A:346:TYR:CE1	2.48	0.48
1:A:579:SER:HA	1:A:612:ILE:HD13	1.96	0.48
1:A:397:PRO:HD2	2:B:109:MET:O	2.15	0.47
2:B:562:THR:O	2:B:563:ASP:OD1	2.33	0.47
1:A:577:LEU:HD23	1:A:614:ILE:HG12	1.96	0.47
1:A:317:LYS:HB3	1:A:318:PRO:HD2	1.97	0.47
1:A:311:GLN:O	1:A:484:ARG:HD3	2.15	0.46
1:A:594:CYS:O	1:A:601:GLU:HA	2.16	0.46
1:A:633:LEU:HG	1:A:634:GLU:H	1.80	0.46
2:B:60:MET:HG2	2:B:71:ALA:HB3	1.97	0.46
2:B:534:GLY:N	2:B:545:LEU:HD11	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:HIS:CE1	2:B:96:THR:HG1	2.34	0.46
1:A:297:PRO:HG2	1:A:418:PRO:HA	1.96	0.46
2:B:66:ARG:NH2	2:B:493:ASP:OD1	2.45	0.46
1:A:540:ARG:HD3	6:A:3171:HOH:O	2.16	0.46
2:B:434:ASN:ND2	3:B:1434:NAG:C7	2.79	0.46
2:B:245:THR:O	2:B:246:MET:CB	2.64	0.45
1:A:73:LEU:HD23	1:A:79:ILE:HA	1.98	0.45
2:B:55:ARG:O	2:B:73:ARG:NH2	2.50	0.45
2:B:527:ALA:O	2:B:529:ARG:HG3	2.17	0.45
2:B:364:PRO:HG3	2:B:378:TYR:CE2	2.51	0.45
2:B:342:ARG:HE	2:B:355:PRO:CB	2.29	0.44
1:A:294:VAL:CG2	4:A:2001:GOL:H2	2.46	0.44
2:B:332:MET:CE	2:B:335:ILE:HD12	2.48	0.44
2:B:132:LEU:HG	2:B:149:VAL:HG22	2.00	0.44
2:B:301:ASP:H	4:B:2004:GOL:C3	2.31	0.44
2:B:284:SER:HB3	2:B:292:TYR:CD1	2.53	0.44
2:B:551:LEU:N	2:B:551:LEU:HD12	2.32	0.44
1:A:292:SER:O	1:A:294:VAL:HG23	2.18	0.43
1:A:233:LEU:HD23	1:A:239:PHE:HB3	1.99	0.43
2:B:536:VAL:HG12	2:B:538:GLU:H	1.83	0.43
1:A:469:GLN:HE22	1:A:472:MET:HE2	1.83	0.43
2:B:375:LEU:HD12	2:B:375:LEU:N	2.33	0.43
1:A:574:HIS:ND1	1:A:618:PRO:HD3	2.33	0.43
2:B:162:MET:O	2:B:163:ALA:HB3	2.18	0.43
2:B:39:PRO:HA	2:B:87:GLU:O	2.18	0.43
1:A:398:VAL:HA	1:A:399:PRO:HD3	1.92	0.43
1:A:536:MET:CE	1:A:538:SER:HB3	2.49	0.43
1:A:469:GLN:HE22	1:A:472:MET:CE	2.32	0.43
2:B:366:PRO:HB3	2:B:392:ILE:HB	2.00	0.42
2:B:322:ILE:HA	2:B:323:PRO:HD3	1.79	0.42
1:A:565:HIS:HA	1:A:566:PRO:HA	1.86	0.42
2:B:431:PRO:HG3	2:B:545:LEU:HD23	2.01	0.42
1:A:345:GLN:HG2	1:A:348:HIS:CE1	2.54	0.42
2:B:286:PRO:HA	2:B:290:HIS:ND1	2.35	0.42
2:B:97:TRP:CD1	2:B:145:ARG:NH1	2.88	0.42
1:A:189:ASP:O	1:A:191:LYS:HD2	2.19	0.42
1:A:605:GLN:O	1:A:611:VAL:HA	2.20	0.41
1:A:222:VAL:HG11	1:A:289:LYS:HG2	2.02	0.41
1:A:277:THR:HG22	1:A:279:ARG:HG3	2.01	0.41
2:B:109:MET:HE2	2:B:109:MET:HB3	1.95	0.41
2:B:250:VAL:O	2:B:294:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:LEU:O	2:B:199:ARG:HA	2.20	0.41
1:A:274:LEU:N	1:A:274:LEU:HD23	2.36	0.41
1:A:156:GLU:HB3	1:A:215:TYR:CE2	2.56	0.41
2:B:344:LYS:HD3	2:B:353:TRP:HB3	2.03	0.41
1:A:121:TYR:CB	4:A:2006:GOL:H32	2.48	0.41
1:A:577:LEU:CD2	1:A:614:ILE:HG12	2.50	0.41
1:A:555:SER:O	1:A:557:SER:N	2.54	0.41
1:A:536:MET:HE1	1:A:538:SER:HB3	2.03	0.41
2:B:227:ASP:OD1	2:B:227:ASP:C	2.59	0.41
2:B:405:ILE:O	2:B:406:ILE:CB	2.69	0.40
2:B:34:TYR:CZ	2:B:517:ARG:HD3	2.56	0.40
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.04	0.40
2:B:38:TYR:HA	2:B:39:PRO:HD3	1.90	0.40
1:A:97:PRO:HB3	1:A:133:TYR:HB3	2.04	0.40
1:A:57:ARG:O	1:A:490:ILE:HG12	2.22	0.40
1:A:525:ASP:HA	1:A:526:PRO:HD3	1.88	0.40
2:B:431:PRO:HG3	2:B:545:LEU:HD22	2.03	0.40
2:B:363:LYS:HA	2:B:364:PRO:C	2.42	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	603/681 (88%)	580 (96%)	21 (4%)	2 (0%)	46	50
2	B	532/565 (94%)	508 (96%)	21 (4%)	3 (1%)	30	29
All	All	1135/1246 (91%)	1088 (96%)	42 (4%)	5 (0%)	39	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	406	ILE
1	A	160	SER
2	B	246	MET
2	B	347	LYS
1	A	556	ILE

### 5.3.2 Protein sidechains ⓘ

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	534/597 (89%)	529 (99%)	5 (1%)	84	92
2	B	476/495 (96%)	473 (99%)	3 (1%)	90	95
All	All	1010/1092 (92%)	1002 (99%)	8 (1%)	86	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	298	PHE
1	A	438	TYR
1	A	451	LYS
1	A	501	ARG
2	B	347	LYS
2	B	514	ARG
2	B	517	ARG

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

Mol	Chain	Res	Type
1	A	558	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 ⓘ

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	1282	2,5	14,14,15	0.51	0	15,19,21	0.93	1 (6%)
5	NAG	B	1283	5	14,14,15	0.48	0	15,19,21	0.95	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
5	NAG	B	1282	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1283	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1283	NAG	C2-N2-C7	-2.66	119.62	123.04
5	B	1282	NAG	C1-O5-C5	2.82	115.83	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

11 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	$\# Z  > 2$
3	NAG	A	1076	1	14,14,15	0.43	0	15,19,21	1.24	1 (6%)
3	NAG	A	1163	1	14,14,15	0.51	0	15,19,21	0.77	0
3	NAG	A	1327	1	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
3	NAG	A	1598	1	14,14,15	0.56	0	15,19,21	0.62	0
4	GOL	A	2001	-	5,5,5	0.49	0	5,5,5	0.24	0
4	GOL	A	2003	-	5,5,5	0.35	0	5,5,5	0.22	0
4	GOL	A	2006	-	5,5,5	0.28	0	5,5,5	0.28	0
3	NAG	B	1065	2	14,14,15	0.55	0	15,19,21	0.97	1 (6%)
3	NAG	B	1434	2	14,14,15	0.48	0	15,19,21	1.44	2 (13%)
4	GOL	B	2002	-	5,5,5	0.29	0	5,5,5	0.38	0
4	GOL	B	2004	-	5,5,5	0.34	0	5,5,5	0.39	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	1076	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1163	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1327	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1598	1	-	0/6/23/26	0/1/1/1
4	GOL	A	2001	-	-	0/4/4/4	0/0/0/0
4	GOL	A	2003	-	-	0/4/4/4	0/0/0/0
4	GOL	A	2006	-	-	0/4/4/4	0/0/0/0
3	NAG	B	1065	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1434	2	-	0/6/23/26	0/1/1/1
4	GOL	B	2002	-	-	0/4/4/4	0/0/0/0
4	GOL	B	2004	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.



All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1434	NAG	C2-N2-C7	-3.50	118.54	123.04
3	B	1434	NAG	C4-C3-C2	-2.43	107.44	111.23
3	A	1327	NAG	C1-O5-C5	2.01	114.80	112.25
3	B	1065	NAG	C1-O5-C5	2.46	115.37	112.25
3	A	1076	NAG	C1-O5-C5	3.62	116.84	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	GOL	2	0
4	A	2006	GOL	6	0
3	B	1434	NAG	1	0
4	B	2002	GOL	3	0
4	B	2004	GOL	2	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	609/681 (89%)	0.38	60 (9%) 9 8	23, 44, 104, 141	0
2	B	540/565 (95%)	0.20	23 (4%) 39 38	24, 41, 96, 166	0
All	All	1149/1246 (92%)	0.30	83 (7%) 18 18	23, 43, 102, 166	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	567	ASP	8.3
2	B	568	CYS	8.1
1	A	656	CYS	7.9
1	A	630	TRP	7.7
1	A	572	SER	7.5
1	A	625	PRO	7.2
2	B	460	LEU	7.1
1	A	569	ILE	7.0
1	A	565	HIS	6.8
1	A	577	LEU	6.7
1	A	623	VAL	6.2
1	A	654	TYR	5.9
1	A	653	PHE	5.9
1	A	617	GLY	5.6
1	A	631	PHE	5.5
2	B	462	GLY	4.9
1	A	633	LEU	4.9
1	A	632	GLY	4.9
2	B	454	ILE	4.7
1	A	651	PHE	4.6
1	A	622	PRO	4.6
2	B	461	ASN	4.5
1	A	621	VAL	4.3
1	A	570	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	599	LEU	4.1
1	A	574	HIS	4.0
1	A	568	SER	4.0
1	A	624	ILE	3.9
1	A	655	ASN	3.8
1	A	571	VAL	3.8
1	A	274	LEU	3.8
1	A	612	ILE	3.7
1	A	616	PRO	3.7
2	B	519	GLY	3.7
2	B	521	CYS	3.6
2	B	562	THR	3.4
1	A	657	SER	3.3
1	A	465	HIS	3.3
1	A	598	ASN	3.3
2	B	523	LYS	3.2
1	A	556	ILE	3.2
2	B	537	ARG	3.1
1	A	348	HIS	3.1
2	B	540	GLY	3.1
1	A	652	LYS	3.0
2	B	520	LYS	3.0
2	B	29	ILE	2.9
1	A	628	GLN	2.9
1	A	429	ARG	2.9
1	A	619	LYS	2.9
1	A	262	THR	2.9
1	A	618	PRO	2.9
2	B	563	ASP	2.9
2	B	566	GLY	2.9
1	A	614	ILE	2.9
2	B	552	THR	2.9
1	A	579	SER	2.8
2	B	526	ILE	2.8
2	B	48	ARG	2.7
1	A	573	ASP	2.7
2	B	51	THR	2.7
1	A	576	ARG	2.7
1	A	629	ASP	2.7
1	A	567	ASN	2.7
2	B	550	ARG	2.7
2	B	453	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	566	PRO	2.6
1	A	347	HIS	2.6
1	A	263	PRO	2.5
1	A	613	CYS	2.5
1	A	37	GLN	2.5
1	A	602	VAL	2.5
1	A	578	LEU	2.5
1	A	564	VAL	2.4
1	A	575	SER	2.3
2	B	417	ARG	2.3
1	A	596	PHE	2.3
1	A	562	LEU	2.2
1	A	116	LEU	2.2
1	A	557	SER	2.1
1	A	554	ALA	2.1
1	A	547	TRP	2.0
1	A	646	PHE	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	1282	14/15	0.96	0.10	0.39	33,39,50,51	0
5	NAG	B	1283	14/15	0.92	0.17	-	40,60,72,73	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<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	2001	6/6	0.89	0.23	6.86	32,40,50,56	0
4	GOL	B	2004	6/6	0.89	0.24	4.45	63,71,75,77	0
4	GOL	A	2006	6/6	0.88	0.18	4.13	68,73,74,81	0
4	GOL	A	2003	6/6	0.78	0.18	2.57	72,75,80,84	0
3	NAG	A	1163	14/15	0.86	0.23	1.92	74,85,95,96	0
4	GOL	B	2002	6/6	0.89	0.18	1.12	39,57,64,66	0
3	NAG	A	1598	14/15	0.60	0.43	-	120,134,140,143	0
3	NAG	B	1434	14/15	0.80	0.26	-	92,107,115,119	0
3	NAG	B	1065	14/15	0.73	0.35	-	102,110,114,115	0
3	NAG	A	1327	14/15	0.83	0.21	-	52,80,106,113	0
3	NAG	A	1076	14/15	0.77	0.37	-	109,120,124,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.