



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:49 pm GMT

PDB ID : 3AL8
Title : Plexin A2 / Semaphorin 6A complex
Authors : Nogi, T.; Yasui, N.; Mihara, E.; Takagi, J.
Deposited on : 2010-07-28
Resolution : 3.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

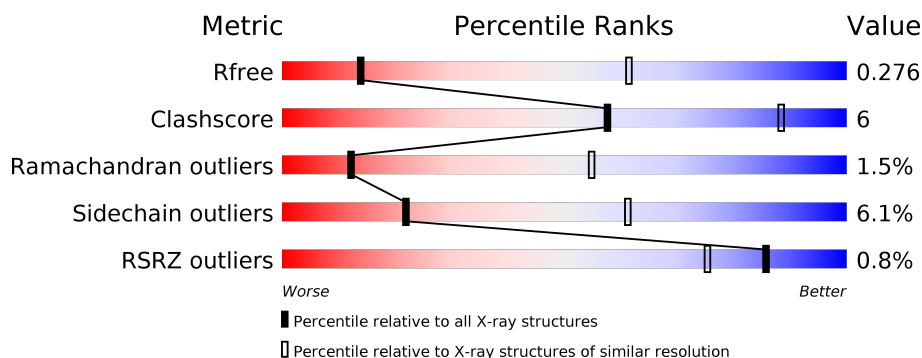
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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 $\leq 5\%$. 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	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 80%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 15% • • </div> </div>
2	B	539	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 71%, yellow 20%, orange 7%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 71% 20% • 7% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8329 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	537	Total	C	N	O	S	0	0	0
			4224	2679	721	792	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	EXPRESSION TAG	UNP O35464
A	16	SER	-	EXPRESSION TAG	UNP O35464
A	17	SER	-	EXPRESSION TAG	UNP O35464
A	18	ARG	-	EXPRESSION TAG	UNP O35464

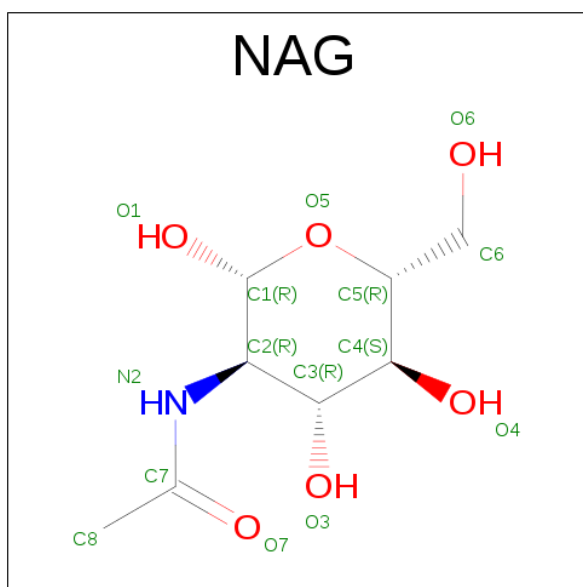
- Molecule 2 is a protein called Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	499	Total	C	N	O	S	0	0	0
			3924	2497	664	740	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	562	SER	-	EXPRESSION TAG	UNP P70207
B	563	ARG	-	EXPRESSION TAG	UNP P70207
B	564	GLU	-	EXPRESSION TAG	UNP P70207
B	565	ASN	-	EXPRESSION TAG	UNP P70207
B	566	LEU	-	EXPRESSION TAG	UNP P70207
B	567	TYR	-	EXPRESSION TAG	UNP P70207
B	568	PHE	-	EXPRESSION TAG	UNP P70207
B	569	GLN	-	EXPRESSION TAG	UNP P70207

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

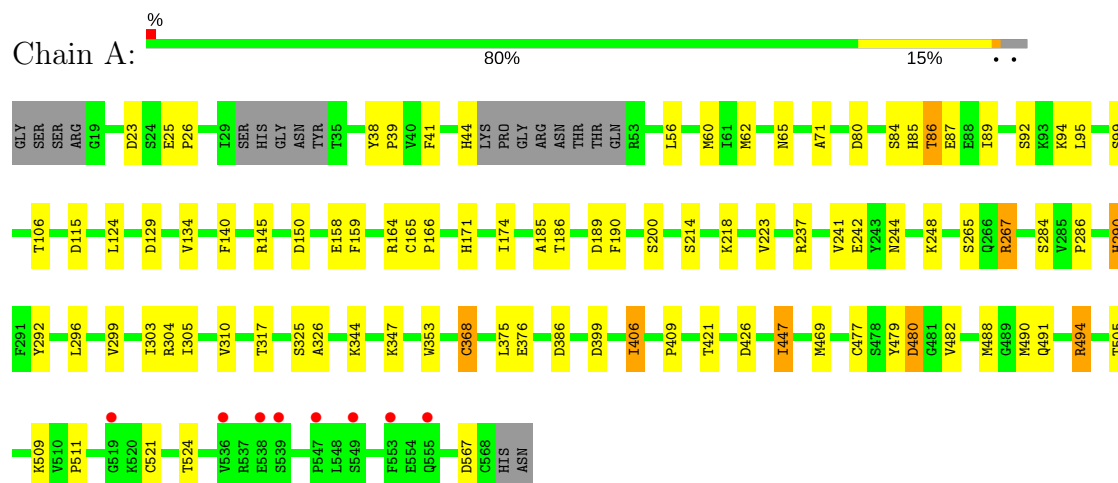
- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			83	46	2	35		

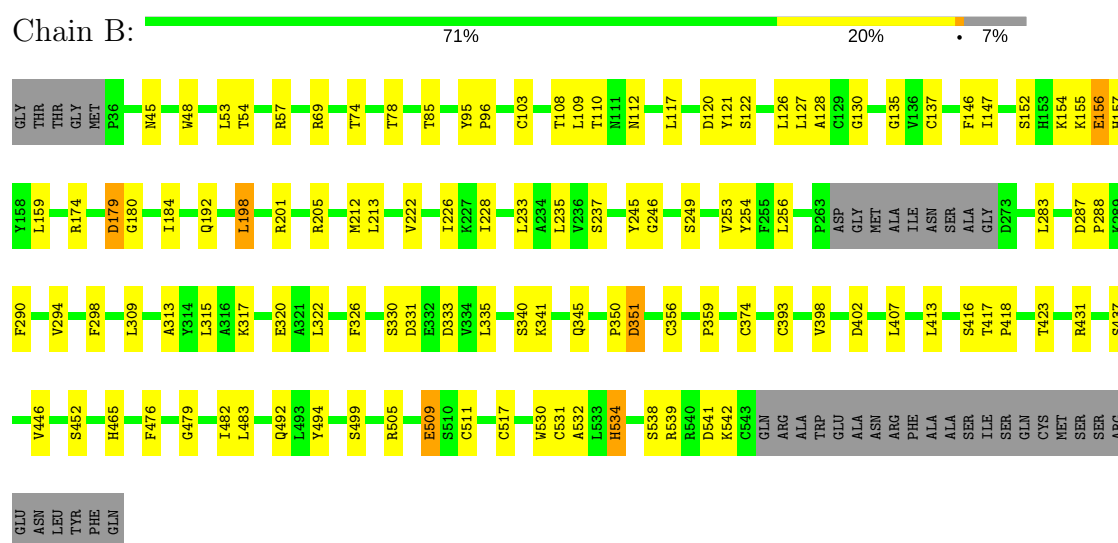
3 Residue-property plots

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



• Molecule 2: Plexin-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	240.87Å 240.87Å 146.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 3.60 49.14 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-3.60) 99.2 (49.14-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.287 0.222 , 0.276	Depositor DCC
R_{free} test set	1483 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8329	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: BMA, NAG, 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	0.39	0/4324	0.54	0/5858
2	B	0.38	0/4019	0.56	0/5454
All	All	0.38	0/8343	0.55	0/11312

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	4224	0	4083	37	0
2	B	3924	0	3835	55	0
3	A	28	0	26	0	0
3	B	14	0	13	1	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	B	83	0	70	0	0
All	All	8329	0	8077	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (92) 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:25:GLU:HG3	1:A:26:PRO:HD2	1.69	0.74
2:B:313:ALA:HB1	2:B:335:LEU:HD11	1.71	0.73
1:A:284:SER:HB3	1:A:292:TYR:CD2	2.27	0.70
2:B:198:LEU:HD21	2:B:283:LEU:HD11	1.74	0.69
1:A:477:CYS:O	1:A:505:THR:HG21	1.98	0.63
1:A:480:ASP:C	1:A:482:VAL:H	2.04	0.61
2:B:531:CYS:SG	2:B:534:HIS:HB2	2.41	0.61
2:B:74:THR:OG1	2:B:78:THR:HG22	1.99	0.60
1:A:145:ARG:HG2	1:A:158:GLU:HG2	1.85	0.58
2:B:120:ASP:OD2	2:B:174:ARG:NH2	2.37	0.58
1:A:60:MET:HG2	1:A:71:ALA:HB3	1.86	0.58
2:B:452:SER:O	2:B:479:GLY:HA2	2.04	0.57
1:A:41:PHE:HB2	1:A:89:ILE:HB	1.84	0.57
1:A:86:THR:OG1	1:A:87:GLU:N	2.38	0.57
2:B:192:GLN:HB2	2:B:228:ILE:O	2.05	0.57
2:B:155:LYS:HG2	2:B:156:GLU:OE2	2.05	0.56
2:B:309:LEU:HB2	2:B:340:SER:HB2	1.87	0.56
2:B:509:GLU:HG2	2:B:539:ARG:NH1	2.21	0.56
2:B:356:CYS:HB3	2:B:423:THR:HA	1.89	0.55
1:A:344:LYS:HG3	1:A:399:ASP:HA	1.90	0.54
1:A:447:ILE:HG22	1:A:469:MET:HG3	1.91	0.53
2:B:226:ILE:HG12	2:B:290:PHE:HD2	1.74	0.53
2:B:174:ARG:HG3	2:B:180:GLY:HA3	1.89	0.53
2:B:157:HIS:CE1	2:B:212:MET:O	2.62	0.53
2:B:476:PHE:HE2	2:B:482:ILE:HG12	1.74	0.52
2:B:538:SER:HB2	2:B:542:LYS:HE3	1.92	0.52
1:A:62:MET:HA	1:A:491:GLN:HE21	1.74	0.52
2:B:159:LEU:HD13	2:B:184:ILE:HD13	1.91	0.52
1:A:214:SER:HB2	1:A:218:LYS:HD2	1.92	0.51
2:B:174:ARG:NH1	2:B:179:ASP:O	2.39	0.51
2:B:85:THR:HB	2:B:112:ASN:HD22	1.76	0.51
2:B:511:CYS:HB2	2:B:538:SER:HA	1.93	0.51
1:A:174:ILE:HB	1:A:185:ALA:HB3	1.93	0.50
1:A:344:LYS:CG	1:A:399:ASP:HA	2.41	0.50
2:B:245:TYR:HB3	2:B:256:LEU:HD12	1.92	0.50
2:B:476:PHE:CE2	2:B:499:SER:HB3	2.48	0.49
2:B:317:LYS:HD2	2:B:331:ASP:O	2.13	0.49
2:B:137:CYS:SG	2:B:159:LEU:CD1	3.01	0.49
2:B:246:GLY:HA2	2:B:254:TYR:O	2.12	0.48
2:B:137:CYS:SG	2:B:159:LEU:HD11	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:CYS:SG	1:A:166:PRO:HD2	2.54	0.48
2:B:315:LEU:HD11	2:B:333:ASP:HB3	1.95	0.48
1:A:56:LEU:HD13	1:A:479:TYR:OH	2.13	0.47
2:B:108:THR:HG22	2:B:109:LEU:N	2.29	0.47
2:B:117:LEU:HD11	2:B:126:LEU:HD21	1.96	0.47
2:B:539:ARG:HG2	2:B:542:LYS:HG2	1.95	0.47
2:B:130:GLY:O	2:B:135:GLY:HA2	2.14	0.47
2:B:122:SER:HB3	2:B:174:ARG:HE	1.80	0.46
2:B:374:CYS:O	2:B:393:CYS:HB3	2.16	0.46
1:A:164:ARG:HH21	1:A:200:SER:HB2	1.81	0.46
1:A:326:ALA:HB1	1:A:409:PRO:HB3	1.97	0.46
1:A:447:ILE:HD11	1:A:490:MET:SD	2.55	0.46
2:B:476:PHE:CE2	2:B:482:ILE:HG12	2.51	0.46
2:B:249:SER:HB3	2:B:254:TYR:CE2	2.51	0.45
2:B:179:ASP:HA	2:B:205:ARG:HD3	1.98	0.45
1:A:39:PRO:HG2	1:A:509:LYS:HD3	1.99	0.45
2:B:494:TYR:CD1	2:B:505:ARG:HG2	2.52	0.45
1:A:124:LEU:HD13	1:A:134:VAL:HG22	1.99	0.45
1:A:248:LYS:HG3	1:A:248:LYS:O	2.17	0.44
1:A:296:LEU:HD11	1:A:299:VAL:HG23	2.00	0.44
1:A:38:TYR:CD1	1:A:511:PRO:HD2	2.52	0.44
2:B:320:GLU:HA	2:B:320:GLU:OE1	2.16	0.44
2:B:154:LYS:HB3	2:B:157:HIS:CD2	2.52	0.44
2:B:74:THR:OG1	2:B:78:THR:CG2	2.64	0.44
2:B:326:PHE:CD1	2:B:359:PRO:HG3	2.53	0.43
2:B:398:VAL:HG11	2:B:407:LEU:HD11	1.99	0.43
1:A:223:VAL:HG21	1:A:296:LEU:HG	2.01	0.43
1:A:94:LYS:HG2	1:A:95:LEU:H	1.83	0.43
1:A:267:ARG:HD3	1:A:386:ASP:OD1	2.18	0.43
2:B:57:ARG:HG2	2:B:121:TYR:CE2	2.53	0.43
1:A:480:ASP:C	1:A:482:VAL:N	2.70	0.43
2:B:294:VAL:HG23	2:B:413:LEU:HB3	2.00	0.43
2:B:95:TYR:HA	2:B:96:PRO:C	2.39	0.43
1:A:242:GLU:HA	1:A:353:TRP:CD1	2.54	0.43
2:B:249:SER:HB3	2:B:254:TYR:HE2	1.84	0.43
1:A:286:PRO:HA	1:A:290:HIS:HB3	2.01	0.42
1:A:305:ILE:HD12	1:A:310:VAL:HG21	2.01	0.42
2:B:437:SER:HB2	2:B:446:VAL:HG22	1.99	0.42
2:B:53:LEU:HD23	2:B:54:THR:N	2.34	0.42
2:B:517:CYS:HB2	2:B:530:TRP:CE2	2.54	0.42
1:A:140:PHE:HB3	1:A:190:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:HB3	1:A:292:TYR:HD2	1.82	0.41
2:B:78:THR:HG21	3:B:9101:NAG:H3	2.02	0.41
2:B:127:LEU:HD12	2:B:128:ALA:N	2.35	0.41
1:A:368:CYS:HB3	1:A:375:LEU:HD22	2.01	0.41
2:B:201:ARG:HB3	2:B:213:LEU:HA	2.02	0.41
1:A:237:ARG:NH1	1:A:296:LEU:O	2.51	0.41
2:B:287:ASP:HA	2:B:288:PRO:HD3	1.76	0.41
1:A:189:ASP:N	1:A:189:ASP:OD1	2.53	0.41
2:B:351:ASP:HA	2:B:431:ARG:HG3	2.03	0.41
1:A:426:ASP:OD1	1:A:494:ARG:NH2	2.55	0.40
2:B:45:ASN:HB3	2:B:48:TRP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/556 (96%)	478 (90%)	46 (9%)	7 (1%)	14	57
2	B	495/539 (92%)	435 (88%)	52 (10%)	8 (2%)	11	53
All	All	1026/1095 (94%)	913 (89%)	98 (10%)	15 (2%)	12	55

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	237	SER
1	A	84	SER
1	A	92	SER
1	A	347	LYS
2	B	345	GLN
2	B	152	SER
2	B	350	PRO

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Mol	Chain	Res	Type
1	A	265	SER
2	B	418	PRO
2	B	532	ALA
1	A	65	ASN
1	A	186	THR
2	B	147	ILE
2	B	534	HIS
1	A	406	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	463/487 (95%)	432 (93%)	31 (7%)	19	58
2	B	438/468 (94%)	414 (94%)	24 (6%)	25	64
All	All	901/955 (94%)	846 (94%)	55 (6%)	22	61

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	44	HIS
1	A	80	ASP
1	A	85	HIS
1	A	86	THR
1	A	99	SER
1	A	106	THR
1	A	115	ASP
1	A	129	ASP
1	A	150	ASP
1	A	159	PHE
1	A	171	HIS
1	A	241	VAL
1	A	244	ASN
1	A	267	ARG

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Mol	Chain	Res	Type
1	A	290	HIS
1	A	303	ILE
1	A	304	ARG
1	A	317	THR
1	A	325	SER
1	A	368	CYS
1	A	376	GLU
1	A	406	ILE
1	A	421	THR
1	A	447	ILE
1	A	480	ASP
1	A	488	MET
1	A	494	ARG
1	A	521	CYS
1	A	524	THR
1	A	567	ASP
2	B	69	ARG
2	B	103	CYS
2	B	110	THR
2	B	146	PHE
2	B	156	GLU
2	B	179	ASP
2	B	198	LEU
2	B	222	VAL
2	B	233	LEU
2	B	235	LEU
2	B	253	VAL
2	B	298	PHE
2	B	322	LEU
2	B	330	SER
2	B	341	LYS
2	B	351	ASP
2	B	402	ASP
2	B	416	SER
2	B	417	THR
2	B	465	HIS
2	B	483	LEU
2	B	492	GLN
2	B	509	GLU
2	B	541	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

11 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	$\# Z > 2$
4	NAG	A	9601	1,4	14,14,15	0.46	0	15,19,21	1.65	4 (26%)
4	NAG	A	9602	4	14,14,15	0.48	0	15,19,21	1.19	1 (6%)
4	NAG	B	9201	2,4	14,14,15	0.49	0	15,19,21	0.97	0
4	NAG	B	9202	4	14,14,15	0.60	0	15,19,21	1.02	1 (6%)
5	NAG	B	9301	2,5	14,14,15	0.58	0	15,19,21	0.97	1 (6%)
5	NAG	B	9302	5	14,14,15	0.53	0	15,19,21	0.67	0
5	BMA	B	9303	5	11,11,12	0.41	0	13,15,17	1.38	2 (15%)
5	MAN	B	9304	5	11,11,12	0.55	0	13,15,17	0.93	0
5	MAN	B	9305	5	11,11,12	0.43	0	13,15,17	1.31	1 (7%)
5	MAN	B	9306	5	11,11,12	0.37	0	13,15,17	1.15	2 (15%)
5	MAN	B	9307	5	11,11,12	0.59	0	13,15,17	0.78	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
4	NAG	A	9601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	9602	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	9201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	9202	4	-	0/6/23/26	0/1/1/1
5	NAG	B	9301	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	9302	5	-	0/6/23/26	0/1/1/1
5	BMA	B	9303	5	-	0/2/19/22	0/1/1/1
5	MAN	B	9304	5	-	0/2/19/22	0/1/1/1
5	MAN	B	9305	5	-	0/2/19/22	0/1/1/1
5	MAN	B	9306	5	-	0/2/19/22	0/1/1/1
5	MAN	B	9307	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	9601	NAG	O5-C1-C2	-3.23	106.98	111.47
4	A	9601	NAG	C4-C3-C2	-2.01	108.07	111.02
5	B	9306	MAN	C1-O5-C5	2.24	115.25	112.17
5	B	9303	BMA	C1-O5-C5	2.25	115.27	112.17
5	B	9301	NAG	C4-C3-C2	2.52	114.72	111.02
4	B	9202	NAG	C1-O5-C5	2.69	115.87	112.17
5	B	9306	MAN	C1-C2-C3	2.75	113.14	109.65
4	A	9602	NAG	C1-O5-C5	2.83	116.07	112.17
4	A	9601	NAG	C1-O5-C5	2.98	116.27	112.17
5	B	9305	MAN	C1-C2-C3	3.01	113.47	109.65
4	A	9601	NAG	C1-C2-N2	3.14	115.85	110.49
5	B	9303	BMA	C1-C2-C3	3.46	114.04	109.65

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

3 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	9401	1	14,14,15	0.49	0	15,19,21	1.53	3 (20%)
3	NAG	A	9501	1	14,14,15	0.45	0	15,19,21	1.35	1 (6%)
3	NAG	B	9101	2	14,14,15	0.61	0	15,19,21	1.01	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
3	NAG	A	9401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	9501	1	-	0/6/23/26	0/1/1/1
3	NAG	B	9101	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	9401	NAG	O5-C1-C2	-2.12	108.52	111.47
3	A	9401	NAG	C3-C4-C5	-2.04	106.63	110.22
3	B	9101	NAG	C2-N2-C7	2.35	126.37	122.94
3	A	9401	NAG	C1-O5-C5	3.88	117.51	112.17
3	A	9501	NAG	C1-O5-C5	3.91	117.55	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	9101	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	537/556 (96%)	-0.05	8 (1%) 74 61	71, 96, 150, 158	0
2	B	499/539 (92%)	-0.22	0 100 100	71, 95, 132, 144	0
All	All	1036/1095 (94%)	-0.13	8 (0%) 86 75	71, 96, 142, 158	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	GLU	3.0
1	A	555	GLN	2.5
1	A	553	PHE	2.4
1	A	519	GLY	2.3
1	A	536	VAL	2.2
1	A	547	PRO	2.2
1	A	549	SER	2.2
1	A	539	SER	2.2

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, 95th 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(\AA^2)	Q<0.9
5	MAN	B	9307	11/12	0.94	0.21	-0.61	103,104,104,104	0
5	MAN	B	9304	11/12	0.92	0.29	-	113,114,114,114	0
4	NAG	B	9202	14/15	0.89	0.33	-	119,120,120,120	0
4	NAG	B	9201	14/15	0.94	0.18	-	109,111,113,116	0
5	BMA	B	9303	11/12	0.94	0.12	-	106,108,110,112	0
5	MAN	B	9306	11/12	0.94	0.16	-	106,106,106,107	0
4	NAG	A	9601	14/15	0.84	0.39	-	134,137,138,140	0
5	NAG	B	9302	14/15	0.94	0.17	-	104,106,107,107	0
5	MAN	B	9305	11/12	0.96	0.14	-	104,105,106,106	0
5	NAG	B	9301	14/15	0.95	0.12	-	100,101,103,104	0
4	NAG	A	9602	14/15	0.82	0.42	-	142,142,143,143	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, 95th 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(\AA^2)	Q<0.9
3	NAG	A	9401	14/15	0.89	0.24	0.31	89,90,91,92	0
3	NAG	A	9501	14/15	0.88	0.33	-	123,125,126,126	0
3	NAG	B	9101	14/15	0.78	0.26	-	119,121,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.