



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2021 – 07:14 pm GMT

PDB ID : 7NE0
Title : Structure of the ternary complex between Netrin-1, Repulsive-Guidance Molecule-B (RGMB) and Neogenin
Authors : Robinson, R.A.; Griffiths, S.C.; van de Haar, L.L.; Malinauskas, T.; van Battum, E.Y.; Zelina, P.; Schwab, R.A.; Karia, D.; Malinauskaite, L.; Brignani, S.; van den Munkhof, M.; Dudukcu, O.; De Ruiter, A.A.; Van den Heuvel, D.M.A.; Bishop, B.; Elegheert, J.; Aricescu, A.R.; Pasterkamp, R.J.; Siebold, C.
Deposited on : 2021-02-02
Resolution : 3.25 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.2.dev2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.2.dev2

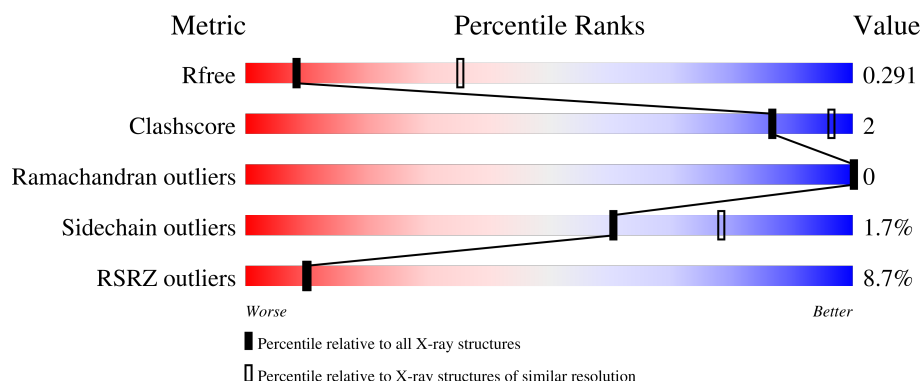
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



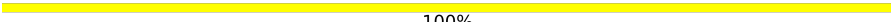


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	444	<div> <div>2%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
2	B	354	<div> <div>6%</div> <div>79%</div> <div>6%</div> <div>16%</div> </div>
3	C	35	<div> <div>29%</div> <div>40%</div> <div>•</div> <div>57%</div> </div>
4	D	165	<div> <div>21%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
5	I	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	J	2	 100%
5	K	2	 100%
5	L	2	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7253 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 Netrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3267	1996	623	608	40			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	-	expression tag	UNP O95631
A	23	THR	-	expression tag	UNP O95631
A	454	GLY	-	expression tag	UNP O95631
A	455	THR	-	expression tag	UNP O95631
A	456	LYS	-	expression tag	UNP O95631
A	457	THR	-	expression tag	UNP O95631
A	458	GLU	-	expression tag	UNP O95631
A	459	THR	-	expression tag	UNP O95631
A	460	SER	-	expression tag	UNP O95631
A	461	GLN	-	expression tag	UNP O95631
A	462	VAL	-	expression tag	UNP O95631
A	463	ALA	-	expression tag	UNP O95631
A	464	PRO	-	expression tag	UNP O95631
A	465	ALA	-	expression tag	UNP O95631

- Molecule 2 is a protein called Neogenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2358	1505	402	445	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	763	GLU	-	expression tag	UNP Q7TQG5
B	764	THR	-	expression tag	UNP Q7TQG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	765	GLY	-	expression tag	UNP Q7TQG5
B	1108	GLY	-	expression tag	UNP Q7TQG5
B	1109	THR	-	expression tag	UNP Q7TQG5
B	1110	LYS	-	expression tag	UNP Q7TQG5
B	1111	HIS	-	expression tag	UNP Q7TQG5
B	1112	HIS	-	expression tag	UNP Q7TQG5
B	1113	HIS	-	expression tag	UNP Q7TQG5
B	1114	HIS	-	expression tag	UNP Q7TQG5
B	1115	HIS	-	expression tag	UNP Q7TQG5
B	1116	HIS	-	expression tag	UNP Q7TQG5

- Molecule 3 is a protein called Repulsive Guidance Molecule B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	S	0	0	0
			121	80	18	21	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	134	GLU	-	expression tag	UNP Q6NW40
C	136	GLY	HIS	conflict	UNP Q6NW40

- Molecule 4 is a protein called Repulsive Guidance Molecule B C-terminal region (chain D).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	161	Total	C	N	O	S	0	0	0
			1225	767	213	238	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	225	GLY	GLU	conflict	UNP Q6NW40

- Molecule 5 is an oligosaccharide called 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	O	S	0	0	0
			55	12	35	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	2	Total	C	O	S	0	0	0
			55	12	35	8			
5	K	2	Total	C	O	S	0	0	0
			55	12	35	8			
5	L	2	Total	C	O	S	0	0	0
			55	12	35	8			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

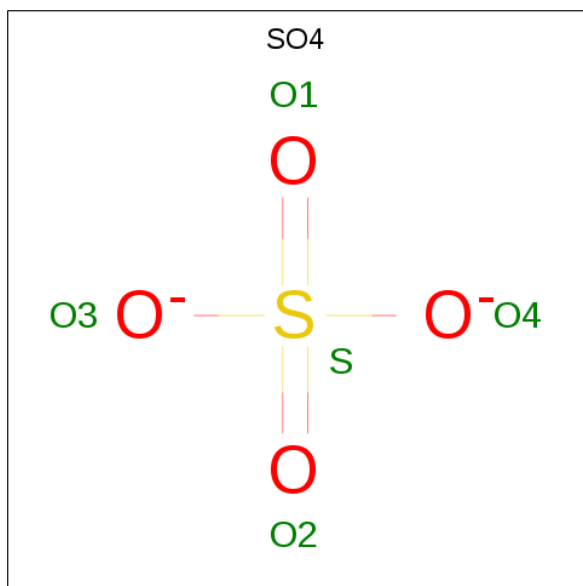


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

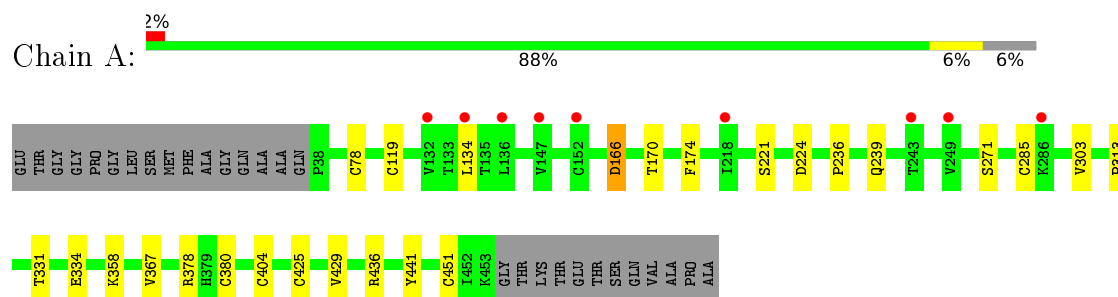


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

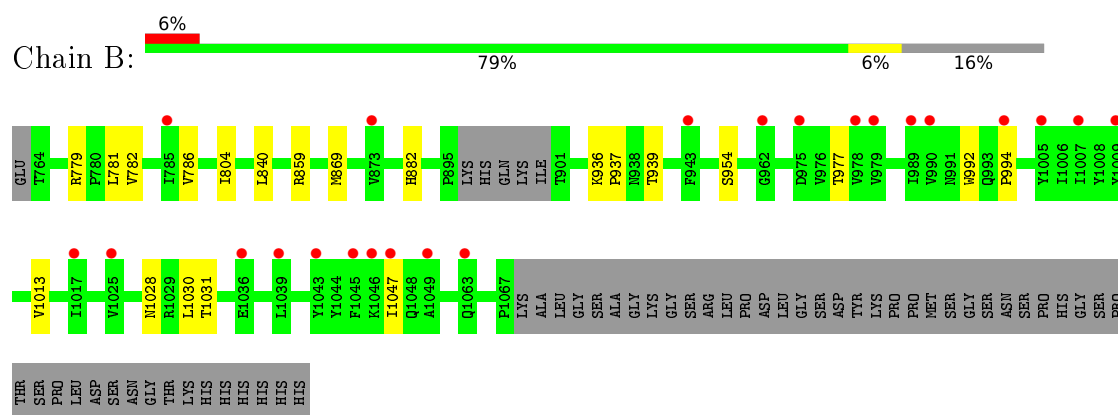
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

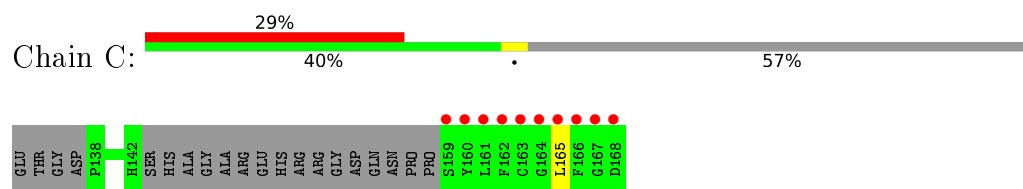
• Molecule 1: Netrin-1



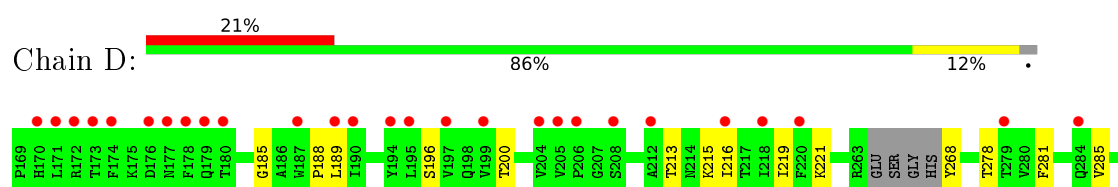
• Molecule 2: Neogenin

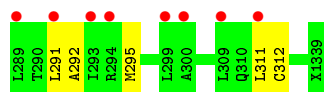


• Molecule 3: Repulsive Guidance Molecule B



• Molecule 4: Repulsive Guidance Molecule B C-terminal region (chain D)





- Molecule 5: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain I:  100%



- Molecule 5: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain J:  100%



- Molecule 5: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain K:  100%



- Molecule 5: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

Chain L:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	136.78 Å 136.78 Å 430.11 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.96 – 3.25 79.62 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-3.25) 99.9 (79.62-3.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.26 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.249 , 0.263 0.271 , 0.291	Depositor DCC
R_{free} test set	1277 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	126.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 105.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YYJ, SO4, NAG, CA, GU4

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	0.36	0/3349	0.56	0/4531
2	B	0.37	0/2425	0.55	0/3324
3	C	0.34	0/125	0.49	0/166
4	D	0.38	0/1197	0.53	0/1626
All	All	0.37	0/7096	0.55	0/9647

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 [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	3267	0	3072	11	0
2	B	2358	0	2339	10	0
3	C	121	0	100	1	0
4	D	1225	0	1162	11	0
5	I	55	0	6	0	0
5	J	55	0	6	0	0
5	K	55	0	6	1	0
5	L	55	0	6	0	0
6	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
All	All	7253	0	6749	29	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 2.

All (29) 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:1031:THR:HG21	4:D:188:PRO:HG3	1.72	0.69
2:B:869:MET:HB2	2:B:954:SER:HB2	1.80	0.63
5:K:1:GU4:O5	5:K:2:YYJ:C1	2.46	0.62
1:A:221:SER:HB3	1:A:224:ASP:HB2	1.91	0.52
4:D:196:SER:HB3	4:D:219:ILE:HB	1.92	0.52
2:B:977:THR:HG21	4:D:185:GLY:HA3	1.92	0.52
3:C:165:LEU:HD21	4:D:213:THR:HG21	1.92	0.52
4:D:189:LEU:HD23	4:D:311:LEU:HB2	1.91	0.51
1:A:303:VAL:HG13	1:A:313:PRO:HA	1.91	0.51
2:B:779:ARG:HB3	2:B:786:VAL:HB	1.92	0.50
2:B:994:PRO:HD3	2:B:1030:LEU:HD21	1.93	0.49
1:A:429:VAL:HG13	1:A:436:ARG:O	2.14	0.48
4:D:200:THR:HG22	4:D:215:LYS:HB3	1.96	0.47
2:B:992:TRP:HB3	2:B:1047:ILE:HD13	1.96	0.47
1:A:367:VAL:HG23	1:A:378:ARG:HA	1.97	0.47
1:A:441:TYR:HB3	1:A:451:CYS:HB3	1.96	0.47
1:A:331:THR:HG23	1:A:334:GLU:H	1.79	0.46
2:B:1028:ASN:HB2	4:D:221:LYS:HD3	1.98	0.46
1:A:166:ASP:OD2	1:A:170:THR:HG22	2.16	0.46
4:D:216:ILE:HD13	4:D:291:LEU:HD13	1.98	0.45
2:B:882:HIS:HB2	2:B:937:PRO:HB3	2.00	0.43
4:D:278:THR:HB	4:D:295:MET:HG3	2.01	0.42
4:D:281:PHE:HB2	4:D:292:ALA:HB3	2.02	0.42
1:A:78:CYS:HB2	1:A:271:SER:HB3	2.01	0.42
1:A:358:LYS:HB3	4:D:285:VAL:HG13	2.01	0.41
2:B:936:LYS:HB2	2:B:939:THR:HG21	2.03	0.41
1:A:425:CYS:HB3	1:A:429:VAL:HB	2.03	0.40
2:B:782:VAL:HA	2:B:859:ARG:O	2.21	0.40
1:A:236:PRO:HA	1:A:239:GLN: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	414/444 (93%)	400 (97%)	14 (3%)	0	100	100
2	B	295/354 (83%)	285 (97%)	10 (3%)	0	100	100
3	C	11/35 (31%)	11 (100%)	0	0	100	100
4	D	147/165 (89%)	138 (94%)	9 (6%)	0	100	100
All	All	867/998 (87%)	834 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	360/378 (95%)	353 (98%)	7 (2%)	57	76
2	B	267/313 (85%)	263 (98%)	4 (2%)	65	80
3	C	13/28 (46%)	13 (100%)	0	100	100
4	D	131/134 (98%)	129 (98%)	2 (2%)	65	80
All	All	771/853 (90%)	758 (98%)	13 (2%)	60	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	CYS
1	A	134	LEU
1	A	166	ASP
1	A	174	PHE
1	A	285	CYS
1	A	380	CYS
1	A	404	CYS
2	B	781	LEU
2	B	804	ILE
2	B	840	LEU
2	B	1013	VAL
4	D	268	TYR
4	D	312	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	121	GLN
1	A	150	GLN
1	A	397	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 monosaccharides 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	GU4	I	1	5	27,27,28	1.78	5 (18%)	29,43,45	1.28	3 (10%)
5	YYJ	I	2	5	27,28,28	1.79	5 (18%)	28,46,46	0.98	2 (7%)
5	GU4	J	1	5	27,27,28	1.78	5 (18%)	29,43,45	2.95	8 (27%)
5	YYJ	J	2	5	27,28,28	1.44	5 (18%)	28,46,46	0.96	2 (7%)
5	GU4	K	1	5	27,27,28	1.78	5 (18%)	29,43,45	1.15	2 (6%)
5	YYJ	K	2	5	27,28,28	1.76	4 (14%)	28,46,46	0.74	1 (3%)
5	GU4	L	1	5	27,27,28	1.77	5 (18%)	29,43,45	1.69	5 (17%)
5	YYJ	L	2	5	27,28,28	1.58	5 (18%)	28,46,46	0.75	1 (3%)

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	GU4	I	1	5	-	0/21/38/41	0/1/1/1
5	YYJ	I	2	5	-	5/23/42/42	0/1/1/1
5	GU4	J	1	5	-	4/21/38/41	0/1/1/1
5	YYJ	J	2	5	-	6/23/42/42	0/1/1/1
5	GU4	K	1	5	-	4/21/38/41	0/1/1/1
5	YYJ	K	2	5	-	10/23/42/42	0/1/1/1
5	GU4	L	1	5	-	2/21/38/41	0/1/1/1
5	YYJ	L	2	5	-	5/23/42/42	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	YYJ	O3S1-S1	4.45	1.64	1.45
5	I	1	GU4	O22-S6	4.43	1.64	1.45
5	I	2	YYJ	O2S3-S3	4.43	1.64	1.45
5	I	1	GU4	O28-S3	4.43	1.64	1.45
5	L	1	GU4	O27-S3	4.42	1.64	1.45
5	L	1	GU4	O25-S4	4.41	1.64	1.45
5	K	2	YYJ	O3S4-S4	4.40	1.64	1.45
5	J	1	GU4	O23-S6	4.40	1.64	1.45
5	J	1	GU4	O25-S4	4.40	1.64	1.45
5	L	2	YYJ	O2S6-S6	4.39	1.64	1.45
5	J	1	GU4	O27-S3	4.39	1.64	1.45
5	L	2	YYJ	O3S1-S1	4.39	1.64	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	GU4	O26-S4	4.37	1.64	1.45
5	I	2	YYJ	O2S1-S1	4.37	1.64	1.45
5	I	2	YYJ	O3S4-S4	4.37	1.64	1.45
5	L	1	GU4	O23-S6	4.37	1.63	1.45
5	K	1	GU4	O12-S2	4.36	1.63	1.45
5	K	1	GU4	O22-S6	4.36	1.63	1.45
5	K	1	GU4	O28-S3	4.36	1.63	1.45
5	K	2	YYJ	O3S6-S6	4.34	1.63	1.45
5	K	2	YYJ	O3S1-S1	4.32	1.63	1.45
5	I	2	YYJ	O2-C2	3.21	1.46	1.40
5	J	2	YYJ	O2-C2	2.93	1.45	1.40
5	K	1	GU4	O2-C2	-2.86	1.42	1.47
5	I	1	GU4	O2-C2	-2.48	1.43	1.47
5	L	2	YYJ	O2-C2	2.27	1.44	1.40
5	L	1	GU4	O2-C2	-2.27	1.43	1.47
5	J	2	YYJ	O1S3-S3	2.24	1.64	1.50
5	L	1	GU4	O10-S2	2.24	1.64	1.50
5	L	2	YYJ	O1S4-S4	2.23	1.64	1.50
5	J	1	GU4	O2-C2	-2.23	1.43	1.47
5	J	1	GU4	O10-S2	2.23	1.64	1.50
5	J	2	YYJ	O1S4-S4	2.22	1.64	1.50
5	I	1	GU4	O10-S2	2.22	1.64	1.50
5	K	1	GU4	O24-S4	2.22	1.64	1.50
5	J	2	YYJ	O1S6-S6	2.22	1.64	1.50
5	L	2	YYJ	O1S3-S3	2.21	1.64	1.50
5	I	2	YYJ	O1S6-S6	2.21	1.64	1.50
5	K	2	YYJ	O1S3-S3	2.20	1.63	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1	GU4	O10-S2-O11	-8.59	78.62	108.49
5	J	1	GU4	O12-S2-O11	-8.28	79.00	112.22
5	J	1	GU4	O10-S2-O12	6.56	131.29	108.49
5	L	1	GU4	C1-O5-C5	5.10	119.11	112.19
5	J	1	GU4	C1-O5-C5	4.78	118.67	112.19
5	L	1	GU4	O2-C2-C3	4.65	111.80	106.65
5	I	1	GU4	O2-C2-C3	3.82	110.88	106.65
5	K	1	GU4	O2-C2-C3	3.71	110.76	106.65
5	L	1	GU4	C2-O2-S2	3.54	122.52	117.91
5	I	1	GU4	C2-O2-S2	3.31	122.23	117.91
5	J	1	GU4	O2-C2-C3	3.04	110.02	106.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1	GU4	C2-O2-S2	2.97	121.79	117.91
5	I	1	GU4	C1-O5-C5	2.97	116.22	112.19
5	K	1	GU4	C1-O5-C5	2.86	116.07	112.19
5	J	2	YYJ	O5-C5-C4	2.50	107.66	103.49
5	K	2	YYJ	O5-C5-C4	2.36	107.43	103.49
5	J	1	GU4	C3-O3-S3	2.31	123.33	118.88
5	L	1	GU4	O3-C3-C4	2.25	113.41	108.48
5	J	1	GU4	C3-C4-C5	2.21	115.16	110.55
5	I	2	YYJ	O5-C5-C4	2.14	107.07	103.49
5	L	1	GU4	C4-O4-S4	2.11	122.94	118.88
5	J	2	YYJ	C4-O4-S4	2.09	122.91	118.88
5	I	2	YYJ	O3-C3-C2	2.08	117.31	111.50
5	L	2	YYJ	O5-C5-C4	2.01	106.85	103.49

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	YYJ	C6-O6-S6-O1S6
5	I	2	YYJ	C6-O6-S6-O2S6
5	I	2	YYJ	C6-O6-S6-O3S6
5	J	1	GU4	O5-C5-C6-O6
5	J	1	GU4	C4-C5-C6-O6
5	J	2	YYJ	O1-C1-C2-C3
5	J	2	YYJ	C4-C5-C6-O6
5	K	1	GU4	C6-O6-S6-O21
5	K	2	YYJ	O1-C1-C2-O2
5	K	2	YYJ	O1-C1-C2-O5
5	K	2	YYJ	C4-C5-C6-O6
5	K	2	YYJ	C1-O1-S1-O1S1
5	L	2	YYJ	O1-C1-C2-C3
5	L	2	YYJ	O1-C1-C2-O2
5	L	2	YYJ	O1-C1-C2-O5
5	L	2	YYJ	C4-C5-C6-O6
5	J	2	YYJ	C1-O1-S1-O2S1
5	K	1	GU4	C6-O6-S6-O22
5	K	2	YYJ	C1-O1-S1-O2S1
5	K	2	YYJ	C1-O1-S1-O3S1
5	K	2	YYJ	C6-O6-S6-O3S6
5	L	1	GU4	O5-C5-C6-O6
5	J	2	YYJ	O5-C5-C6-O6
5	J	2	YYJ	C1-O1-S1-O1S1

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Mol	Chain	Res	Type	Atoms
5	K	2	YYJ	C6-O6-S6-O1S6
5	J	1	GU4	C2-O2-S2-O12
5	K	1	GU4	C6-O6-S6-O23
5	K	2	YYJ	C6-O6-S6-O2S6
5	K	2	YYJ	O5-C5-C6-O6
5	L	2	YYJ	O5-C5-C6-O6
5	J	2	YYJ	C1-O1-S1-O3S1
5	L	1	GU4	C4-C5-C6-O6
5	J	1	GU4	C2-O2-S2-O10
5	I	2	YYJ	O1-C1-C2-C3
5	I	2	YYJ	C2-C1-O1-S1
5	K	1	GU4	C5-C6-O6-S6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	GU4	1	0
5	K	2	YYJ	1	0

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
6	NAG	B	1201	2	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
6	NAG	A	503	1	14,14,15	0.32	0	17,19,21	0.68	0
6	NAG	A	501	1	14,14,15	0.31	0	17,19,21	0.71	0
8	SO4	A	505	-	4,4,4	0.13	0	6,6,6	0.08	0
6	NAG	A	502	1	14,14,15	0.31	0	17,19,21	0.97	2 (11%)

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
6	NAG	A	501	1	-	1/6/23/26	0/1/1/1
6	NAG	A	503	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1201	2	-	0/6/23/26	0/1/1/1
6	NAG	A	502	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	502	NAG	C1-C2-N2	2.38	114.55	110.49
6	B	1201	NAG	C1-O5-C5	2.33	115.35	112.19
6	A	502	NAG	C2-N2-C7	2.07	125.85	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	NAG	O5-C5-C6-O6
6	A	503	NAG	O5-C5-C6-O6
6	A	502	NAG	C3-C2-N2-C7
6	A	502	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	323:ASP	C	1330:UNK	N	15.77

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, 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	416/444 (93%)	0.26	9 (2%) 62 59	91, 142, 186, 211	0
2	B	299/354 (84%)	0.51	23 (7%) 13 12	98, 154, 226, 239	0
3	C	15/35 (42%)	2.48	10 (66%) 0 0	186, 201, 237, 241	0
4	D	151/165 (91%)	1.24	35 (23%) 0 1	159, 196, 240, 253	0
All	All	881/998 (88%)	0.55	77 (8%) 10 10	91, 155, 225, 253	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	989	ILE	10.8
4	D	194	TYR	8.3
4	D	199	VAL	7.0
4	D	195	LEU	6.7
4	D	187	TRP	6.4
2	B	1045	PHE	6.0
3	C	161	LEU	5.9
4	D	176	ASP	5.9
3	C	164	GLY	5.7
4	D	177	ASN	5.7
4	D	178	PHE	5.2
2	B	1005	TYR	5.2
4	D	279	THR	5.1
4	D	212	ALA	4.9
3	C	165	LEU	4.9
4	D	171	LEU	4.8
2	B	1063	GLN	4.7
3	C	166	PHE	4.7
4	D	300	ALA	4.6
4	D	204	VAL	4.6
2	B	978	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
4	D	170	HIS	4.2
4	D	216	ILE	4.1
4	D	293	ILE	4.1
4	D	197	VAL	4.0
3	C	163	CYS	3.9
2	B	1009	TYR	3.8
4	D	220	PHE	3.7
4	D	299	LEU	3.7
2	B	1047	ILE	3.7
2	B	979	VAL	3.6
4	D	174	PHE	3.5
4	D	205	VAL	3.4
4	D	289	LEU	3.3
4	D	179	GLN	3.3
4	D	218	ILE	3.2
4	D	311	LEU	3.1
4	D	180	THR	3.1
2	B	1025	VAL	3.1
4	D	189	LEU	3.1
2	B	1043	TYR	3.0
2	B	1049	ALA	3.0
2	B	1039	LEU	2.9
2	B	1007	ILE	2.9
4	D	206	PRO	2.9
2	B	990	VAL	2.9
3	C	160	TYR	2.8
4	D	172	ARG	2.8
1	A	147	VAL	2.7
2	B	873	VAL	2.6
4	D	291	LEU	2.5
4	D	309	LEU	2.4
3	C	168	ASP	2.4
2	B	1017	ILE	2.4
3	C	167	GLY	2.4
3	C	159	SER	2.4
2	B	1036	GLU	2.3
4	D	190	ILE	2.2
4	D	173	THR	2.2
1	A	249	VAL	2.2
1	A	243	THR	2.2
2	B	785	ILE	2.2
1	A	132	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	2.2
1	A	134	LEU	2.1
2	B	975	ASP	2.1
4	D	208	SER	2.1
2	B	994	PRO	2.1
1	A	136	LEU	2.1
2	B	943	PHE	2.1
2	B	962	GLY	2.1
1	A	152	CYS	2.0
3	C	162	PHE	2.0
1	A	286	LYS	2.0
4	D	284	GLN	2.0
2	B	1046	LYS	2.0
4	D	294	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
5	YYJ	J	2	28/28	0.45	0.20	280,281,283,283	0
5	YYJ	K	2	28/28	0.67	0.27	184,187,191,191	28
5	GU4	L	1	27/28	0.68	0.22	264,264,265,265	0
5	GU4	J	1	27/28	0.70	0.17	277,278,280,280	0
5	YYJ	L	2	28/28	0.73	0.31	263,266,267,267	0
5	YYJ	I	2	28/28	0.74	0.19	195,202,210,211	0
5	GU4	I	1	27/28	0.83	0.17	196,201,208,208	0
5	GU4	K	1	27/28	0.85	0.22	190,194,197,197	27

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. 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	B-factors(\AA^2)	Q<0.9
6	NAG	A	501	14/15	0.76	0.24	149,152,153,153	0
6	NAG	B	1201	14/15	0.84	0.20	141,142,144,144	0
6	NAG	A	502	14/15	0.85	0.31	140,141,142,142	0
6	NAG	A	503	14/15	0.90	0.21	159,161,162,163	0
7	CA	A	504	1/1	0.90	0.25	111,111,111,111	0
8	SO4	A	505	5/5	0.92	0.32	148,148,148,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.