



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:50 pm GMT

PDB ID : 3AL9
Title : Mouse Plexin A2 extracellular domain
Authors : Nogi, T.; Yasui, N.; Mihara, E.; Takagi, J.
Deposited on : 2010-07-28
Resolution : 2.10 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

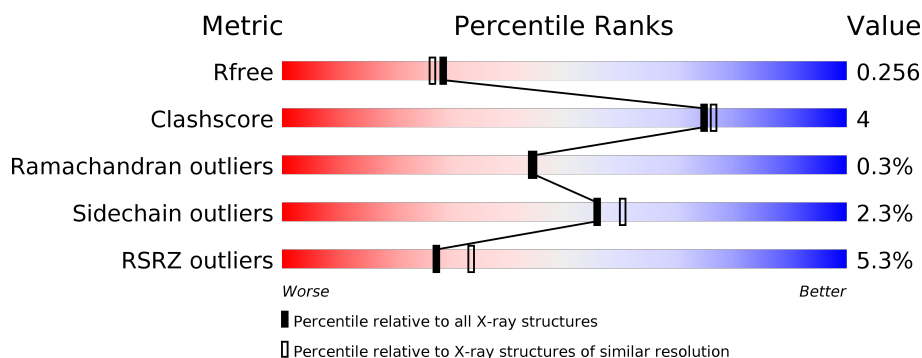
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	539	<div> <div>6%</div> <div>87%</div> <div>8%</div> <div>• •</div> </div>
1	B	539	<div> <div>5%</div> <div>83%</div> <div>13%</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
3	NAG	B	9101	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8604 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	516	Total	C	N	O	S	0	0	0
			4059	2578	693	763	25			
1	B	516	Total	C	N	O	S	0	0	0
			4059	2578	693	763	25			

There are 16 discrepancies between the modelled and reference sequences:

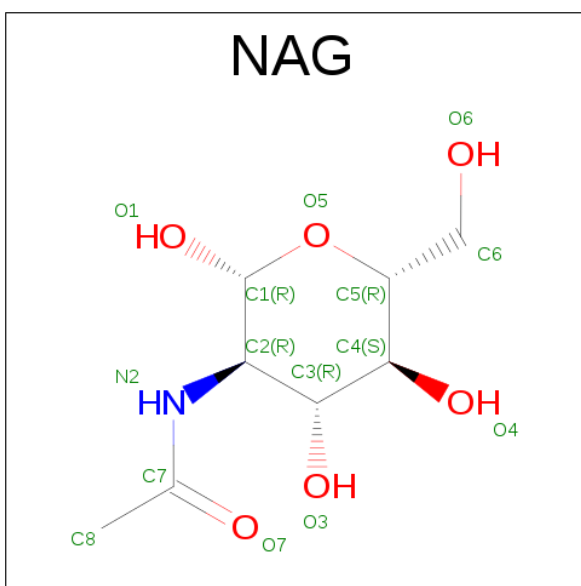
Chain	Residue	Modelled	Actual	Comment	Reference
A	562	SER	-	EXPRESSION TAG	UNP P70207
A	563	ARG	-	EXPRESSION TAG	UNP P70207
A	564	GLU	-	EXPRESSION TAG	UNP P70207
A	565	ASN	-	EXPRESSION TAG	UNP P70207
A	566	LEU	-	EXPRESSION TAG	UNP P70207
A	567	TYR	-	EXPRESSION TAG	UNP P70207
A	568	PHE	-	EXPRESSION TAG	UNP P70207
A	569	GLN	-	EXPRESSION TAG	UNP P70207
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 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

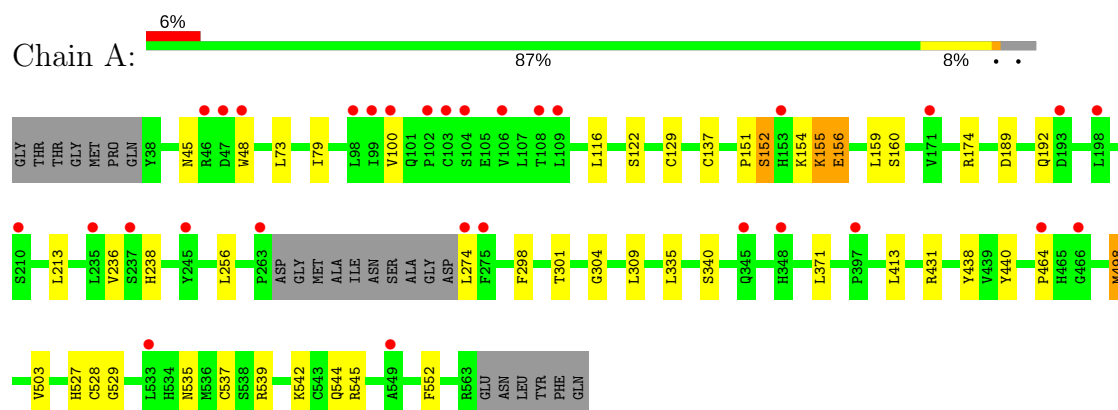
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	235	Total	O	0	0
			235	235		

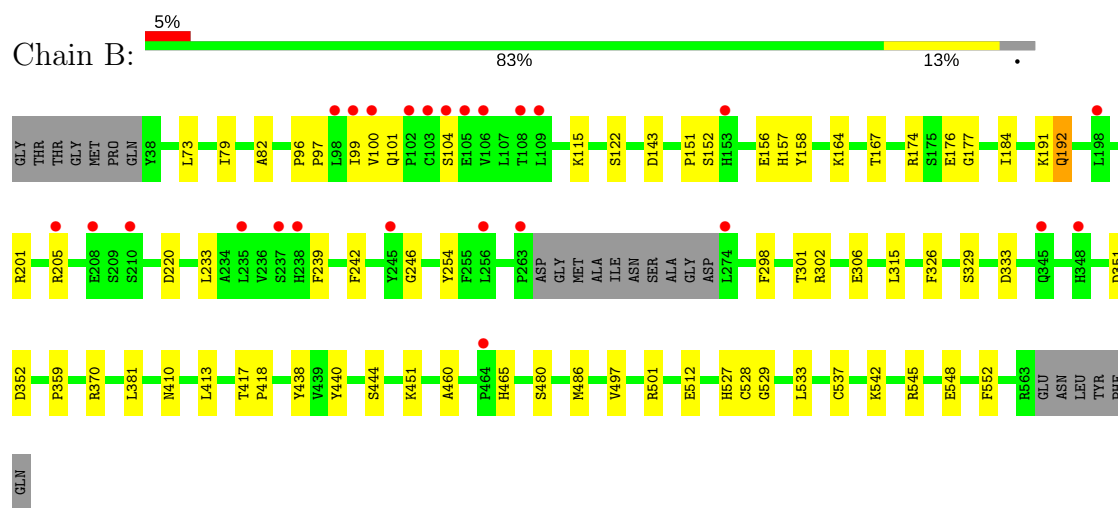
3 Residue-property plots

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: Plexin-A2



• Molecule 1: Plexin-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.70Å 60.68Å 95.39Å 109.80° 92.47° 112.53°	Depositor
Resolution (Å)	42.56 – 2.10 42.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.56-2.10) 83.9 (42.55-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.205 , 0.257 0.204 , 0.256	Depositor DCC
R_{free} test set	3075 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8604	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% 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: NAG, EDO

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	0.53	0/4156	0.63	0/5637
1	B	0.54	0/4156	0.63	0/5637
All	All	0.54	0/8312	0.63	0/11274

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	4059	0	3967	26	0
1	B	4059	0	3966	34	0
2	A	8	0	12	3	0
2	B	4	0	6	0	0
3	B	14	0	13	0	0
4	A	225	0	0	1	0
4	B	235	0	0	2	0
All	All	8604	0	7964	59	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 4.

All (59) 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:512:GLU:HG3	4:B:8028:HOH:O	1.58	1.03
1:B:177:GLY:HA2	1:B:205:ARG:HH21	1.28	0.96
1:A:304:GLY:H	2:A:8302:EDO:H22	1.44	0.82
1:A:154:LYS:HB3	1:A:156:GLU:OE2	1.87	0.75
1:B:177:GLY:HA2	1:B:205:ARG:NH2	2.05	0.72
1:B:233:LEU:HD23	1:B:239:PHE:HB3	1.73	0.71
1:A:304:GLY:N	2:A:8302:EDO:H22	2.11	0.65
1:B:96:PRO:HB2	1:B:100:VAL:HG21	1.81	0.63
1:B:79:ILE:HD11	1:B:82:ALA:HB2	1.79	0.63
1:A:73:LEU:HD23	1:A:79:ILE:HA	1.82	0.61
1:A:122:SER:HB3	1:A:174:ARG:HD2	1.86	0.58
1:A:301:THR:HB	2:A:8302:EDO:H21	1.85	0.57
1:A:544:GLN:HG2	1:A:545:ARG:HG3	1.87	0.57
1:B:351:ASP:OD1	1:B:451:LYS:CE	2.57	0.53
1:A:151:PRO:HG2	1:A:213:LEU:HD12	1.91	0.52
1:B:529:GLY:HA3	1:B:552:PHE:CZ	2.44	0.51
1:A:137:CYS:SG	1:A:159:LEU:HD12	2.50	0.51
1:A:539:ARG:HD3	1:A:542:LYS:HD3	1.93	0.51
1:B:156:GLU:HB2	1:B:201:ARG:NH1	2.26	0.51
1:A:100:VAL:HG11	1:A:152:SER:O	2.10	0.50
1:A:528:CYS:HB3	1:A:537:CYS:SG	2.52	0.50
1:B:480:SER:OG	1:B:501:ARG:NH2	2.45	0.50
1:B:301:THR:HG22	1:B:306:GLU:HA	1.94	0.49
1:B:381:LEU:HD21	1:B:410:ASN:HA	1.95	0.49
1:A:440:TYR:CE2	1:A:527:HIS:HA	2.48	0.49
1:B:370:ARG:HG3	1:B:413:LEU:HD21	1.96	0.48
1:B:73:LEU:HD23	1:B:79:ILE:HA	1.96	0.47
1:B:326:PHE:CG	1:B:359:PRO:HG3	2.48	0.47
1:B:122:SER:HB3	1:B:174:ARG:HD2	1.96	0.47
1:B:440:TYR:CE2	1:B:527:HIS:HA	2.50	0.46
1:B:545:ARG:NH1	1:B:548:GLU:OE1	2.48	0.46
1:B:246:GLY:HA2	1:B:254:TYR:O	2.15	0.46
1:A:256:LEU:HD11	1:A:335:LEU:HD21	1.98	0.45
1:B:444:SER:HB2	1:B:460:ALA:HB3	1.99	0.45
1:A:116:LEU:HB3	1:A:129:CYS:HB2	1.98	0.44
1:B:486:MET:SD	1:B:497:VAL:HG22	2.57	0.44
1:B:99:ILE:HG21	1:B:152:SER:HB2	2.00	0.44
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.53	0.44
1:B:315:LEU:HD11	1:B:333:ASP:HB3	2.00	0.44
1:B:97:PRO:HG2	1:B:158:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:CYS:SG	1:A:159:LEU:CD1	3.06	0.43
1:B:100:VAL:HG23	1:B:101:GLN:H	1.82	0.43
1:A:236:VAL:HG13	1:A:238:HIS:CE1	2.54	0.43
1:A:155:LYS:HD2	1:B:220:ASP:CG	2.39	0.43
1:B:115:LYS:HB3	1:B:115:LYS:HE2	1.72	0.43
1:B:351:ASP:OD1	1:B:451:LYS:HE2	2.18	0.42
1:B:192:GLN:NE2	4:B:8192:HOH:O	2.52	0.42
1:B:151:PRO:O	1:B:157:HIS:HB3	2.19	0.42
1:A:238:HIS:CE1	1:A:274:LEU:HD22	2.55	0.41
1:B:167:THR:HG22	1:B:242:PHE:HD1	1.85	0.41
1:B:528:CYS:HB3	1:B:537:CYS:SG	2.60	0.41
1:A:238:HIS:NE2	1:A:274:LEU:HD22	2.36	0.41
1:A:431:ARG:HD3	4:A:8099:HOH:O	2.20	0.41
1:B:417:THR:HA	1:B:418:PRO:HD3	1.93	0.41
1:A:371:LEU:HD23	1:A:413:LEU:HD22	2.03	0.40
1:B:302:ARG:NH2	1:B:465:HIS:O	2.43	0.40
1:A:45:ASN:HB2	1:A:48:TRP:HB2	2.04	0.40
1:A:309:LEU:HB2	1:A:340:SER:HB2	2.04	0.40
1:A:498:MET:HB3	1:A:503:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	512/539 (95%)	501 (98%)	8 (2%)	3 (1%)	28	24
1	B	512/539 (95%)	498 (97%)	14 (3%)	0	100	100
All	All	1024/1078 (95%)	999 (98%)	22 (2%)	3 (0%)	44	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	SER
1	A	160	SER
1	A	464	PRO

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	451/468 (96%)	443 (98%)	8 (2%)	64	70
1	B	451/468 (96%)	438 (97%)	13 (3%)	48	51
All	All	902/936 (96%)	881 (98%)	21 (2%)	56	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	156	GLU
1	A	189	ASP
1	A	192	GLN
1	A	298	PHE
1	A	438	TYR
1	A	498	MET
1	A	535	ASN
1	B	104	SER
1	B	143	ASP
1	B	164	LYS
1	B	176	GLU
1	B	184	ILE
1	B	191	LYS
1	B	192	GLN
1	B	298	PHE
1	B	329	SER
1	B	352	ASP
1	B	438	TYR
1	B	533	LEU
1	B	542	LYS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	EDO	A	8301	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	A	8302	-	3,3,3	0.41	0	2,2,2	0.47	0
2	EDO	B	8301	-	3,3,3	0.52	0	2,2,2	0.27	0
3	NAG	B	9101	1	14,14,15	0.47	0	15,19,21	1.18	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	8301	-	-	0/1/1/1	0/0/0/0
2	EDO	A	8302	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	8301	-	-	0/1/1/1	0/0/0/0
3	NAG	B	9101	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9101	NAG	C1-O5-C5	3.34	116.78	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	8302	EDO	3	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, 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	516/539 (95%)	0.23	30 (5%) 24 30	12, 24, 39, 55	0
1	B	516/539 (95%)	0.26	25 (4%) 31 37	10, 24, 40, 58	0
All	All	1032/1078 (95%)	0.25	55 (5%) 27 33	10, 24, 40, 58	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	ILE	6.8
1	B	103	CYS	6.8
1	A	99	ILE	6.3
1	A	104	SER	5.8
1	A	100	VAL	5.4
1	B	100	VAL	5.2
1	B	104	SER	4.9
1	A	103	CYS	4.7
1	A	106	VAL	3.9
1	B	102	PRO	3.7
1	B	464	PRO	3.7
1	B	238	HIS	3.5
1	A	102	PRO	3.4
1	A	153	HIS	3.4
1	B	153	HIS	3.4
1	A	98	LEU	3.3
1	A	464	PRO	3.3
1	A	466	GLY	3.1
1	B	345	GLN	3.0
1	A	263	PRO	2.9
1	A	47	ASP	2.9
1	A	397	PRO	2.8
1	B	237	SER	2.7
1	B	208	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	348	HIS	2.7
1	B	210	SER	2.7
1	A	348	HIS	2.6
1	B	235	LEU	2.6
1	A	533	LEU	2.6
1	B	274	LEU	2.6
1	A	171	VAL	2.5
1	A	549	ALA	2.5
1	A	198	LEU	2.4
1	A	46	ARG	2.4
1	A	274	LEU	2.4
1	B	245	TYR	2.4
1	A	48	TRP	2.3
1	B	105	GLU	2.3
1	A	245	TYR	2.2
1	B	109	LEU	2.2
1	B	256	LEU	2.2
1	A	210	SER	2.2
1	A	193	ASP	2.2
1	B	198	LEU	2.2
1	A	345	GLN	2.1
1	A	235	LEU	2.1
1	B	205	ARG	2.1
1	A	275	PHE	2.1
1	A	109	LEU	2.1
1	B	263	PRO	2.1
1	B	108	THR	2.1
1	B	98	LEU	2.0
1	A	237	SER	2.0
1	A	108	THR	2.0
1	B	106	VAL	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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
3	NAG	B	9101	14/15	0.86	0.21	2.28	32,36,38,41	0
2	EDO	A	8302	4/4	0.87	0.17	1.38	36,37,38,41	0
2	EDO	B	8301	4/4	0.97	0.18	0.21	19,22,22,23	0
2	EDO	A	8301	4/4	0.94	0.10	-0.53	30,31,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.