WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2017 – 12:53 am GMT

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PDB ID	:	3QEL
Title	:	Crystal structure of amino terminal domains of the NMDA receptor subunit GluN1 and GluN2B in complex with ifenprodil
Authors	:	Karakas, E.; Simorowski, N.; Furukawa, H.
Deposited on	:	2011-01-20
Resolution	:	2.60 Å(reported)

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 2.60 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.
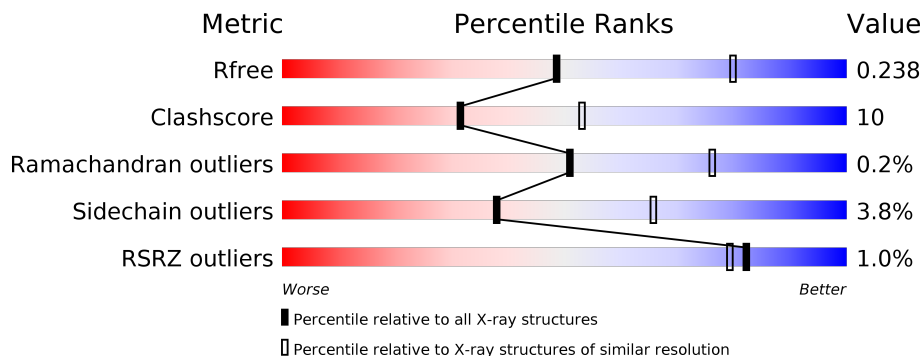
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	383	77% 14% • 7%
1	C	383	2% 73% 18% • 8%
2	B	364	% 76% 19% • •
2	D	364	72% 22% • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	501	X	-	-	-
4	NAG	B	502	X	-	-	-
4	NAG	C	502	X	-	-	X
4	NAG	D	501	X	-	-	-
4	NAG	D	502	X	-	-	-
5	MAN	A	506	-	-	-	X
5	FUC	A	508	X	-	-	-
6	QEL	B	1	X	-	-	-
6	QEL	D	2	X	-	-	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 10737 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 NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2665	1702	460	493	10			
1	C	351	Total	C	N	O	S	0	0	0
			2573	1642	445	476	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	ENGINEERED MUTATION	UNP Q91977
A	371	GLN	ASN	ENGINEERED MUTATION	UNP Q91977
C	61	GLN	ASN	ENGINEERED MUTATION	UNP Q91977
C	371	GLN	ASN	ENGINEERED MUTATION	UNP Q91977

- Molecule 2 is a protein called Glutamate [NMDA] receptor subunit epsilon-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	353	Total	C	N	O	S	0	0	0
			2608	1678	417	498	15			
2	D	345	Total	C	N	O	S	0	0	0
			2549	1644	401	488	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	ENGINEERED MUTATION	UNP Q00960
D	348	ASP	ASN	ENGINEERED MUTATION	UNP Q00960

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).
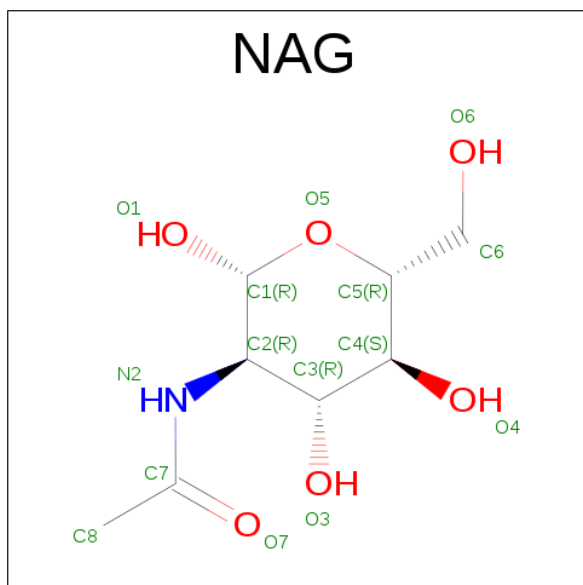
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total Na		0	0
			1 1			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is 4-[(1R,2S)-2-(4-BENZYLPIPERIDIN-1-YL)-1-HYDROXYPROPYL]PHENOL (three-letter code: QEL) (formula: $C_{21}H_{27}NO_2$).
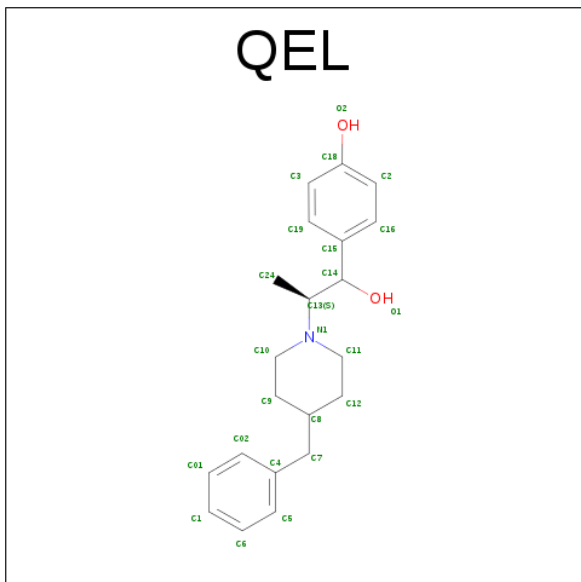
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 24	C 21	N 1	O 2	0	0
6	D	1	Total 24	C 21	N 1	O 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total 68	O 68	0	0
7	B	31	Total 31	O 31	0	0
7	C	24	Total 24	O 24	0	0
7	D	14	Total 14	O 14	0	0

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: NMDA glutamate receptor subunit
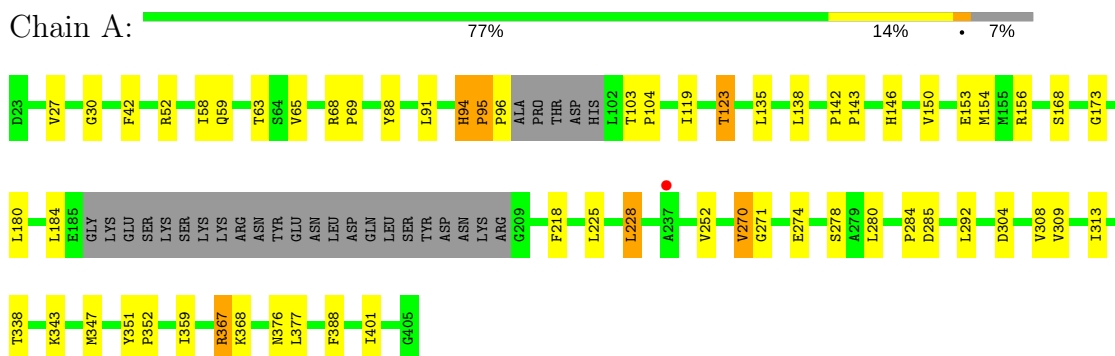
• Molecule 1: NMDA glutamate receptor subunit
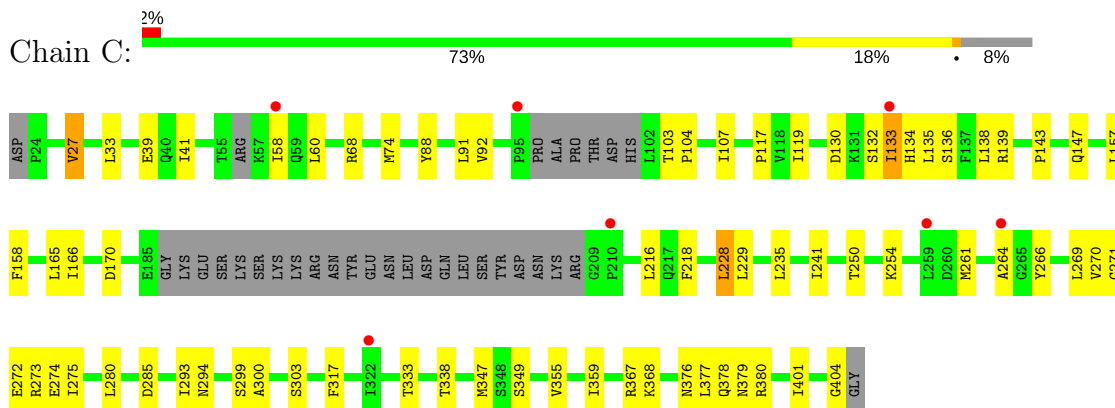
• Molecule 2: Glutamate [NMDA] receptor subunit epsilon-2

I340 N341 V342 T343 F344 E345 G346 D354 G355 Y356 L362 V363 I364 W379 K382 W391 P392 R393 MET
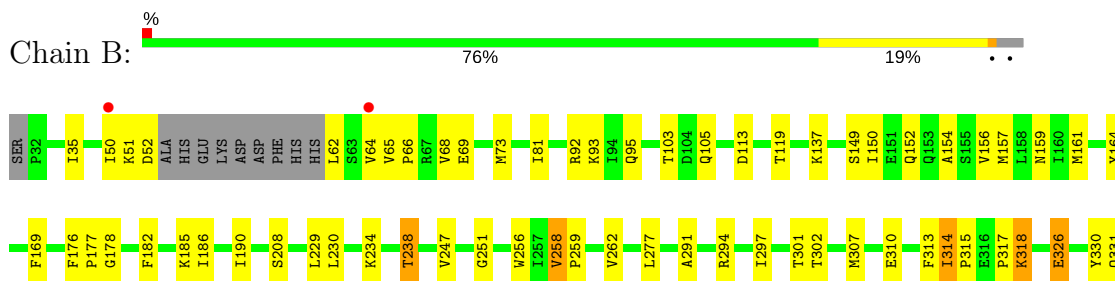
• Molecule 2: Glutamate [NMDA] receptor subunit epsilon-2

Chain D:

72%   22%   5%

SER PRO P33 S34 I35 I40 L41 V42 K51 ASP ALA HIS GLU LYS ASP ASP F59 V64 V65 V68 E69 L70 M73 T76 G96 T103 E106 L124 G125 I126 D138 S141 F144 Q145 F146 S149 M157 L158 N159 I160 M161 F169 T173

T174 Y179 Q180 D181 F182 S188 M207 S208 D211 G212 D213 L220 Q224 S225 P226 I227 I228 L229 L230 Y231 C232 T233 K234 E235 E236 A237 T238 Y239 I240 V243 V247 I257 V258 P259 S260 L261 V262 P270 S271 E272 F273 Y282 Y287 G288 L289 P290 A291 R292

V293 I297 I300 T301 THR A303 H311 S312 F313 E316 P317 K318 N323 THR HIS GLU K327 R328 I329 Y330 Q331 S332 N333 M334 L335 F344 E345 GLY ARG D348 G355 Y356 L362 V363 I364 W379 LYS ASP LYS SER L384 W391 P392 R393 M394

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	267.99Å 60.87Å 144.92Å 90.00° 116.49° 90.00°	Depositor
Resolution (Å)	29.98 – 2.60 48.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.0 (29.98-2.60) 98.1 (48.43-2.60)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	0.51	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.188 , 0.238 0.187 , 0.238	Depositor DCC
R_{free} test set	3253 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10737	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, NA, QEL, FUC, 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	0.46	0/2722	0.60	0/3713
1	C	0.36	0/2626	0.53	0/3589
2	B	0.41	0/2666	0.57	0/3648
2	D	0.36	0/2602	0.57	2/3555 (0.1%)
All	All	0.40	0/10616	0.57	2/14505 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	224	GLN	CB-CA-C	-5.39	99.62	110.40
2	D	103	THR	CB-CA-C	-5.08	97.89	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	508	FUC	C1

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	2665	0	2569	40	0
1	C	2573	0	2425	52	0
2	B	2608	0	2386	65	0
2	D	2549	0	2330	56	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
4	C	14	0	13	2	0
4	D	28	0	26	0	0
5	A	71	0	61	0	0
6	B	24	0	25	0	0
6	D	24	0	25	1	0
7	A	68	0	0	1	0
7	B	31	0	0	3	0
7	C	24	0	0	1	0
7	D	14	0	0	0	0
All	All	10737	0	9899	208	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 10.

The worst 5 of 208 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:318:LYS:H	2:B:318:LYS:HE2	1.21	1.06
2:D:161:MET:HE1	2:D:229:LEU:HD21	1.49	0.93
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.59	0.82
1:C:147:GLN:HE22	1:C:272:GLU:H	1.32	0.78
2:B:119:THR:O	2:B:318:LYS:HD2	1.84	0.77

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	349/383 (91%)	338 (97%)	10 (3%)	1 (0%)	44	70
1	C	343/383 (90%)	320 (93%)	23 (7%)	0	100	100
2	B	349/364 (96%)	321 (92%)	27 (8%)	1 (0%)	44	70
2	D	333/364 (92%)	315 (95%)	17 (5%)	1 (0%)	44	70
All	All	1374/1494 (92%)	1294 (94%)	77 (6%)	3 (0%)	51	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	LYS
2	D	318	LYS
1	A	95	PRO

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	272/329 (83%)	263 (97%)	9 (3%)	43	70
1	C	253/329 (77%)	244 (96%)	9 (4%)	40	68
2	B	258/327 (79%)	251 (97%)	7 (3%)	50	77
2	D	255/327 (78%)	241 (94%)	14 (6%)	25	49
All	All	1038/1312 (79%)	999 (96%)	39 (4%)	38	66

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	133	ILE
1	C	303	SER
2	D	287	TYR
1	C	170	ASP
1	C	228	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	94	HIS
1	C	147	GLN
2	D	127	HIS
2	B	333	ASN
1	C	38	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 ⓘ

6 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	A	503	1,5	14,14,15	0.62	0	15,19,21	0.76	0
5	NAG	A	504	5	14,14,15	0.71	0	15,19,21	0.87	0
5	BMA	A	505	5	11,11,12	1.00	1 (9%)	13,15,17	2.22	4 (30%)
5	MAN	A	506	5	11,11,12	0.78	0	13,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	MAN	A	507	5	11,11,12	0.74	0	13,15,17	0.81	0
5	FUC	A	508	5	9,10,11	1.93	2 (22%)	13,14,16	1.67	4 (30%)

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	A	503	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	504	5	-	0/6/23/26	0/1/1/1
5	BMA	A	505	5	-	0/2/19/22	0/1/1/1
5	MAN	A	506	5	-	0/2/19/22	0/1/1/1
5	MAN	A	507	5	-	0/2/19/22	0/1/1/1
5	FUC	A	508	5	1/1/4/5	0/0/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	508	FUC	C2-C3	-4.64	1.46	1.52
5	A	508	FUC	C4-C3	-2.57	1.45	1.52
5	A	505	BMA	C4-C5	2.18	1.57	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	505	BMA	O4-C4-C3	2.06	114.84	110.36
5	A	508	FUC	O5-C1-C2	2.31	114.41	110.79
5	A	508	FUC	C1-O5-C5	2.41	117.72	112.39
5	A	508	FUC	C1-C2-C3	2.62	112.97	109.65
5	A	508	FUC	O5-C5-C4	2.82	114.27	109.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	508	FUC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#|Z| > 2$
4	NAG	A	502	1	14,14,15	0.65	0	15,19,21	1.30	2 (13%)
6	QEL	B	1	-	26,26,26	2.55	9 (34%)	34,35,35	2.14	8 (23%)
4	NAG	B	501	2	14,14,15	0.40	0	15,19,21	1.11	1 (6%)
4	NAG	B	502	2	14,14,15	0.59	0	15,19,21	1.17	1 (6%)
4	NAG	C	502	1	14,14,15	0.52	0	15,19,21	0.63	0
6	QEL	D	2	-	26,26,26	2.69	11 (42%)	34,35,35	2.08	9 (26%)
4	NAG	D	501	2	14,14,15	0.45	0	15,19,21	0.69	0
4	NAG	D	502	2	14,14,15	0.61	0	15,19,21	1.46	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
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
6	QEL	B	1	-	1/1/4/4	0/16/26/26	0/3/3/3
4	NAG	B	501	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	502	1	1/1/5/7	0/6/23/26	0/1/1/1
6	QEL	D	2	-	1/1/4/4	0/16/26/26	0/3/3/3
4	NAG	D	501	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	502	2	1/1/5/7	0/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	QEL	O1-C14	-10.00	1.23	1.42
6	B	1	QEL	O1-C14	-9.52	1.23	1.42
6	B	1	QEL	C14-C13	-3.49	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	QEL	C3-C18	-3.45	1.32	1.38
6	B	1	QEL	C3-C18	-3.15	1.32	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	2	QEL	C24-C13-C14	-5.24	103.69	111.82
6	B	1	QEL	C24-C13-C14	-4.63	104.64	111.82
6	B	1	QEL	C12-C8-C7	-4.40	102.13	111.85
6	D	2	QEL	C19-C15-C14	-3.48	115.64	120.73
6	D	2	QEL	C12-C8-C7	-3.46	104.19	111.85

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	502	NAG	C1
4	B	502	NAG	C1
6	B	1	QEL	C14
6	D	2	QEL	C14
4	B	501	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	NAG	2	0
6	D	2	QEL	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 ⓘ

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	355/383 (92%)	-0.32	1 (0%)	93	93	28, 45, 80, 100	0
1	C	351/383 (91%)	-0.05	7 (1%)	65	59	46, 70, 102, 122	0
2	B	353/364 (96%)	-0.19	5 (1%)	75	71	30, 62, 100, 125	0
2	D	345/364 (94%)	-0.23	1 (0%)	93	93	44, 70, 116, 133	0
All	All	1404/1494 (93%)	-0.20	14 (0%)	82	79	28, 64, 102, 133	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	344	PHE	3.6
1	C	210	PRO	3.3
2	B	342	VAL	2.8
1	C	58	ILE	2.7
2	B	346	GLY	2.5

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

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

6.3 Carbohydrates ⓘ

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
5	MAN	A	506	11/12	0.96	0.24	4.65	45,48,52,53	0
5	NAG	A	503	14/15	0.94	0.14	-0.72	42,54,57,60	0
5	FUC	A	508	10/11	0.83	0.21	-	63,71,77,79	10
5	MAN	A	507	11/12	0.78	0.30	-	72,81,83,85	0
5	NAG	A	504	14/15	0.96	0.16	-	50,56,61,65	0
5	BMA	A	505	11/12	0.91	0.23	-	47,55,62,68	0

6.4 Ligands ⓘ

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
4	NAG	C	502	14/15	0.81	0.20	2.28	65,71,75,80	4
6	QEL	B	1	24/24	0.95	0.20	0.36	31,40,48,58	0
3	NA	C	501	1/1	0.89	0.17	-0.12	63,63,63,63	0
6	QEL	D	2	24/24	0.95	0.16	-0.40	48,56,61,63	0
3	NA	A	501	1/1	0.96	0.15	-1.02	48,48,48,48	0
4	NAG	D	502	14/15	0.73	0.38	-	105,115,116,121	0
4	NAG	B	502	14/15	0.90	0.32	-	96,106,109,112	0
4	NAG	B	501	14/15	0.85	0.19	-	97,101,107,109	0
4	NAG	D	501	14/15	0.66	0.34	-	96,106,111,112	0
4	NAG	A	502	14/15	0.91	0.19	-	47,51,60,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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