



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:55 AM GMT

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)

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

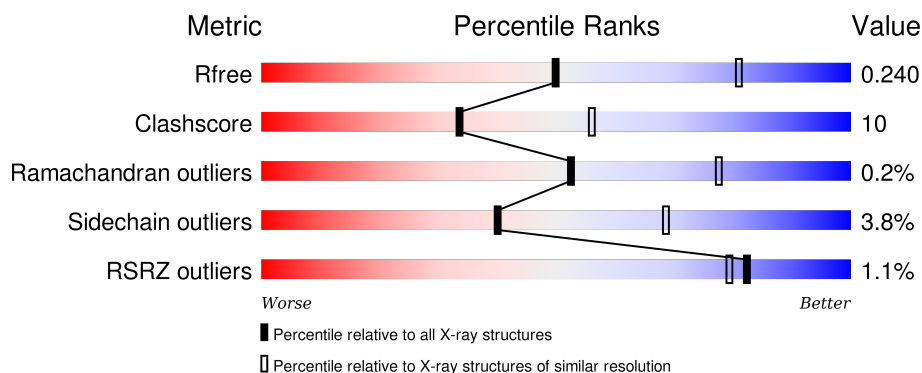
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 $\leq 5\%$. 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	383	
1	C	383	
2	B	364	
2	D	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	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 [i](#)

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: $C_8H_{15}NO_6$).

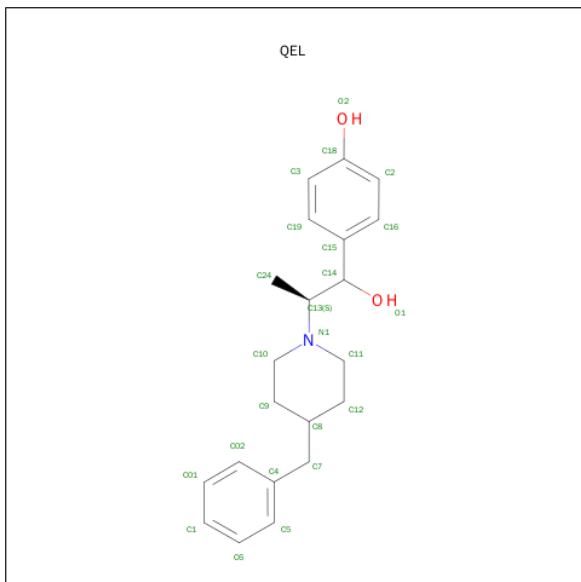


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	1	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- 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: C₂₁H₂₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			24	21	1	2		
6	D	1	Total	C	N	O	0	0
			24	21	1	2		

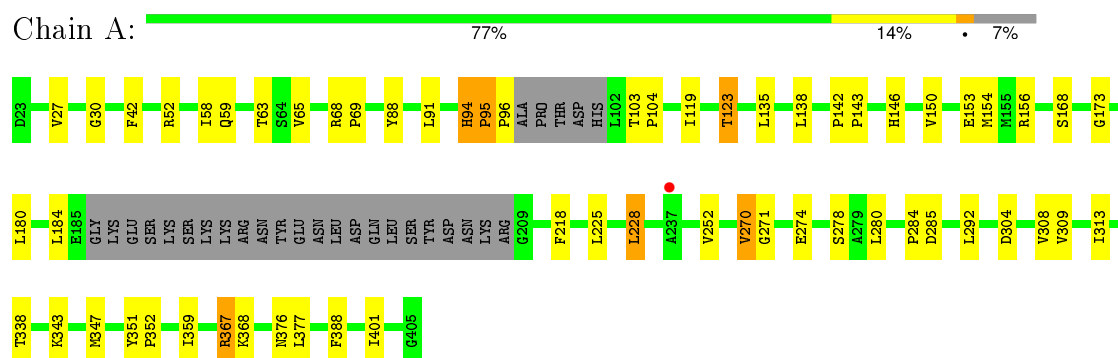
- Molecule 7 is water.

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

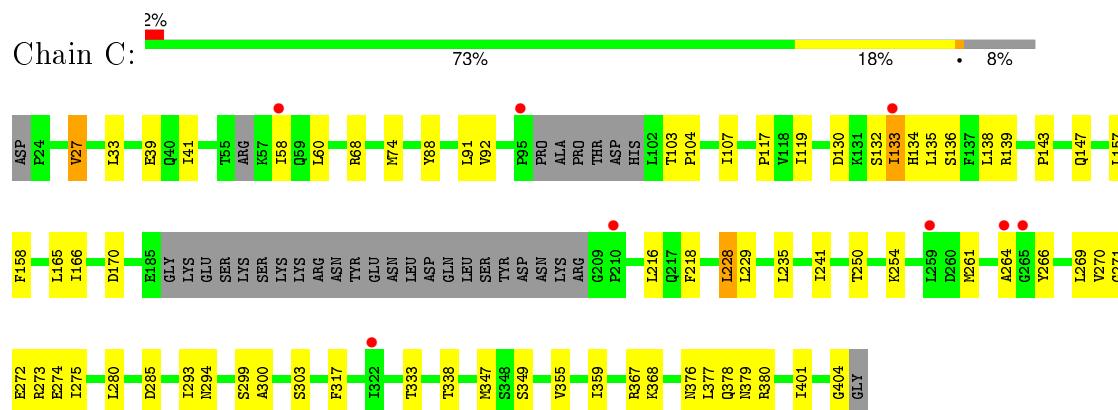
3 Residue-property plots [i](#)

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

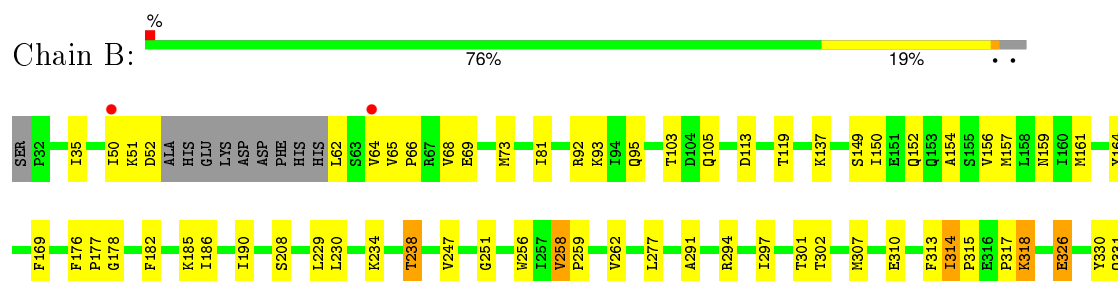
• Molecule 1: NMDA glutamate receptor subunit



• Molecule 1: NMDA glutamate receptor subunit



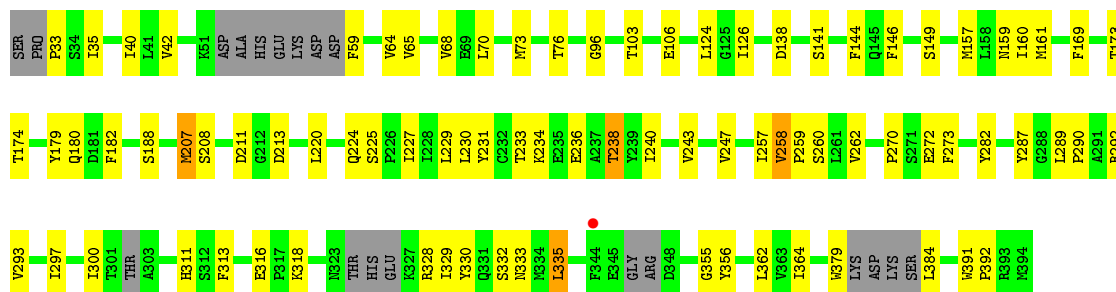
• Molecule 2: Glutamate [NMDA] receptor subunit epsilon-2





- Molecule 2: Glutamate [NMDA] receptor subunit epsilon-2

Chain D: 72% 22% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	267.99 Å 60.87 Å 144.92 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.188 , 0.238 0.193 , 0.240	Depositor DCC
R_{free} test set	3252 reflections (5.36%)	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 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63992 reflections	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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 ⓘ

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.

All (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
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.66	0.77
2:B:379:TRP:CZ2	2:B:382:LYS:HA	2.21	0.76
1:A:94:HIS:CE1	1:A:123:THR:HG23	2.20	0.75
1:C:270:VAL:HG13	1:C:274:GLU:HB2	1.70	0.74
1:C:147:GLN:HE22	1:C:272:GLU:N	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:HE1	1:A:123:THR:HG23	1.55	0.72
2:D:159:ASN:HD22	2:D:379:TRP:HZ3	1.38	0.70
1:C:355:VAL:HG11	4:C:502:NAG:H82	1.72	0.70
1:C:376:ASN:HD21	1:C:401:ILE:H	1.39	0.69
2:B:157:MET:HE3	2:B:229:LEU:HD22	1.75	0.69
2:D:96:GLY:HA3	2:D:300:ILE:HD13	1.75	0.68
1:C:378:GLN:HG2	1:C:401:ILE:HD12	1.77	0.67
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.76	0.67
1:C:92:VAL:HG21	1:C:107:ILE:HG21	1.78	0.66
1:A:367:ARG:HD2	1:A:368:LYS:O	1.96	0.65
2:D:35:ILE:HG23	2:D:64:VAL:HG21	1.77	0.65
2:B:318:LYS:HD3	2:B:331:GLN:OE1	1.96	0.65
2:D:258:VAL:HG22	2:D:262:VAL:HG21	1.80	0.64
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.80	0.64
2:D:220:LEU:HD12	2:D:243:VAL:HG12	1.78	0.63
1:A:135:LEU:HD22	2:B:208:SER:HB3	1.80	0.62
1:A:103:THR:HB	1:A:104:PRO:HD2	1.81	0.62
2:D:157:MET:HE3	2:D:229:LEU:HD22	1.81	0.62
1:C:133:ILE:HG13	1:C:134:HIS:CD2	2.34	0.62
2:B:161:MET:HE1	2:B:229:LEU:HD11	1.81	0.61
2:B:152:GLN:O	2:B:156:VAL:HG23	2.00	0.61
2:B:169:PHE:HZ	2:B:190:ILE:HD11	1.64	0.61
2:D:293:VAL:O	2:D:297:ILE:HG13	2.00	0.60
2:B:68:VAL:HG21	2:B:297:ILE:HD13	1.83	0.59
1:C:92:VAL:CG2	1:C:107:ILE:HG21	2.32	0.59
1:A:68:ARG:NH1	7:A:443:HOH:O	2.33	0.59
2:D:68:VAL:HG21	2:D:297:ILE:HD13	1.84	0.59
1:C:27:VAL:HG23	1:C:60:LEU:HD23	1.85	0.59
2:B:318:LYS:CE	2:B:318:LYS:H	2.07	0.59
1:C:270:VAL:CG1	1:C:274:GLU:HB2	2.32	0.58
2:B:310:GLU:O	2:B:310:GLU:HG2	2.02	0.58
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.85	0.57
2:B:119:THR:O	2:B:318:LYS:CD	2.51	0.57
1:A:65:VAL:HB	1:A:68:ARG:NH2	2.20	0.56
2:D:174:THR:HG21	2:D:207:MET:HG3	1.88	0.55
1:A:30:GLY:HA2	1:A:63:THR:O	2.06	0.55
2:D:159:ASN:HB3	2:D:384:LEU:HD22	1.87	0.55
1:C:293:ILE:O	1:C:294:ASN:HB2	2.06	0.55
2:D:174:THR:CG2	2:D:207:MET:HG3	2.38	0.54
2:D:233:THR:OG1	2:D:236:GLU:HG3	2.07	0.54
1:A:150:VAL:HG12	1:A:154:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:PHE:CD2	2:D:332:SER:HB2	2.43	0.54
2:B:258:VAL:HG22	2:B:262:VAL:HG21	1.89	0.54
2:B:230:LEU:HB3	2:B:258:VAL:HG23	1.90	0.54
1:C:275:ILE:HB	1:C:280:LEU:HD13	1.90	0.54
1:A:270:VAL:HG13	1:A:271:GLY:N	2.24	0.54
1:C:367:ARG:HD2	1:C:368:LYS:O	2.08	0.53
1:A:309:VAL:O	1:A:313:ILE:HG12	2.08	0.53
2:B:291:ALA:O	2:B:294:ARG:HB3	2.08	0.53
2:B:247:VAL:HG12	2:B:247:VAL:O	2.08	0.53
2:B:95:GLN:NE2	2:B:315:PRO:O	2.40	0.53
1:C:376:ASN:ND2	1:C:401:ILE:H	2.06	0.53
2:B:65:VAL:CG2	2:B:66:PRO:HD2	2.39	0.53
1:C:228:LEU:HD23	1:C:229:LEU:HG	1.91	0.52
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.90	0.52
2:B:182:PHE:O	2:B:186:ILE:HG12	2.10	0.52
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.90	0.52
2:D:227:ILE:HD12	2:D:227:ILE:N	2.24	0.52
2:D:35:ILE:HG13	2:D:35:ILE:O	2.10	0.52
1:C:58:ILE:HD12	1:C:317:PHE:CD1	2.45	0.52
2:B:65:VAL:HG22	2:B:66:PRO:HD2	1.91	0.51
2:D:157:MET:HE1	2:D:182:PHE:HZ	1.74	0.51
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.93	0.51
1:A:103:THR:HB	1:A:104:PRO:CD	2.41	0.51
2:B:149:SER:HB3	2:B:356:TYR:CD1	2.46	0.51
1:C:119:ILE:HA	1:C:138:LEU:O	2.11	0.51
2:B:169:PHE:CZ	2:B:190:ILE:HD11	2.45	0.50
1:C:359:ILE:HG12	1:C:367:ARG:NH2	2.27	0.50
2:B:364:ILE:HD12	2:B:364:ILE:N	2.27	0.50
2:B:256:TRP:O	2:B:277:LEU:HD12	2.12	0.50
2:B:159:ASN:ND2	2:B:379:TRP:CZ3	2.80	0.50
2:B:149:SER:HB3	2:B:356:TYR:CG	2.47	0.50
2:B:35:ILE:HG23	2:B:64:VAL:HG21	1.93	0.50
1:C:117:PRO:HA	1:C:136:SER:HB2	1.94	0.50
1:C:300:ALA:HA	4:C:502:NAG:C8	2.41	0.49
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.47	0.49
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.95	0.49
1:C:157:LEU:HD23	1:C:158:PHE:HE2	1.78	0.49
2:D:258:VAL:HG21	2:D:262:VAL:HG11	1.94	0.49
1:C:165:LEU:HD12	1:C:166:ILE:N	2.28	0.49
1:A:65:VAL:HB	1:A:68:ARG:HH21	1.76	0.49
1:C:139:ARG:NH2	1:C:143:PRO:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:ILE:HD11	2:D:364:ILE:HG12	1.94	0.49
2:B:157:MET:HE1	2:B:229:LEU:HB3	1.95	0.48
1:C:132:SER:O	6:D:2:QEL:H19	2.14	0.48
2:D:106:GLU:OE1	2:D:106:GLU:N	2.44	0.48
1:C:103:THR:HB	1:C:104:PRO:HD2	1.96	0.48
1:C:27:VAL:HG12	1:C:88:TYR:CE1	2.49	0.48
2:B:354:ASP:HB2	2:B:356:TYR:CE2	2.49	0.48
2:B:230:LEU:O	2:B:259:PRO:HD3	2.14	0.48
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.49	0.48
2:D:159:ASN:ND2	2:D:379:TRP:HZ3	2.11	0.47
1:A:95:PRO:HB2	1:A:96:PRO:HD2	1.96	0.47
1:C:135:LEU:HD22	2:D:208:SER:HB3	1.95	0.47
2:B:150:ILE:HD13	2:B:178:GLY:HA3	1.95	0.47
1:C:103:THR:HB	1:C:104:PRO:CD	2.44	0.47
2:B:68:VAL:CG2	2:B:297:ILE:HD13	2.45	0.47
2:D:391:TRP:HA	2:D:392:PRO:HD3	1.69	0.47
2:D:149:SER:HB3	2:D:356:TYR:CD2	2.50	0.47
1:A:338:THR:O	1:A:338:THR:HG22	2.15	0.47
1:A:225:LEU:HD13	1:A:252:VAL:HG22	1.95	0.47
1:C:130:ASP:OD2	1:C:132:SER:HB3	2.13	0.47
2:D:270:PRO:HG2	2:D:273:PHE:CE1	2.50	0.47
2:B:62:LEU:HD13	2:B:301:THR:HG22	1.97	0.47
2:B:157:MET:HE2	2:B:229:LEU:HD13	1.96	0.47
2:B:314:ILE:HD12	2:B:314:ILE:HA	1.74	0.46
2:D:229:LEU:CD2	2:D:257:ILE:HB	2.46	0.46
1:A:143:PRO:HG2	1:A:146:HIS:CD2	2.50	0.46
2:D:35:ILE:HG23	2:D:64:VAL:CG2	2.45	0.46
2:D:328:ARG:C	2:D:330:TYR:H	2.19	0.46
2:D:33:PRO:HB2	2:D:64:VAL:HG23	1.97	0.46
1:A:68:ARG:HA	1:A:68:ARG:HD3	1.63	0.46
1:A:168:SER:O	1:A:173:GLY:HA3	2.16	0.46
2:D:311:HIS:O	2:D:313:PHE:HD2	1.99	0.46
1:C:379:ASN:C	1:C:380:ARG:HG2	2.36	0.45
2:D:234:LYS:O	2:D:238:THR:HG23	2.16	0.45
2:D:332:SER:OG	2:D:333:ASN:N	2.50	0.45
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.77	0.45
1:C:270:VAL:HG13	1:C:271:GLY:N	2.31	0.45
2:B:391:TRP:HA	2:B:392:PRO:HD3	1.72	0.45
2:D:42:VAL:HG11	2:D:76:THR:CG2	2.47	0.45
2:B:234:LYS:HD2	2:B:262:VAL:O	2.17	0.45
1:C:157:LEU:HD23	1:C:158:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:ND2	1:A:401:ILE:H	2.14	0.45
1:A:308:VAL:HG21	1:A:359:ILE:HG21	1.98	0.45
1:C:261:MET:HA	1:C:266:TYR:CE1	2.52	0.44
2:D:213:ASP:N	2:D:213:ASP:OD1	2.46	0.44
1:C:165:LEU:HD12	1:C:166:ILE:H	1.82	0.44
1:C:41:ILE:HD13	1:C:299:SER:OG	2.18	0.44
1:C:241:ILE:HA	1:C:269:LEU:O	2.17	0.44
1:C:250:THR:HG22	1:C:254:LYS:HD2	2.00	0.44
2:B:92:ARG:HG2	2:B:93:LYS:H	1.82	0.44
2:B:35:ILE:HG23	2:B:64:VAL:CG2	2.48	0.44
2:D:157:MET:CE	2:D:229:LEU:HD22	2.48	0.44
2:D:68:VAL:CG2	2:D:297:ILE:HD13	2.48	0.44
2:B:258:VAL:HG13	2:B:262:VAL:HB	2.00	0.44
1:A:376:ASN:HD21	1:A:401:ILE:H	1.65	0.44
2:B:50:ILE:O	2:B:52:ASP:N	2.49	0.44
2:D:144:PHE:HD1	2:D:355:GLY:HA2	1.82	0.44
1:A:351:TYR:HA	1:A:352:PRO:HD3	1.83	0.44
1:C:33:LEU:HD12	1:C:39:GLU:HA	1.99	0.43
2:B:307:MET:O	2:B:307:MET:HG2	2.17	0.43
1:A:58:ILE:CD1	1:A:313:ILE:HG22	2.47	0.43
2:B:154:ALA:HB1	2:B:186:ILE:HD11	1.99	0.43
1:A:304:ASP:HB3	1:A:359:ILE:HD11	1.99	0.43
2:B:113:ASP:OD1	2:B:137:LYS:HB3	2.18	0.43
2:D:159:ASN:HB3	2:D:384:LEU:CD2	2.48	0.43
2:B:315:PRO:O	2:B:317:PRO:HD3	2.19	0.43
1:C:285:ASP:HA	1:C:377:LEU:HD23	2.00	0.43
1:C:91:LEU:HD12	1:C:91:LEU:N	2.34	0.43
2:B:302:THR:HG21	2:B:342:VAL:HG13	2.00	0.43
1:A:343:LYS:O	1:A:347:MET:HG2	2.18	0.43
1:A:119:ILE:HA	1:A:138:LEU:O	2.19	0.43
2:B:313:PHE:CG	2:D:332:SER:HB2	2.54	0.42
2:B:157:MET:CE	2:B:229:LEU:HD13	2.48	0.42
1:C:235:LEU:N	1:C:235:LEU:HD23	2.34	0.42
1:A:180:LEU:O	1:A:184:LEU:HG	2.19	0.42
1:C:280:LEU:HD12	1:C:280:LEU:HA	1.86	0.42
2:D:124:LEU:HD22	2:D:144:PHE:HB2	2.01	0.42
1:C:68:ARG:HG2	1:C:74:MET:HE3	2.00	0.42
2:D:282:TYR:CE2	2:D:292:ARG:NH1	2.87	0.42
2:D:126:ILE:HG22	2:D:146:PHE:CE1	2.54	0.42
2:B:152:GLN:HB2	2:B:152:GLN:HE21	1.52	0.42
1:A:142:PRO:HD2	1:A:292:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LYS:O	2:B:238:THR:HG23	2.20	0.42
1:A:58:ILE:O	1:A:58:ILE:HG13	2.20	0.42
1:A:376:ASN:HD21	1:A:401:ILE:N	2.18	0.42
2:B:185:LYS:HD2	2:B:185:LYS:O	2.20	0.42
2:B:164:TYR:CZ	2:B:391:TRP:CE3	3.08	0.42
2:B:326:GLU:H	2:B:326:GLU:HG3	1.51	0.42
2:B:73:MET:HE1	2:B:81:ILE:HG12	2.01	0.42
2:D:230:LEU:O	2:D:259:PRO:HD3	2.19	0.42
1:A:156:ARG:HH11	1:A:156:ARG:HB2	1.85	0.41
2:B:105:GLN:NE2	7:B:24:HOH:O	2.53	0.41
2:D:138:ASP:O	2:D:141:SER:HB3	2.20	0.41
1:A:42:PHE:CE1	1:A:91:LEU:HD22	2.56	0.41
1:C:264:ALA:HB2	1:C:404:GLY:HA3	2.02	0.41
2:B:330:TYR:CD2	2:D:316:GLU:HG3	2.55	0.41
2:B:247:VAL:CG1	2:B:247:VAL:O	2.67	0.41
1:C:147:GLN:NE2	7:C:21:HOH:O	2.52	0.41
1:A:68:ARG:HB3	1:A:69:PRO:CD	2.50	0.41
2:D:157:MET:CE	2:D:182:PHE:HZ	2.33	0.41
1:C:216:LEU:N	1:C:216:LEU:HD23	2.35	0.41
1:C:338:THR:HG22	1:C:338:THR:O	2.21	0.41
2:B:251:GLY:N	7:B:403:HOH:O	2.53	0.41
2:B:68:VAL:HG12	2:B:69:GLU:N	2.36	0.41
2:D:173:THR:HA	2:D:231:TYR:O	2.21	0.41
2:B:154:ALA:HB1	2:B:186:ILE:CD1	2.50	0.41
2:D:179:TYR:CE1	2:D:180:GLN:HG3	2.56	0.41
2:D:40:ILE:CG2	2:D:73:MET:HE2	2.51	0.41
1:A:153:GLU:HG3	1:A:388:PHE:HE1	1.86	0.41
2:D:335:LEU:HA	2:D:335:LEU:HD23	1.86	0.40
2:B:103:THR:HB	7:B:411:HOH:O	2.21	0.40
2:D:247:VAL:HG12	2:D:247:VAL:O	2.21	0.40
1:C:218:PHE:HB3	1:C:228:LEU:CD1	2.44	0.40
1:C:27:VAL:CG2	1:C:60:LEU:HD23	2.51	0.40
2:D:169:PHE:HA	2:D:225:SER:HB3	2.04	0.40
1:A:284:PRO:O	1:A:377:LEU:HD23	2.21	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	349/383 (91%)	338 (97%)	10 (3%)	1 (0%)	46	72
1	C	343/383 (90%)	320 (93%)	23 (7%)	0	100	100
2	B	349/364 (96%)	321 (92%)	27 (8%)	1 (0%)	46	72
2	D	333/364 (92%)	315 (95%)	17 (5%)	1 (0%)	46	72
All	All	1374/1494 (92%)	1294 (94%)	77 (6%)	3 (0%)	52	77

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%)	45	73
1	C	253/329 (77%)	244 (96%)	9 (4%)	42	71
2	B	258/327 (79%)	251 (97%)	7 (3%)	52	79
2	D	255/327 (78%)	241 (94%)	14 (6%)	27	51
All	All	1038/1312 (79%)	999 (96%)	39 (4%)	40	68

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	59	GLN
1	A	94	HIS
1	A	123	THR
1	A	228	LEU
1	A	270	VAL
1	A	278	SER
1	A	285	ASP
1	A	367	ARG
2	B	238	THR
2	B	258	VAL
2	B	314	ILE
2	B	318	LYS
2	B	326	GLU
2	B	340	ILE
2	B	393	ARG
1	C	27	VAL
1	C	133	ILE
1	C	170	ASP
1	C	228	LEU
1	C	273	ARG
1	C	303	SER
1	C	333	THR
1	C	347	MET
1	C	349	SER
2	D	59	PHE
2	D	65	VAL
2	D	70	LEU
2	D	188	SER
2	D	207	MET
2	D	211	ASP
2	D	238	THR
2	D	240	ILE
2	D	258	VAL
2	D	260	SER
2	D	272	GLU
2	D	287	TYR
2	D	329	ILE
2	D	335	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	94	HIS
1	A	146	HIS
1	A	376	ASN
2	B	105	GLN
2	B	152	GLN
2	B	311	HIS
2	B	333	ASN
1	C	38	HIS
1	C	94	HIS
1	C	147	GLN
1	C	159	ASN
1	C	376	ASN
1	C	384	GLN
2	D	110	GLN
2	D	118	GLN
2	D	127	HIS
2	D	152	GLN
2	D	218	ASN
2	D	311	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	0.60	0	15,19,21	0.79	1 (6%)
5	NAG	A	504	5	14,14,15	0.69	0	15,19,21	0.72	0
5	BMA	A	505	5	11,11,12	0.97	1 (9%)	14,15,17	2.34	4 (28%)
5	MAN	A	506	5	11,11,12	0.76	0	14,15,17	0.88	0
5	MAN	A	507	5	11,11,12	0.73	0	14,15,17	0.97	0
5	FUC	A	508	5	10,10,11	1.80	2 (20%)	14,14,16	1.95	5 (35%)

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	-4.54	1.46	1.52
5	A	508	FUC	C4-C3	-2.50	1.45	1.52
5	A	505	BMA	C4-C5	2.17	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	NAG	C2-N2-C7	-2.07	120.38	123.04
5	A	508	FUC	O5-C1-C2	2.19	114.41	110.86
5	A	508	FUC	O5-C5-C4	2.73	114.27	109.53
5	A	508	FUC	C1-C2-C3	2.90	112.97	109.54
5	A	508	FUC	O5-C5-C6	3.35	111.67	106.13
5	A	508	FUC	C1-O5-C5	3.46	117.72	112.38
5	A	505	BMA	O3-C3-C4	3.51	118.23	110.34
5	A	505	BMA	O5-C5-C6	3.77	115.51	107.35
5	A	505	BMA	O3-C3-C2	4.25	117.68	110.00
5	A	505	BMA	O2-C2-C3	4.26	118.69	110.12

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	0.64	0	15,19,21	1.38	2 (13%)
6	QEL	B	1	-	26,26,26	2.51	8 (30%)	34,35,35	2.16	8 (23%)
4	NAG	B	501	2	14,14,15	0.39	0	15,19,21	1.22	2 (13%)
4	NAG	B	502	2	14,14,15	0.58	0	15,19,21	0.98	1 (6%)
4	NAG	C	502	1	14,14,15	0.50	0	15,19,21	0.97	1 (6%)
6	QEL	D	2	-	26,26,26	2.64	11 (42%)	34,35,35	2.09	9 (26%)
4	NAG	D	501	2	14,14,15	0.44	0	15,19,21	0.77	0
4	NAG	D	502	2	14,14,15	0.60	0	15,19,21	1.04	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	QEL	O1-C14	-9.71	1.23	1.42
6	B	1	QEL	O1-C14	-9.24	1.23	1.42
6	B	1	QEL	C14-C13	-3.43	1.49	1.54
6	D	2	QEL	C3-C18	-3.34	1.32	1.38
6	B	1	QEL	C3-C18	-3.05	1.32	1.38
6	D	2	QEL	C14-C13	-2.95	1.50	1.54
6	B	1	QEL	C9-C8	-2.92	1.44	1.52
6	D	2	QEL	C9-C8	-2.87	1.44	1.52
6	B	1	QEL	C24-C13	-2.85	1.47	1.52
6	D	2	QEL	C24-C13	-2.60	1.47	1.52
6	B	1	QEL	C16-C15	-2.49	1.34	1.39
6	D	2	QEL	C16-C15	-2.18	1.35	1.39
6	D	2	QEL	C6-C1	2.10	1.43	1.38
6	D	2	QEL	C7-C8	2.19	1.60	1.53
6	D	2	QEL	C3-C19	2.20	1.42	1.38
6	B	1	QEL	C2-C16	2.22	1.42	1.38
6	D	2	QEL	C02-C4	2.26	1.43	1.38
6	B	1	QEL	C3-C19	2.29	1.42	1.38
6	D	2	QEL	C2-C16	2.74	1.43	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	QEL	C24-C13-C14	-5.03	103.69	111.80
6	B	1	QEL	C24-C13-C14	-4.44	104.64	111.80
6	B	1	QEL	C12-C8-C7	-4.33	102.13	111.84
4	A	502	NAG	C2-N2-C7	-3.49	118.55	123.04
6	D	2	QEL	C19-C15-C14	-3.48	115.64	120.72
6	D	2	QEL	C12-C8-C7	-3.41	104.19	111.84
6	B	1	QEL	C19-C15-C14	-2.43	117.17	120.72
4	B	501	NAG	C2-N2-C7	-2.16	120.27	123.04
6	D	2	QEL	C9-C10-N1	2.13	114.93	111.48
4	B	501	NAG	C1-O5-C5	2.17	115.00	112.25
4	B	502	NAG	O5-C5-C6	2.17	112.05	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	NAG	C1-O5-C5	2.24	115.09	112.25
6	D	2	QEL	C11-N1-C13	2.27	120.48	113.29
6	B	1	QEL	C11-N1-C13	2.29	120.52	113.29
4	C	502	NAG	O5-C5-C6	2.34	112.41	107.35
6	B	1	QEL	C4-C7-C8	2.72	118.75	114.62
6	D	2	QEL	C16-C15-C14	3.02	125.15	120.72
6	D	2	QEL	C15-C14-C13	3.07	116.94	112.34
6	B	1	QEL	C10-N1-C11	3.90	116.30	109.23
6	D	2	QEL	O1-C14-C13	5.02	120.28	108.38
6	D	2	QEL	O1-C14-C15	5.13	122.50	111.16
6	B	1	QEL	O1-C14-C13	5.26	120.84	108.38
6	B	1	QEL	O1-C14-C15	5.80	123.98	111.16

All (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
4	D	501	NAG	C1
4	C	502	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%)	-0.29	1 (0%) 94 93	28, 45, 80, 100	0
1	C	351/383 (91%)	-0.02	8 (2%) 64 57	46, 70, 102, 122	0
2	B	353/364 (96%)	-0.16	5 (1%) 78 74	30, 62, 100, 125	0
2	D	345/364 (94%)	-0.20	1 (0%) 94 93	44, 70, 116, 133	0
All	All	1404/1494 (93%)	-0.17	15 (1%) 82 79	28, 64, 102, 133	0

All (15) 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
1	A	237	ALA	2.5
2	B	50	ILE	2.4
1	C	322	ILE	2.3
1	C	264	ALA	2.3
1	C	259	LEU	2.3
2	D	344	PHE	2.2
1	C	95	PRO	2.2
1	C	133	ILE	2.1
2	B	64	VAL	2.0
1	C	265	GLY	2.0

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	-0.41	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.