



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:56 am GMT

PDB ID : 5EWJ
Title : CRYSTAL STRUCTURE OF AMINO TERMINAL DOMAINS OF THE
NMDA RECEPTOR SUBUNIT GLUN1 AND GLUN2B IN COMPLEX
WITH IFENPRODIL
Authors : Pandit, J.
Deposited on : 2015-11-20
Resolution : 2.77 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

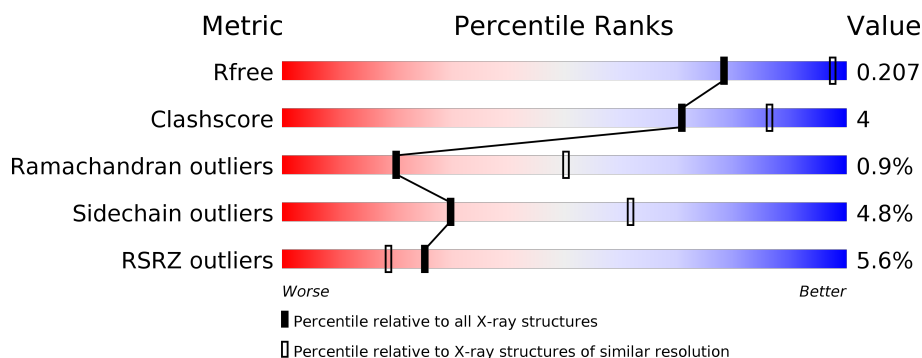
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	3276 (2.80-2.76)
Clashscore	112137	3771 (2.80-2.76)
Ramachandran outliers	110173	3707 (2.80-2.76)
Sidechain outliers	110143	3709 (2.80-2.76)
RSRZ outliers	101464	3307 (2.80-2.76)

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	390	<div> <div>2%</div> <div>80% 10% • 8%</div> </div>
1	C	390	<div> <div>7%</div> <div>78% 11% • 9%</div> </div>
2	B	364	<div> <div>5%</div> <div>84% 12% • •</div> </div>
2	D	364	<div> <div>7%</div> <div>83% 13% • •</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	C	501	-	-	-	X
4	NAG	C	502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11563 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	357	Total	C	N	O	S	0	0	0
			2752	1753	477	511	11			
1	C	356	Total	C	N	O	S	0	0	0
			2737	1741	479	507	10			

There are 12 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
A	409	LEU	-	expression tag	UNP Q91977
A	410	VAL	-	expression tag	UNP Q91977
A	411	PRO	-	expression tag	UNP Q91977
A	412	ARG	-	expression tag	UNP Q91977
C	61	GLN	ASN	engineered mutation	UNP Q91977
C	371	GLN	ASN	engineered mutation	UNP Q91977
C	409	LEU	-	expression tag	UNP Q91977
C	410	VAL	-	expression tag	UNP Q91977
C	411	PRO	-	expression tag	UNP Q91977
C	412	ARG	-	expression tag	UNP Q91977

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	353	Total	C	N	O	S	0	0	0
			2750	1772	436	527	15			
2	D	355	Total	C	N	O	S	0	0	0
			2778	1791	436	535	16			

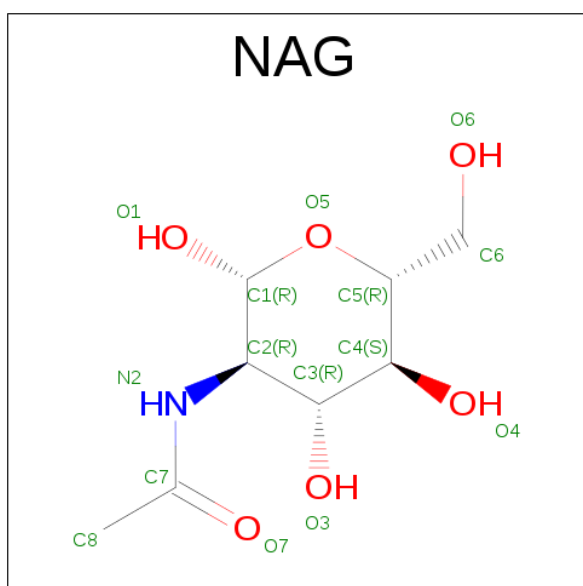
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q13224
D	348	ASP	ASN	engineered mutation	UNP Q13224

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



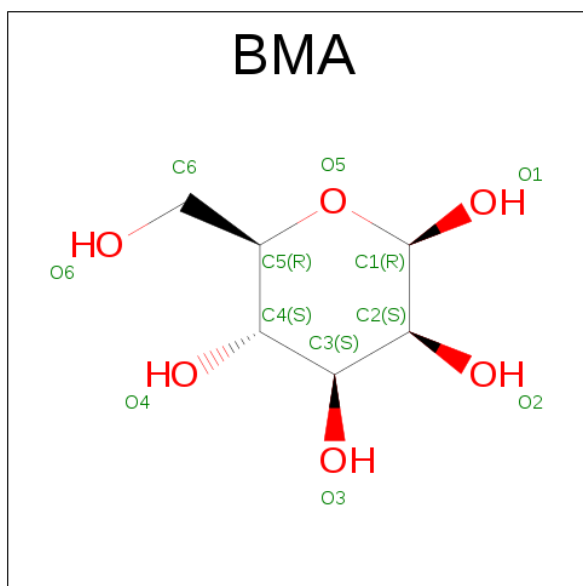
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

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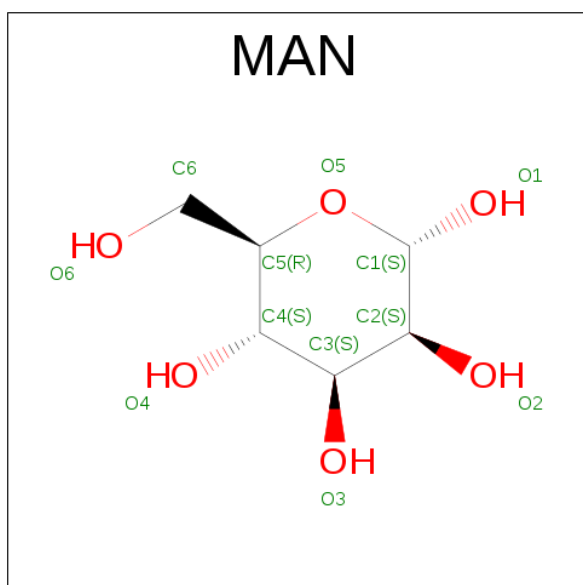
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



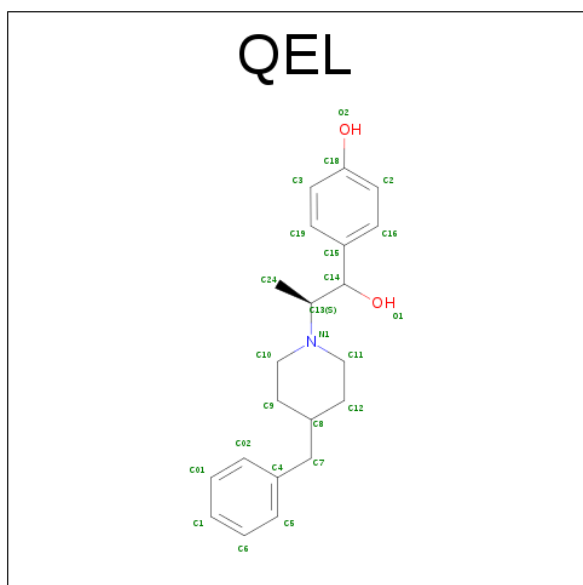
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (three-letter code: QEL) (formula: C₂₁H₂₇NO₂).



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

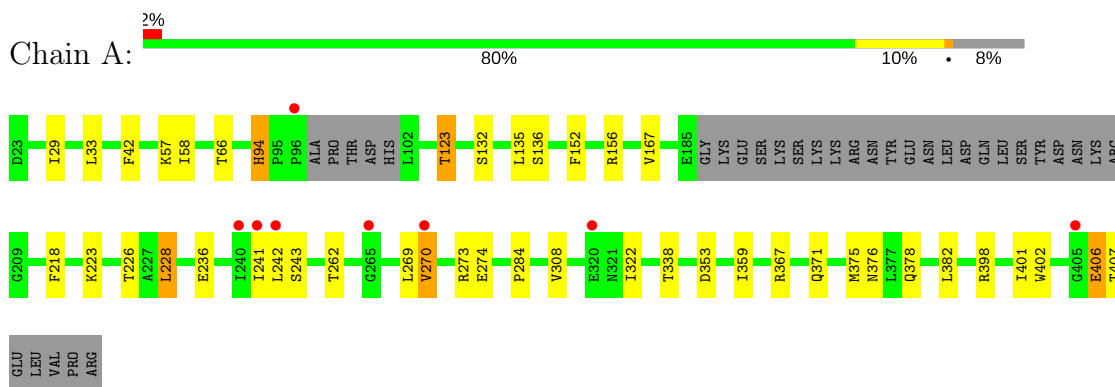
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	158	Total	O	0	0
			158	158		
8	B	80	Total	O	0	0
			80	80		
8	C	53	Total	O	0	0
			53	53		
8	D	60	Total	O	0	0
			60	60		

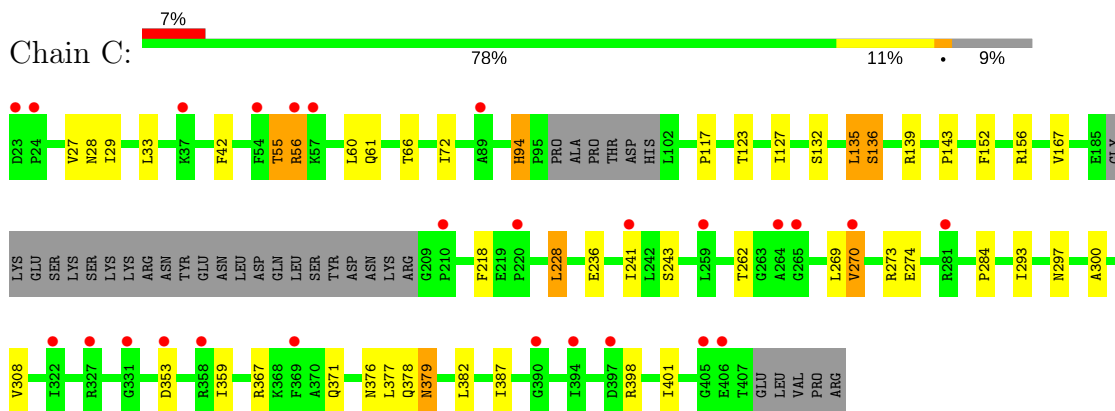
3 Residue-property plots

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.

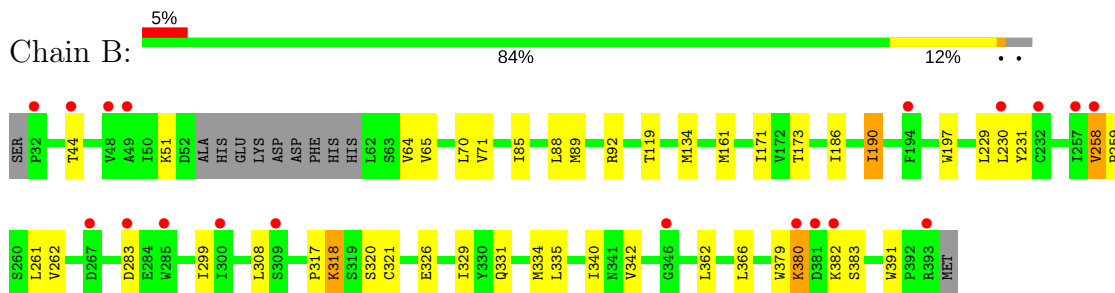
- Molecule 1: NMDA glutamate receptor subunit



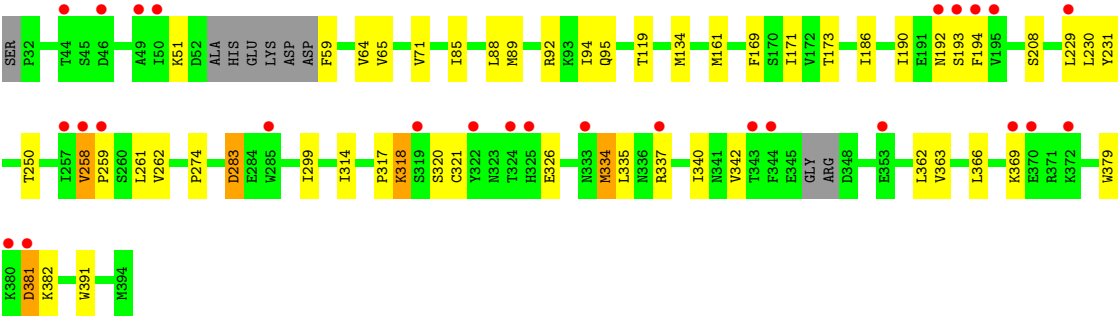
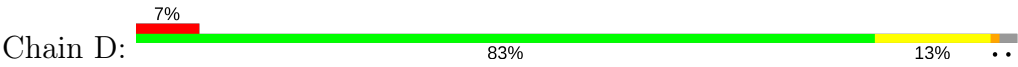
- Molecule 1: NMDA glutamate receptor subunit



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.46Å 60.10Å 145.00Å 90.00° 116.22° 90.00°	Depositor
Resolution (Å)	27.92 – 2.77 27.82 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.92-2.77) 98.9 (27.82-2.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.76Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.174 , 0.211 0.175 , 0.207	Depositor DCC
R_{free} test set	2685 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NA, BMA, NAG, QEL

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	0.57	0/2809	0.73	1/3819 (0.0%)
1	C	0.47	0/2792	0.69	1/3794 (0.0%)
2	B	0.51	0/2812	0.71	0/3828
2	D	0.50	0/2841	0.74	1/3864 (0.0%)
All	All	0.51	0/11254	0.72	3/15305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	381	ASP	C-N-CA	5.53	135.52	121.70
1	C	270	VAL	N-CA-CB	-5.14	100.19	111.50
1	A	270	VAL	N-CA-CB	-5.00	100.49	111.50

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	2752	0	2717	22	0
1	C	2737	0	2705	26	0
2	B	2750	0	2662	21	0
2	D	2778	0	2691	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	42	0	37	0	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
4	D	28	0	26	0	0
5	A	11	0	8	0	0
6	A	22	0	20	0	0
7	B	24	0	27	2	0
7	D	24	0	27	1	0
8	A	158	0	0	0	0
8	B	80	0	0	0	0
8	C	53	0	0	0	0
8	D	60	0	0	0	0
All	All	11563	0	10959	91	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 (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:HD22	1:A:378:GLN:HE21	1.27	0.82
1:C:55:THR:HG22	1:C:56:ARG:H	1.43	0.79
1:A:94:HIS:HE1	1:A:123:THR:HG23	1.46	0.79
1:A:402:TRP:HD1	1:A:406:GLU:HA	1.52	0.75
1:C:28:ASN:HD21	1:C:61:GLN:HE21	1.40	0.69
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.74	0.67
1:C:376:ASN:HD21	1:C:401:ILE:H	1.44	0.66
1:A:376:ASN:ND2	1:A:378:GLN:HE21	1.93	0.64
1:A:376:ASN:HD21	1:A:401:ILE:H	1.45	0.63
1:C:27:VAL:HG23	1:C:60:LEU:HD23	1.79	0.63
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.83	0.60
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.84	0.60
2:B:51:LYS:HE3	2:B:70:LEU:HD22	1.85	0.59
1:C:270:VAL:HG13	1:C:274:GLU:HB2	1.86	0.58
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.86	0.58
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.84	0.58
2:D:171:ILE:HD11	2:D:186:ILE:HG21	1.85	0.58
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.86	0.57
2:B:258:VAL:HG13	2:B:262:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:HIS:HE1	1:C:123:THR:HG23	1.69	0.56
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.88	0.55
2:B:329:ILE:HD12	2:D:314:ILE:HD11	1.88	0.54
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.73	0.54
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.89	0.54
1:C:167:VAL:HG12	1:C:243:SER:HB3	1.89	0.53
2:B:161:MET:HE1	2:B:229:LEU:HD11	1.91	0.52
1:A:322:ILE:HG23	1:A:338:THR:HG21	1.91	0.52
1:A:402:TRP:CD1	1:A:406:GLU:HA	2.41	0.52
1:C:28:ASN:HD21	1:C:61:GLN:NE2	2.07	0.51
2:B:317:PRO:HA	2:B:318:LYS:HE2	1.93	0.51
1:C:262:THR:HB	1:C:284:PRO:HB3	1.93	0.51
1:C:378:GLN:HG2	1:C:401:ILE:HD12	1.93	0.50
1:C:241:ILE:HA	1:C:269:LEU:O	2.12	0.50
1:C:72:ILE:HG21	2:D:321:CYS:HB3	1.93	0.50
1:C:376:ASN:HD22	1:C:378:GLN:HE21	1.58	0.49
1:A:241:ILE:HA	1:A:269:LEU:O	2.12	0.49
2:D:95:GLN:NE2	2:D:314:ILE:HD12	2.28	0.49
2:D:317:PRO:HA	2:D:318:LYS:HE2	1.93	0.49
2:B:299:ILE:HA	2:B:342:VAL:HG11	1.94	0.49
1:A:33:LEU:O	1:A:66:THR:HA	2.13	0.49
2:B:318:LYS:HD2	2:B:331:GLN:OE1	2.14	0.48
2:B:119:THR:O	2:B:318:LYS:HD2	2.14	0.47
1:C:33:LEU:O	1:C:66:THR:HA	2.15	0.47
2:D:366:LEU:HD13	2:D:391:TRP:HZ2	1.79	0.47
2:D:230:LEU:O	2:D:259:PRO:HD3	2.15	0.47
2:D:169:PHE:CZ	2:D:190:ILE:HD11	2.50	0.47
2:B:230:LEU:O	2:B:259:PRO:HD3	2.15	0.46
1:A:57:LYS:HG2	1:A:58:ILE:HG23	1.98	0.46
2:B:318:LYS:H	2:B:318:LYS:CD	2.28	0.46
2:D:119:THR:O	2:D:318:LYS:HD2	2.15	0.46
1:A:262:THR:HB	1:A:284:PRO:HB3	1.97	0.46
1:A:308:VAL:HG21	1:A:359:ILE:HG21	1.98	0.46
2:D:94:ILE:O	2:D:317:PRO:HB3	2.16	0.46
1:A:132:SER:O	7:B:503:QEL:H19	2.15	0.45
2:B:366:LEU:HD13	2:B:391:TRP:HZ2	1.82	0.45
1:C:117:PRO:HA	1:C:136:SER:HB3	1.98	0.45
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.98	0.45
2:B:161:MET:HE2	2:B:229:LEU:HD21	1.98	0.44
2:D:334:MET:HG3	2:D:337:ARG:HH21	1.82	0.44
1:A:135:LEU:HB2	7:B:503:QEL:H24	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:THR:HG22	1:C:56:ARG:N	2.23	0.44
2:D:318:LYS:H	2:D:318:LYS:CD	2.30	0.44
1:C:132:SER:O	7:D:503:QEL:H19	2.18	0.44
1:A:94:HIS:CE1	1:A:123:THR:HG23	2.37	0.44
2:D:250:THR:HB	2:D:274:PRO:HB3	2.00	0.44
1:A:152:PHE:CE2	1:A:156:ARG:HD2	2.53	0.43
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.99	0.43
2:D:283:ASP:HB3	2:D:363:VAL:HG23	2.00	0.43
1:A:29:ILE:HG22	1:A:42:PHE:HZ	1.82	0.43
2:D:173:THR:HA	2:D:231:TYR:O	2.19	0.43
2:B:85:ILE:HG22	2:B:89:MET:CE	2.49	0.42
2:B:89:MET:HE3	2:B:321:CYS:SG	2.59	0.42
1:C:29:ILE:HG22	1:C:42:PHE:HZ	1.84	0.42
2:D:161:MET:HE2	2:D:229:LEU:HD21	2.02	0.42
1:C:152:PHE:CE2	1:C:156:ARG:HD2	2.55	0.41
2:D:85:ILE:HG22	2:D:89:MET:CE	2.50	0.41
1:C:382:LEU:HA	1:C:382:LEU:HD23	1.96	0.41
1:C:297:ASN:HB3	1:C:300:ALA:HB3	2.03	0.41
2:B:71:VAL:HG11	2:B:88:LEU:HD11	2.02	0.41
2:D:362:LEU:HB2	2:D:379:TRP:HB3	2.01	0.41
2:B:190:ILE:HG13	2:B:197:TRP:CG	2.56	0.41
2:B:173:THR:HG22	2:B:231:TYR:HB3	2.02	0.41
2:B:173:THR:HA	2:B:231:TYR:O	2.21	0.41
1:C:139:ARG:NH2	1:C:143:PRO:HB3	2.36	0.41
1:C:135:LEU:HD22	2:D:208:SER:HB3	2.01	0.41
2:D:71:VAL:HG11	2:D:88:LEU:HD11	2.01	0.41
1:C:293:ILE:HD11	1:C:387:ILE:HG12	2.02	0.41
1:A:242:LEU:HB3	1:A:270:VAL:HG22	2.03	0.40
2:D:89:MET:HE3	2:D:321:CYS:SG	2.61	0.40
2:B:380:LYS:HD2	2:B:383:SER:HB3	2.03	0.40
1:A:375:MET:HB3	1:A:382:LEU:HD22	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	351/390 (90%)	336 (96%)	15 (4%)	0	100	100
1	C	350/390 (90%)	333 (95%)	13 (4%)	4 (1%)	17	44
2	B	349/364 (96%)	329 (94%)	18 (5%)	2 (1%)	28	60
2	D	349/364 (96%)	327 (94%)	16 (5%)	6 (2%)	11	31
All	All	1399/1508 (93%)	1325 (95%)	62 (4%)	12 (1%)	20	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	ASP
1	C	56	ARG
1	C	135	LEU
2	D	382	LYS
1	C	55	THR
1	C	379	ASN
2	D	283	ASP
2	D	381	ASP
2	B	334	MET
2	D	334	MET
2	D	193	SER
2	D	51	LYS

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	292/336 (87%)	278 (95%)	14 (5%)	30	62
1	C	289/336 (86%)	277 (96%)	12 (4%)	34	67
2	B	298/326 (91%)	282 (95%)	16 (5%)	26	56
2	D	305/326 (94%)	290 (95%)	15 (5%)	29	61
All	All	1184/1324 (89%)	1127 (95%)	57 (5%)	30	62

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	123	THR
1	A	136	SER
1	A	223	LYS
1	A	226	THR
1	A	228	LEU
1	A	236	GLU
1	A	273	ARG
1	A	353	ASP
1	A	367	ARG
1	A	371	GLN
1	A	398	ARG
1	A	406	GLU
1	A	407	THR
2	B	44	THR
2	B	64	VAL
2	B	65	VAL
2	B	92	ARG
2	B	134	MET
2	B	190	ILE
2	B	258	VAL
2	B	261	LEU
2	B	308	LEU
2	B	318	LYS
2	B	320	SER
2	B	326	GLU
2	B	335	LEU
2	B	340	ILE
2	B	380	LYS
2	B	382	LYS
1	C	94	HIS
1	C	127	ILE
1	C	136	SER
1	C	228	LEU
1	C	236	GLU
1	C	273	ARG
1	C	353	ASP
1	C	367	ARG
1	C	371	GLN
1	C	377	LEU
1	C	379	ASN
1	C	398	ARG

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Mol	Chain	Res	Type
2	D	59	PHE
2	D	64	VAL
2	D	65	VAL
2	D	92	ARG
2	D	134	MET
2	D	192	ASN
2	D	194	PHE
2	D	258	VAL
2	D	261	LEU
2	D	318	LYS
2	D	320	SER
2	D	326	GLU
2	D	335	LEU
2	D	340	ILE
2	D	369	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	376	ASN
2	B	105	GLN
2	B	311	HIS
1	C	28	ASN
1	C	94	HIS
1	C	376	ASN
1	C	379	ASN
2	D	95	GLN
2	D	105	GLN
2	D	118	GLN
2	D	219	GLN
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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	0.27	0	15,19,21	1.08	1 (6%)
4	NAG	A	503	1,4	14,14,15	0.29	0	15,19,21	0.66	0
4	NAG	A	504	5,4	14,14,15	0.26	0	15,19,21	1.04	1 (6%)
5	BMA	A	505	4,6	11,11,12	0.28	0	13,15,17	1.01	1 (7%)
6	MAN	A	506	5	11,11,12	0.42	0	13,15,17	0.98	0
6	MAN	A	507	5	11,11,12	0.41	0	13,15,17	0.73	0
4	NAG	B	501	2	14,14,15	0.31	0	15,19,21	0.67	0
4	NAG	B	502	2	14,14,15	0.25	0	15,19,21	2.08	2 (13%)
7	QEL	B	503	-	26,26,26	0.38	0	34,35,35	0.56	1 (2%)
4	NAG	C	502	1	14,14,15	0.38	0	15,19,21	0.73	1 (6%)
4	NAG	D	501	2	14,14,15	0.32	0	15,19,21	0.54	0
4	NAG	D	502	2	14,14,15	0.35	0	15,19,21	0.57	0
7	QEL	D	503	-	26,26,26	0.30	0	34,35,35	0.57	1 (2%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	507	5	-	0/2/19/22	0/1/1/1
4	NAG	B	501	2	-	0/6/23/26	0/1/1/1
4	NAG	B	502	2	-	0/6/23/26	0/1/1/1
7	QEL	B	503	-	-	0/16/26/26	0/3/3/3
4	NAG	C	502	1	-	0/6/23/26	0/1/1/1
4	NAG	D	501	2	-	0/6/23/26	0/1/1/1
4	NAG	D	502	2	-	0/6/23/26	0/1/1/1
7	QEL	D	503	-	-	0/16/26/26	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	NAG	C1-C2-N2	-3.25	104.94	110.49
4	C	502	NAG	C1-C2-N2	2.24	114.32	110.49
7	B	503	QEL	C10-N1-C13	2.49	121.66	113.37
7	D	503	QEL	C10-N1-C13	2.61	122.08	113.37
5	A	505	BMA	C1-O5-C5	2.91	116.17	112.17
4	A	502	NAG	C1-O5-C5	3.92	117.56	112.17
4	B	502	NAG	C1-O5-C5	4.97	119.02	112.17
4	B	502	NAG	O5-C1-C2	6.19	120.08	111.47

There are no chirality outliers.

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
7	B	503	QEL	2	0
7	D	503	QEL	1	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	357/390 (91%)	-0.20	8 (2%) 62 56	34, 52, 82, 101	0
1	C	356/390 (91%)	0.21	26 (7%) 16 10	55, 82, 111, 145	0
2	B	353/364 (96%)	0.17	19 (5%) 26 20	38, 72, 108, 125	0
2	D	355/364 (97%)	0.28	27 (7%) 15 9	55, 80, 121, 144	0
All	All	1421/1508 (94%)	0.11	80 (5%) 25 19	34, 73, 111, 145	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	381	ASP	6.1
2	D	380	LYS	5.6
2	D	193	SER	5.6
1	C	56	ARG	5.1
2	B	381	ASP	4.7
1	C	54	PHE	4.5
2	D	194	PHE	4.4
2	D	192	ASN	4.4
2	B	32	PRO	4.3
1	C	57	LYS	4.2
2	B	380	LYS	3.8
2	D	353	GLU	3.8
2	D	195	VAL	3.6
2	D	285	TRP	3.6
2	B	285	TRP	3.5
2	D	44	THR	3.3
1	A	405	GLY	3.3
2	D	343	THR	3.3
1	C	394	ILE	3.3
1	C	327	ARG	3.3
2	D	50	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	319	SER	3.2
2	D	324	THR	3.1
2	D	344	PHE	3.1
1	A	96	PRO	3.1
1	C	353	ASP	3.1
2	B	382	LYS	3.0
2	B	48	VAL	3.0
2	B	49	ALA	3.0
2	D	257	ILE	2.9
2	D	49	ALA	2.9
1	C	264	ALA	2.9
1	C	406	GLU	2.9
2	B	257	ILE	2.9
2	D	322	TYR	2.8
2	D	258	VAL	2.8
1	C	220	PRO	2.8
1	C	397	ASP	2.8
1	C	358	ARG	2.7
1	C	241	ILE	2.7
2	D	337	ARG	2.6
2	D	229	LEU	2.6
1	C	405	GLY	2.6
2	D	259	PRO	2.6
2	B	346	GLY	2.5
1	A	242	LEU	2.5
2	D	325	HIS	2.5
1	C	270	VAL	2.5
1	C	210	PRO	2.5
1	C	265	GLY	2.5
2	B	258	VAL	2.5
1	C	24	PRO	2.4
1	A	320	GLU	2.4
1	C	331	GLY	2.4
1	A	270	VAL	2.4
2	B	309	SER	2.3
1	C	369	PHE	2.3
1	A	241	ILE	2.3
2	B	44	THR	2.3
1	C	259	LEU	2.3
2	B	232	CYS	2.3
2	D	372	LYS	2.2
2	B	283	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	240	ILE	2.2
2	B	230	LEU	2.2
1	C	23	ASP	2.2
2	B	267	ASP	2.2
1	A	265	GLY	2.2
2	D	333	ASN	2.1
1	C	281	ARG	2.1
2	B	393	ARG	2.1
1	C	37	LYS	2.1
2	B	300	ILE	2.1
2	B	194	PHE	2.1
2	D	46	ASP	2.1
1	C	322	ILE	2.1
2	D	370	GLU	2.1
1	C	89	ALA	2.1
1	C	390	GLY	2.0
2	D	369	LYS	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	NA	C	501	1/1	0.80	0.62	9.53	100,100,100,100	0
4	NAG	C	502	14/15	0.86	0.31	4.01	88,94,97,100	0
4	NAG	A	502	14/15	0.96	0.18	1.71	58,69,76,77	0
3	NA	A	501	1/1	0.91	0.17	0.67	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	QEL	D	503	24/24	0.93	0.18	0.59	64,69,73,77	0
4	NAG	A	503	14/15	0.97	0.16	0.46	50,57,64,70	0
7	QEL	B	503	24/24	0.98	0.14	-0.57	36,45,60,60	0
6	MAN	A	506	11/12	0.95	0.12	-1.66	55,62,68,70	0
4	NAG	A	504	14/15	0.97	0.18	-	62,63,71,73	0
4	NAG	D	502	14/15	0.64	0.48	-	164,170,173,174	0
4	NAG	B	501	14/15	0.84	0.41	-	140,145,148,149	0
6	MAN	A	507	11/12	0.91	0.22	-	80,81,85,85	0
4	NAG	B	502	14/15	0.73	0.36	-	142,147,153,153	0
4	NAG	D	501	14/15	0.71	0.48	-	154,160,163,164	0
5	BMA	A	505	11/12	0.97	0.20	-	62,69,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.