



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2016 – 03:07 PM EDT

PDB ID : 5EWM
Title : CRYSTAL STRUCTURE OF AMINO TERMINAL DOMAINS OF THE
NMDA RECEPTOR SUBUNIT GLUN1 AND GLUN2B IN COMPLEX
WITH EVT-101
Authors : Pandit, J.
Deposited on : 2015-11-20
Resolution : 2.76 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
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) : rb-20027107

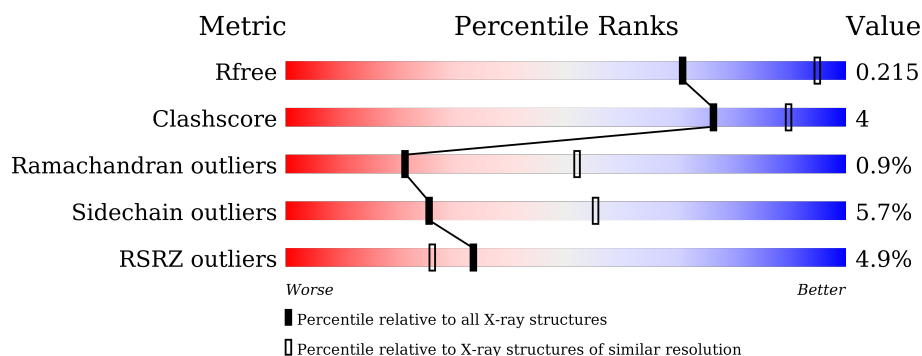
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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>7%</div> <div>80% 12% 8%</div> </div>
1	C	390	<div> <div>7%</div> <div>78% 11% 9%</div> </div>
2	B	364	<div> <div>4%</div> <div>83% 14% ..</div> </div>
2	D	364	<div> <div>7%</div> <div>82% 14% ..</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	A	501	-	-	-	X
3	NA	C	501	-	-	-	X
4	NAG	A	502	-	-	-	X
4	NAG	C	502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11534 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	356	Total	C	N	O	S	0	0	0
			2781	1793	443	530	15			
2	D	355	Total	C	N	O	S	0	0	0
			2778	1791	436	535	16			

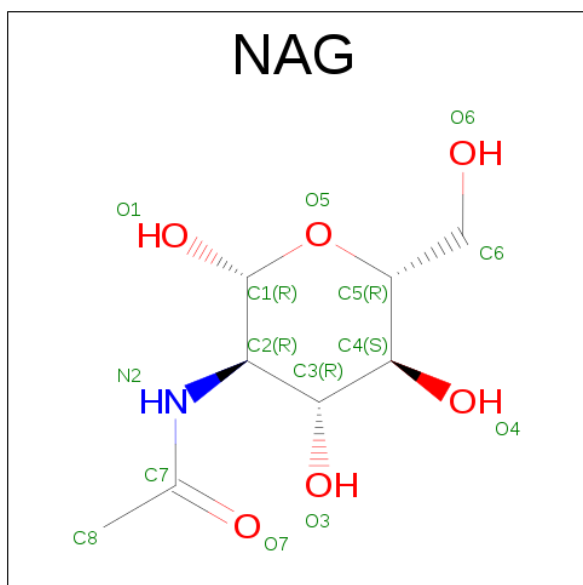
There are 2 discrepancies between the modelled and reference sequences:

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	B	1	Total Na 1 1	0	0
3	A	3	Total Na 3 3	0	0
3	C	1	Total Na 1 1	0	0

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



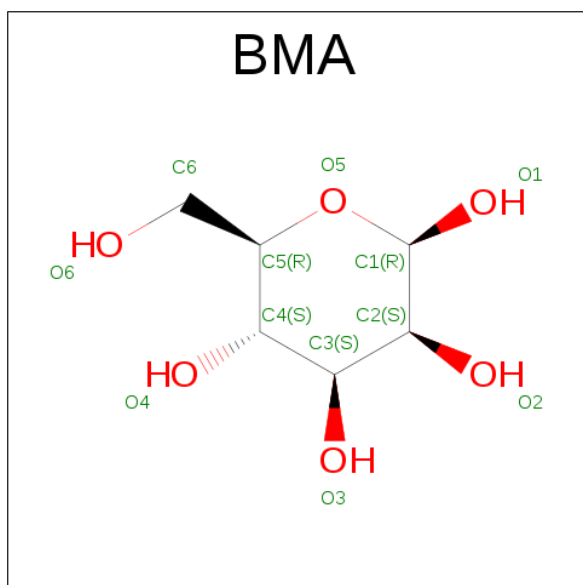
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

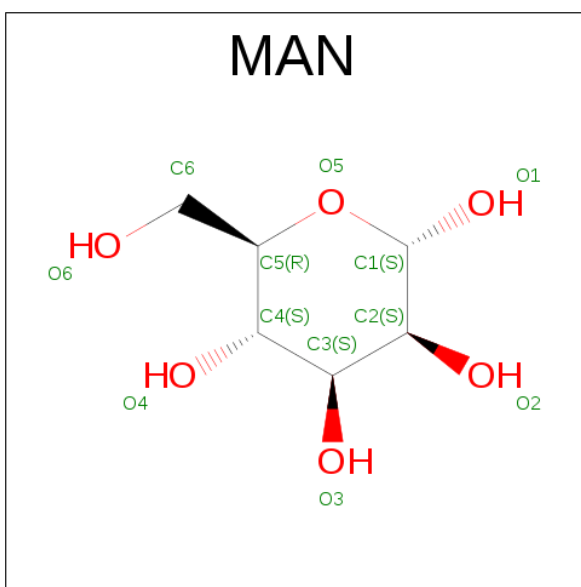
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



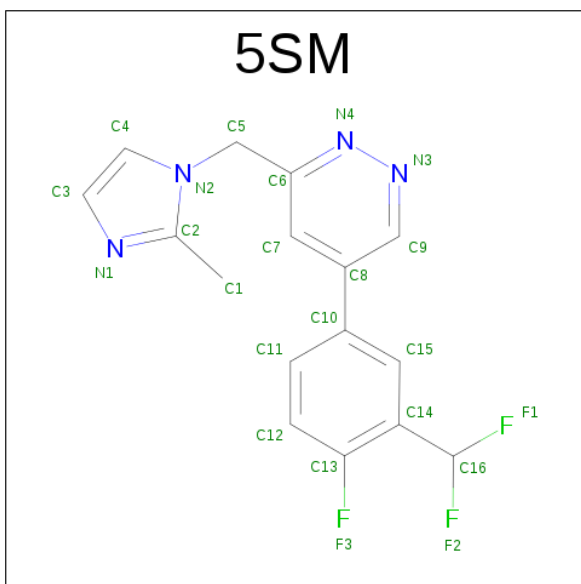
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- 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 5-[3-[bis(fluoranyl)methyl]-4-fluoranyl-phenyl]-3-[(2-methylimidazol-1-yl)methyl]pyridazine (three-letter code: 5SM) (formula: $C_{16}H_{13}F_3N_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	F	N	0	0
			23	16	3	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	F	N	0	0
			23	16	3	4		

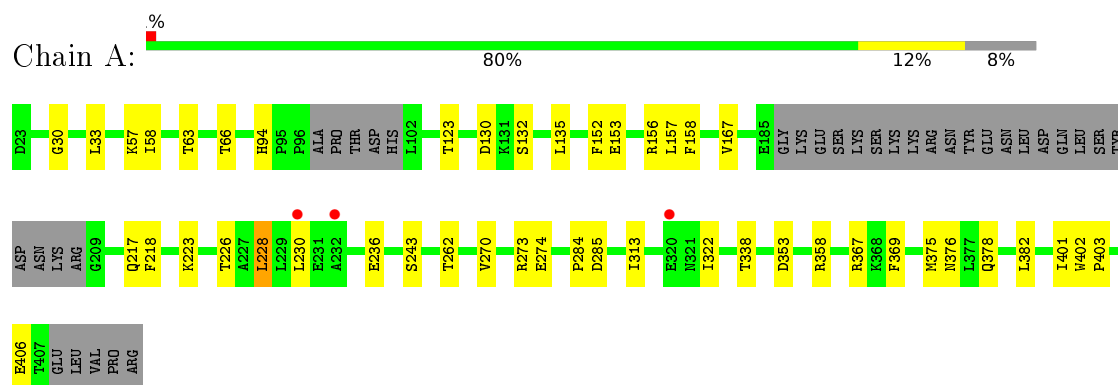
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	115	Total	O	0	0
			115	115		
8	B	86	Total	O	0	0
			86	86		
8	C	39	Total	O	0	0
			39	39		
8	D	50	Total	O	0	0
			50	50		

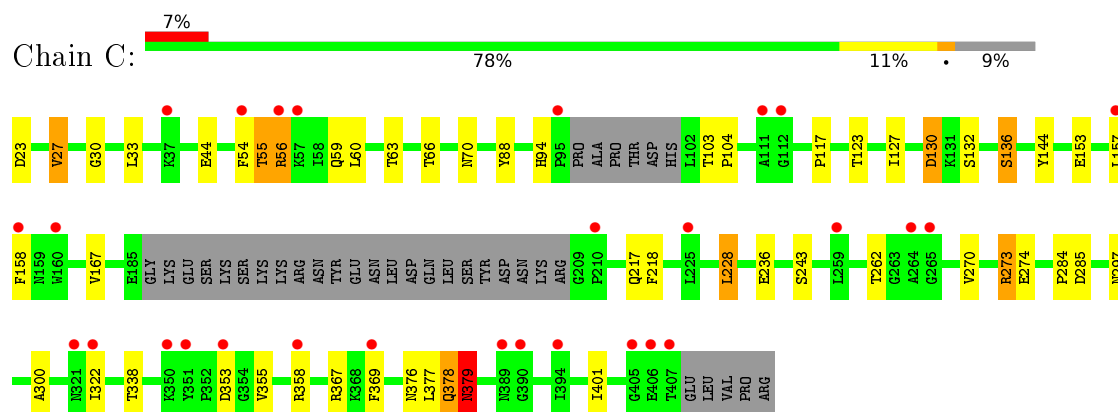
3 Residue-property plots [i](#)

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.

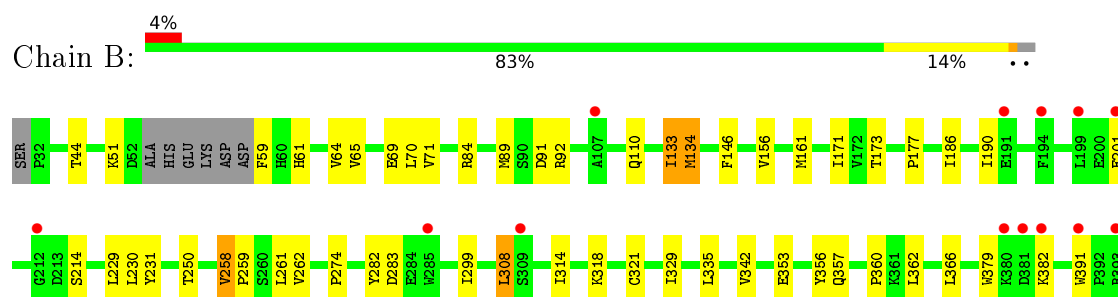
- Molecule 1: NMDA glutamate receptor subunit



- Molecule 1: NMDA glutamate receptor subunit

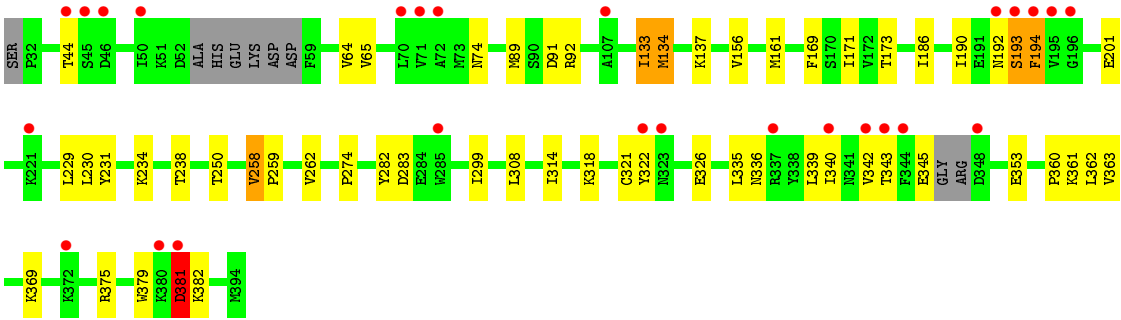
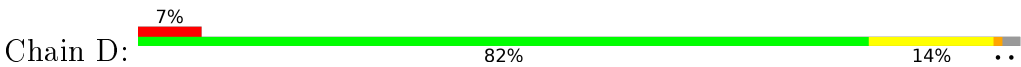


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



MET

- 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	268.40Å 60.61Å 144.50Å 90.00° 116.27° 90.00°	Depositor
Resolution (Å)	40.41 – 2.76 40.11 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.41-2.76) 98.2 (40.11-2.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.171 , 0.211 0.172 , 0.215	Depositor DCC
R_{free} test set	2608 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.4	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 53264 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11534	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: NA, 5SM, BMA, NAG, 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	0.58	0/2809	0.72	0/3819
1	C	0.47	0/2792	0.69	1/3794 (0.0%)
2	B	0.51	0/2846	0.71	1/3874 (0.0%)
2	D	0.49	0/2841	0.72	1/3864 (0.0%)
All	All	0.52	0/11288	0.71	3/15351 (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	B	61	HIS	C-N-CA	5.49	135.41	121.70
2	D	381	ASP	C-N-CA	5.07	134.38	121.70
1	C	130	ASP	C-N-CA	5.05	134.33	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	2717	20	0
1	C	2737	0	2705	25	0
2	B	2781	0	2685	21	0
2	D	2778	0	2691	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	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	1	0
4	D	28	0	26	0	0
5	A	11	0	8	0	0
6	A	22	0	20	0	0
7	B	23	0	0	1	0
7	D	23	0	0	0	0
8	A	115	0	0	1	0
8	B	86	0	0	0	0
8	C	39	0	0	1	0
8	D	50	0	0	0	0
All	All	11534	0	10928	84	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 (84) 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:HD21	1:A:401:ILE:H	1.36	0.73
1:A:402:TRP:HD1	1:A:406:GLU:HA	1.60	0.65
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.81	0.62
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.82	0.62
1:C:270:VAL:HG13	1:C:274:GLU:HB2	1.84	0.60
2:B:230:LEU:O	2:B:259:PRO:HD3	2.02	0.60
2:D:171:ILE:HD11	2:D:186:ILE:HG21	1.84	0.58
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.85	0.58
2:D:230:LEU:O	2:D:259:PRO:HD3	2.03	0.58
1:C:70:ASN:HD21	2:D:322:TYR:HA	1.69	0.57
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.86	0.56
1:C:27:VAL:HG23	1:C:60:LEU:HD23	1.87	0.56
1:C:262:THR:HB	1:C:284:PRO:HB3	1.87	0.56
1:C:358:ARG:HD2	1:C:369:PHE:CD2	2.42	0.55
2:B:110:GLN:HG2	2:B:134:MET:HE2	1.89	0.54
1:C:130:ASP:OD1	1:C:132:SER:HB3	2.08	0.53
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.90	0.53
2:B:258:VAL:HG13	2:B:262:VAL:HB	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.93	0.51
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.92	0.51
1:A:130:ASP:OD1	1:A:132:SER:HB3	2.10	0.51
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.92	0.51
2:D:134:MET:HE2	2:D:137:LYS:HG2	1.92	0.51
2:B:133:ILE:HD11	2:B:261:LEU:HD22	1.92	0.50
1:A:262:THR:HB	1:A:284:PRO:HB3	1.93	0.49
1:C:379:ASN:HB2	8:C:615:HOH:O	2.12	0.49
2:B:161:MET:HE2	2:B:229:LEU:HD21	1.94	0.49
1:C:117:PRO:HA	1:C:136:SER:HB3	1.94	0.49
1:A:57:LYS:HB2	8:A:695:HOH:O	2.13	0.48
2:B:329:ILE:HD12	2:D:314:ILE:HD11	1.95	0.48
1:A:33:LEU:O	1:A:66:THR:HA	2.14	0.48
1:C:55:THR:HG23	1:C:59:GLN:HB2	1.96	0.48
2:B:146:PHE:HA	2:B:357:GLN:HG3	1.95	0.47
1:C:94:HIS:CE1	1:C:123:THR:HG23	2.50	0.47
1:C:27:VAL:HG12	1:C:88:TYR:CE1	2.49	0.47
1:C:33:LEU:O	1:C:66:THR:HA	2.15	0.47
1:A:402:TRP:CD1	1:A:406:GLU:HA	2.47	0.46
2:B:89:MET:CE	2:B:321:CYS:SG	3.04	0.46
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.80	0.46
1:A:30:GLY:HA2	1:A:63:THR:O	2.16	0.46
2:D:161:MET:HE2	2:D:229:LEU:HD21	1.98	0.46
2:D:250:THR:HB	2:D:274:PRO:HB3	1.97	0.46
2:D:89:MET:CE	2:D:321:CYS:SG	3.05	0.45
2:B:299:ILE:HA	2:B:342:VAL:HG11	1.99	0.45
2:B:250:THR:HB	2:B:274:PRO:HB3	1.99	0.44
1:C:157:LEU:HD23	1:C:158:PHE:CE1	2.53	0.44
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.99	0.44
1:C:167:VAL:O	1:C:217:GLN:HA	2.17	0.44
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.99	0.44
2:B:133:ILE:HG22	2:B:356:TYR:CE1	2.53	0.43
2:B:282:TYR:HE1	2:B:360:PRO:HB3	1.84	0.43
1:A:157:LEU:HD23	1:A:158:PHE:CE1	2.53	0.43
1:A:322:ILE:HG23	1:A:338:THR:HG21	2.01	0.43
1:A:376:ASN:HD22	1:A:378:GLN:HE21	1.67	0.43
1:C:297:ASN:HB3	1:C:300:ALA:HB3	2.00	0.43
1:A:167:VAL:O	1:A:217:GLN:HA	2.18	0.43
1:A:375:MET:HB3	1:A:382:LEU:HD22	2.00	0.43
1:C:376:ASN:HD21	1:C:401:ILE:H	1.66	0.43
2:B:177:PRO:HG2	7:B:503:5SM:C1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ILE:HG23	1:C:338:THR:HG21	2.01	0.42
1:C:30:GLY:HA2	1:C:63:THR:O	2.19	0.42
1:A:167:VAL:HG12	1:A:243:SER:HB3	2.02	0.42
1:C:378:GLN:HG2	1:C:401:ILE:HD12	2.01	0.42
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.55	0.42
2:D:282:TYR:HE1	2:D:360:PRO:CB	2.33	0.42
1:A:152:PHE:CE2	1:A:156:ARG:HD2	2.55	0.41
2:B:51:LYS:HE3	2:B:70:LEU:HD22	2.02	0.41
2:D:308:LEU:HB2	2:D:314:ILE:HG23	2.01	0.41
2:D:363:VAL:HG11	2:D:375:ARG:HG2	2.00	0.41
2:B:156:VAL:HG22	2:B:379:TRP:CD2	2.55	0.41
1:C:378:GLN:CG	1:C:401:ILE:HD12	2.50	0.41
1:C:355:VAL:HG11	4:C:502:NAG:H82	2.01	0.41
1:A:58:ILE:HD13	1:A:313:ILE:HG22	2.02	0.41
1:C:167:VAL:HG12	1:C:243:SER:HB3	2.02	0.40
2:D:156:VAL:HG22	2:D:379:TRP:CD2	2.55	0.40
2:B:308:LEU:HB2	2:B:314:ILE:HG23	2.02	0.40
1:A:94:HIS:CE1	1:A:123:THR:HG23	2.57	0.40
1:A:358:ARG:HD3	1:A:369:PHE:CD2	2.56	0.40
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.37	0.40
2:D:234:LYS:O	2:D:238:THR:HG23	2.22	0.40
2:B:366:LEU:HD13	2:B:391:TRP:HZ2	1.86	0.40
1:C:103:THR:HB	1:C:104:PRO:CD	2.52	0.40
2:D:134:MET:CE	2:D:137:LYS:HA	2.51	0.40
2:D:336:ASN:HA	2:D:339:LEU:HD12	2.04	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%)	343 (98%)	7 (2%)	1 (0%)	46 77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	350/390 (90%)	338 (97%)	8 (2%)	4 (1%)	17	46
2	B	352/364 (97%)	334 (95%)	17 (5%)	1 (0%)	46	77
2	D	349/364 (96%)	334 (96%)	9 (3%)	6 (2%)	11	32
All	All	1402/1508 (93%)	1349 (96%)	41 (3%)	12 (1%)	21	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	382	LYS
2	B	283	ASP
1	C	54	PHE
1	C	56	ARG
2	D	194	PHE
2	D	283	ASP
1	C	379	ASN
2	D	381	ASP
2	D	193	SER
1	C	55	THR
2	D	133	ILE
1	A	403	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	292/336 (87%)	281 (96%)	11 (4%)	40	73
1	C	289/336 (86%)	273 (94%)	16 (6%)	27	56
2	B	301/326 (92%)	283 (94%)	18 (6%)	24	53
2	D	305/326 (94%)	282 (92%)	23 (8%)	17	40
All	All	1187/1324 (90%)	1119 (94%)	68 (6%)	25	55

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	153	GLU
1	A	223	LYS
1	A	226	THR
1	A	228	LEU
1	A	230	LEU
1	A	236	GLU
1	A	273	ARG
1	A	285	ASP
1	A	353	ASP
1	A	367	ARG
2	B	44	THR
2	B	59	PHE
2	B	64	VAL
2	B	65	VAL
2	B	69	GLU
2	B	91	ASP
2	B	92	ARG
2	B	133	ILE
2	B	134	MET
2	B	190	ILE
2	B	201	GLU
2	B	214	SER
2	B	258	VAL
2	B	308	LEU
2	B	318	LYS
2	B	335	LEU
2	B	353	GLU
2	B	382	LYS
1	C	23	ASP
1	C	27	VAL
1	C	44	GLU
1	C	56	ARG
1	C	127	ILE
1	C	136	SER
1	C	153	GLU
1	C	228	LEU
1	C	236	GLU
1	C	273	ARG
1	C	285	ASP
1	C	353	ASP
1	C	367	ARG
1	C	377	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	378	GLN
1	C	379	ASN
2	D	44	THR
2	D	64	VAL
2	D	65	VAL
2	D	74	ASN
2	D	91	ASP
2	D	92	ARG
2	D	133	ILE
2	D	134	MET
2	D	192	ASN
2	D	193	SER
2	D	194	PHE
2	D	201	GLU
2	D	258	VAL
2	D	318	LYS
2	D	326	GLU
2	D	335	LEU
2	D	340	ILE
2	D	343	THR
2	D	345	GLU
2	D	353	GLU
2	D	361	LYS
2	D	369	LYS
2	D	381	ASP

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	59	GLN
1	A	376	ASN
2	B	105	GLN
2	B	219	GLN
2	B	311	HIS
1	C	28	ASN
1	C	53	HIS
1	C	146	HIS
1	C	147	GLN
1	C	376	ASN
2	D	105	GLN
2	D	192	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 5 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	0.29	0	15,19,21	1.07	1 (6%)
4	NAG	A	503	1,4	14,14,15	0.35	0	15,19,21	0.49	0
4	NAG	A	504	5,4	14,14,15	0.27	0	15,19,21	0.54	0
5	BMA	A	505	4,6	11,11,12	0.25	0	15,15,17	0.84	1 (6%)
6	MAN	A	506	5	11,11,12	0.31	0	15,15,17	0.84	1 (6%)
6	MAN	A	507	5	11,11,12	0.32	0	15,15,17	0.70	0
4	NAG	B	501	2	14,14,15	0.28	0	15,19,21	0.64	0
4	NAG	B	502	2	14,14,15	0.28	0	15,19,21	0.65	0
7	5SM	B	503	-	20,25,25	0.39	0	24,35,35	0.94	2 (8%)
4	NAG	C	502	1	14,14,15	0.40	0	15,19,21	0.57	0
4	NAG	D	501	2	14,14,15	0.35	0	15,19,21	0.39	0
4	NAG	D	502	2	14,14,15	0.31	0	15,19,21	0.53	0
7	5SM	D	503	-	20,25,25	0.36	0	24,35,35	0.76	1 (4%)

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
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	5SM	B	503	-	-	0/10/12/12	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	5SM	D	503	-	-	0/10/12/12	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	503	5SM	C5-C6-C7	-2.49	119.40	121.96
7	D	503	5SM	C4-N2-C2	-2.17	106.56	108.60
7	B	503	5SM	C4-N2-C2	-2.03	106.69	108.60
6	A	506	MAN	C1-C2-C3	2.20	112.21	109.55
5	A	505	BMA	C1-O5-C5	2.40	115.67	112.14
4	A	502	NAG	C1-O5-C5	3.10	116.70	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503	5SM	1	0
4	C	502	NAG	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	357/390 (91%)	-0.21	3 (0%) 87 83	36, 53, 85, 109	0
1	C	356/390 (91%)	0.32	28 (7%) 15 10	61, 87, 116, 145	0
2	B	356/364 (97%)	0.19	13 (3%) 45 38	44, 73, 109, 142	0
2	D	355/364 (97%)	0.27	26 (7%) 18 13	55, 80, 120, 139	0
All	All	1424/1508 (94%)	0.14	70 (4%) 33 26	36, 76, 113, 145	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	381	ASP	5.3
1	C	259	LEU	5.1
1	C	358	ARG	4.9
2	D	193	SER	4.4
1	C	369	PHE	4.4
1	C	57	LYS	4.4
2	B	382	LYS	4.1
2	D	44	THR	3.8
1	C	353	ASP	3.5
2	D	194	PHE	3.5
2	B	380	LYS	3.4
2	D	323	ASN	3.2
1	C	406	GLU	3.2
2	D	72	ALA	3.2
2	B	381	ASP	3.0
1	C	56	ARG	3.0
2	D	195	VAL	3.0
1	C	54	PHE	3.0
1	C	321	ASN	3.0
1	C	390	GLY	3.0
2	B	285	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	337	ARG	2.8
1	A	232	ALA	2.7
2	B	191	GLU	2.7
2	D	343	THR	2.7
2	B	201	GLU	2.6
2	B	393	ARG	2.6
1	C	407	THR	2.6
2	D	344	PHE	2.6
1	A	320	GLU	2.6
1	C	351	TYR	2.6
1	C	210	PRO	2.5
1	C	111	ALA	2.5
2	D	380	LYS	2.5
2	B	194	PHE	2.5
2	B	309	SER	2.5
1	C	225	LEU	2.5
2	D	322	TYR	2.5
1	C	264	ALA	2.4
1	C	158	PHE	2.4
2	D	50	ILE	2.4
1	C	37	LYS	2.4
1	C	394	ILE	2.4
1	C	160	TRP	2.3
1	C	389	ASN	2.3
1	C	350	LYS	2.3
1	A	230	LEU	2.2
2	D	342	VAL	2.2
2	D	107	ALA	2.2
1	C	265	GLY	2.2
2	D	45	SER	2.2
2	D	340	ILE	2.2
2	B	199	LEU	2.1
2	D	372	LYS	2.1
2	B	391	TRP	2.1
2	D	285	TRP	2.1
2	B	212	GLY	2.1
2	D	71	VAL	2.1
2	B	107	ALA	2.1
1	C	405	GLY	2.1
2	D	70	LEU	2.1
1	C	322	ILE	2.1
2	D	221	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	192	ASN	2.1
1	C	112	GLY	2.1
2	D	348	ASP	2.1
1	C	157	LEU	2.0
2	D	196	GLY	2.0
1	C	95	PRO	2.0
2	D	46	ASP	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	A	501	1/1	0.90	0.42	21.56	67,67,67,67	0
3	NA	C	501	1/1	0.93	0.29	4.18	80,80,80,80	0
4	NAG	A	502	14/15	0.96	0.20	2.70	56,69,75,79	0
4	NAG	C	502	14/15	0.80	0.27	2.05	98,105,107,111	0
6	MAN	A	506	11/12	0.98	0.16	0.89	55,61,69,71	0
7	5SM	D	503	23/23	0.98	0.22	0.25	66,71,72,73	0
7	5SM	B	503	23/23	0.97	0.22	0.03	42,48,57,60	0
3	NA	A	508	1/1	0.94	0.12	-0.68	45,45,45,45	0
4	NAG	A	503	14/15	0.96	0.11	-1.83	45,59,64,68	0
3	NA	B	504	1/1	0.92	0.09	-1.92	57,57,57,57	0
3	NA	A	509	1/1	0.94	0.09	-2.22	62,62,62,62	0
4	NAG	B	501	14/15	0.69	0.27	-	140,143,145,147	0
4	NAG	D	502	14/15	0.71	0.44	-	152,158,161,163	0
4	NAG	D	501	14/15	0.70	0.41	-	150,154,158,160	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	502	14/15	0.81	0.30	-	128,136,142,145	0
5	BMA	A	505	11/12	0.95	0.15	-	62,69,75,83	0
6	MAN	A	507	11/12	0.92	0.17	-	88,89,93,96	0
4	NAG	A	504	14/15	0.96	0.12	-	61,65,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.