Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 01:21 AM EDT

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PDB ID	:	5TPZ
Title	:	Crystal structure of amino terminal domains of the NMDA receptor subunit GluN1 and GluN2B in apo closed state
Authors	:	Romero-Hernandez, A.; Simorwski, N.; Karakas, E.; Furukawa, H.
Deposited on	:	unknown
Resolution	:	3.10 Å(reported)

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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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
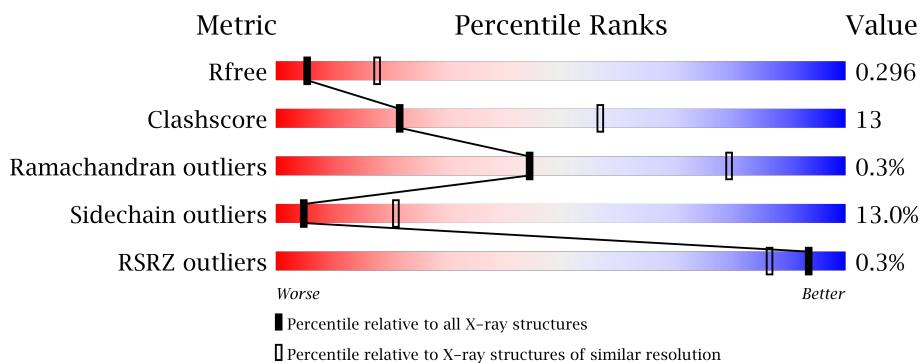
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	62% 27% · 8%
2	D	362	67% 28% · ·
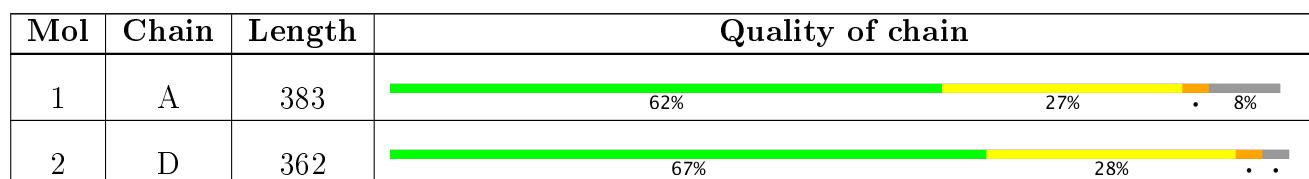
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5023 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	354	Total	C	N	O	S	0	0	0
			2514	1598	428	478	10			

There are 2 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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	352	Total	C	N	O	S	0	1	0
			2449	1556	398	480	15			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
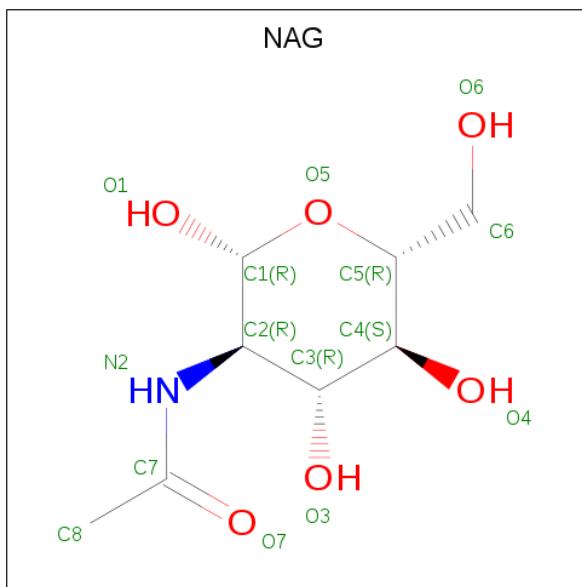
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	D	1	Total 1	O 1	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

Chain A:
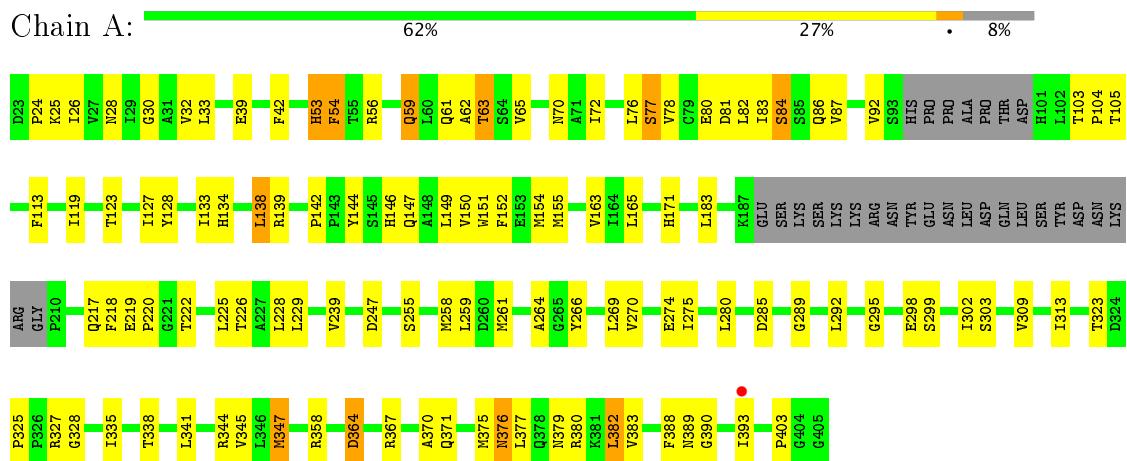
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:
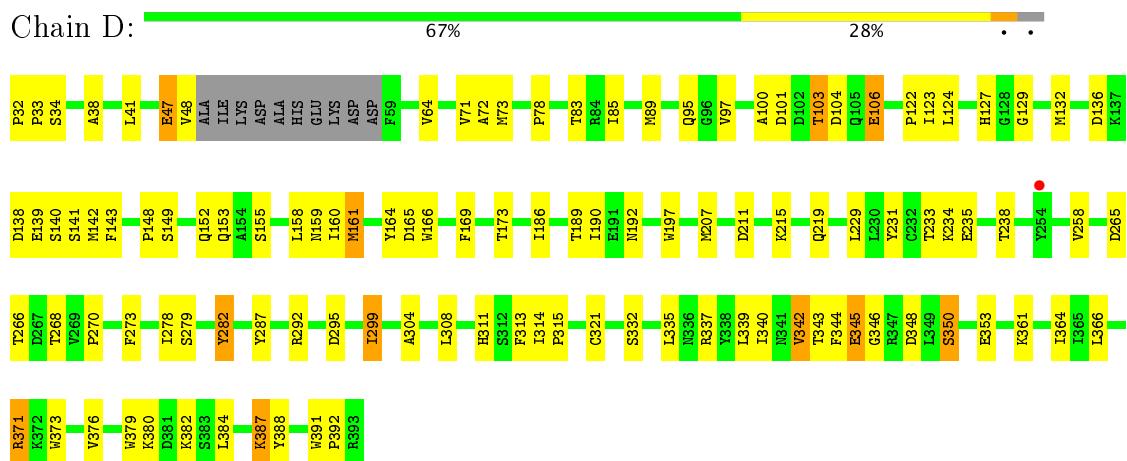
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	75.78Å 75.78Å 548.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.89 – 3.10 47.41 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.89-3.10) 95.3 (47.41-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.240 , 0.300 0.228 , 0.296	Depositor DCC
R_{free} test set	900 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	94.3	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 87.2	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5023	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
NAG

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	0/2566	0.63	0/3519
2	D	0.42	0/2512	0.60	0/3445
All	All	0.44	0/5078	0.61	0/6964

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
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	GLY	Peptide
1	A	53	HIS	Peptide

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	2514	0	2263	64	0
2	D	2449	0	2023	63	0
3	A	42	0	39	0	0
3	D	14	0	13	1	0
4	A	3	0	0	0	0
4	D	1	0	0	0	0
All	All	5023	0	4338	125	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 13.

All (125) 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:D:161:MET:HB3	2:D:166:TRP:HB2	1.60	0.84
2:D:273:PHE:O	2:D:371:ARG:NH2	2.17	0.77
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.66	0.76
1:A:261:MET:HA	1:A:266:TYR:CE2	2.22	0.74
2:D:282:TYR:HE1	2:D:361:LYS:H	1.38	0.72
2:D:366:LEU:HB2	2:D:376:VAL:HG21	1.71	0.72
1:A:358:ARG:O	1:A:367:ARG:NH1	2.25	0.69
2:D:160:ILE:HD11	2:D:364:ILE:HG12	1.75	0.67
1:A:53:HIS:HA	1:A:54:PHE:CD2	2.30	0.66
2:D:350:SER:OG	3:D:401:NAG:O7	2.13	0.66
1:A:128:TYR:HA	1:A:134:HIS:CD2	2.33	0.64
1:A:30:GLY:HA2	1:A:63:THR:O	1.98	0.63
1:A:275:ILE:HD13	1:A:289:GLY:HA3	1.79	0.63
2:D:266:THR:O	2:D:373:TRP:HD1	1.83	0.61
1:A:54:PHE:CD1	1:A:54:PHE:O	2.54	0.61
2:D:287:TYR:CE2	2:D:292:ARG:HG2	2.35	0.61
1:A:280:LEU:HD12	1:A:377:LEU:HD22	1.83	0.60
1:A:376:ASN:HD22	1:A:377:LEU:N	1.99	0.59
1:A:54:PHE:HD1	1:A:54:PHE:O	1.84	0.59
2:D:129:GLY:HA2	2:D:132:MET:SD	2.43	0.58
2:D:33:PRO:HG2	2:D:64:VAL:HG12	1.85	0.58
1:A:77:SER:OG	1:A:81:ASP:OD2	2.21	0.58
2:D:138:ASP:OD1	2:D:139:GLU:N	2.36	0.57
2:D:122:PRO:HB3	2:D:339:LEU:HD11	1.85	0.57
1:A:113:PHE:CE2	2:D:78:PRO:HD3	2.40	0.57
2:D:304:ALA:O	2:D:314:ILE:HD11	2.05	0.56
1:A:259:LEU:HB2	1:A:261:MET:HG3	1.86	0.56
2:D:161:MET:HE1	2:D:229:LEU:HD21	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG12	1:A:289:GLY:HA2	1.88	0.56
1:A:163:VAL:HG12	1:A:239:VAL:HB	1.87	0.55
2:D:345:GLU:OE1	2:D:346:GLY:N	2.39	0.55
1:A:226:THR:HG22	1:A:259:LEU:HD21	1.89	0.54
2:D:106:GLU:H	2:D:106:GLU:CD	2.10	0.54
2:D:104:ASP:OD2	2:D:234:LYS:NZ	2.32	0.54
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.90	0.53
1:A:86:GLN:HG3	1:A:327:ARG:HA	1.89	0.53
2:D:292:ARG:O	2:D:295:ASP:N	2.42	0.53
1:A:53:HIS:HA	1:A:54:PHE:CG	2.44	0.53
1:A:298:GLU:O	1:A:302:ILE:HG13	2.09	0.53
2:D:215:LYS:O	2:D:219:GLN:N	2.40	0.52
1:A:24:PRO:HB3	1:A:56:ARG:O	2.09	0.52
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.74	0.52
1:A:78:VAL:O	1:A:83:ILE:HG12	2.10	0.51
1:A:269:LEU:HD12	1:A:270:VAL:H	1.75	0.51
2:D:391:TRP:CD2	2:D:392:PRO:HD2	2.45	0.51
1:A:119:ILE:HA	1:A:138:LEU:O	2.11	0.51
1:A:144:TYR:O	1:A:147:GLN:HG3	2.10	0.51
2:D:164:TYR:HH	2:D:391:TRP:HZ3	1.59	0.51
2:D:47:GLU:OE1	2:D:48:VAL:N	2.43	0.50
2:D:95:GLN:NE2	2:D:315:PRO:O	2.45	0.49
1:A:84:SER:HA	1:A:327:ARG:O	2.11	0.49
1:A:152:PHE:CD2	1:A:183:LEU:HD22	2.48	0.49
1:A:152:PHE:HD2	1:A:183:LEU:HD22	1.77	0.48
2:D:348:ASP:OD1	2:D:350:SER:OG	2.31	0.48
1:A:364:ASP:OD1	1:A:364:ASP:N	2.47	0.48
2:D:155:SER:O	2:D:159:ASN:ND2	2.47	0.48
1:A:261:MET:HA	1:A:266:TYR:HE2	1.76	0.48
2:D:387:LYS:HB3	2:D:388:TYR:CD1	2.49	0.48
1:A:218:PHE:HB3	1:A:228:LEU:HD12	1.95	0.47
2:D:270:PRO:HD2	2:D:273:PHE:CD2	2.49	0.47
2:D:122:PRO:HA	2:D:142:MET:O	2.14	0.47
2:D:38:ALA:HB3	2:D:97:VAL:HG22	1.96	0.47
1:A:370:ALA:O	1:A:390:GLY:HA2	2.15	0.47
1:A:338:THR:O	1:A:341:LEU:N	2.48	0.47
2:D:344:PHE:CD2	2:D:345:GLU:HG3	2.50	0.47
1:A:151:TRP:O	1:A:155:MET:HG3	2.15	0.46
2:D:148:PRO:HG2	2:D:153:GLN:NE2	2.30	0.46
2:D:315:PRO:HG2	2:D:335:LEU:HD22	1.97	0.46
1:A:70:ASN:OD1	1:A:72:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:LEU:HD13	2:D:314:ILE:HG12	1.97	0.46
1:A:150:VAL:HG12	1:A:154:MET:HE2	1.98	0.45
1:A:347:MET:HB3	1:A:347:MET:HE3	1.84	0.45
1:A:379:ASN:C	1:A:380:ARG:HD3	2.37	0.45
2:D:32:PRO:HA	2:D:33:PRO:HD3	1.82	0.45
2:D:41:LEU:O	2:D:72:ALA:HA	2.17	0.45
1:A:375:MET:HB3	1:A:382:LEU:HD22	1.98	0.45
2:D:85:ILE:O	2:D:89:MET:HG3	2.16	0.45
2:D:299:ILE:HG23	2:D:342:VAL:HG21	1.99	0.45
1:A:142:PRO:HG3	1:A:370:ALA:CB	2.47	0.45
2:D:158:LEU:HD11	2:D:186:ILE:HG12	1.98	0.45
2:D:258:VAL:O	2:D:279:SER:HA	2.16	0.44
2:D:104:ASP:OD2	2:D:234:LYS:HD3	2.18	0.44
2:D:149:SER:CB	2:D:152:GLN:HG3	2.48	0.44
1:A:127:ILE:HA	1:A:171:HIS:CE1	2.53	0.44
1:A:280:LEU:HA	1:A:280:LEU:HD13	1.82	0.44
2:D:100:ALA:HB1	2:D:127:HIS:HB3	1.99	0.44
1:A:86:GLN:HG2	1:A:325:PRO:O	2.17	0.44
1:A:33:LEU:HA	1:A:33:LEU:HD23	1.73	0.44
1:A:264:ALA:HA	1:A:403:PRO:O	2.18	0.44
1:A:28:ASN:HA	1:A:61:GLN:O	2.18	0.44
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.87	0.43
1:A:113:PHE:HE2	2:D:78:PRO:HD3	1.81	0.43
1:A:388:PHE:HD1	1:A:393:ILE:HG12	1.83	0.43
1:A:42:PHE:CE2	1:A:62:ALA:HB1	2.53	0.43
2:D:101:ASP:OD2	2:D:103:THR:HG23	2.18	0.43
1:A:33:LEU:HD12	1:A:39:GLU:HA	2.00	0.43
2:D:384:LEU:H	2:D:384:LEU:HD23	1.83	0.43
1:A:32:VAL:HG13	1:A:65:VAL:HG23	2.00	0.43
2:D:371:ARG:NH1	2:D:371:ARG:HG2	2.34	0.43
2:D:265:ASP:HB3	2:D:268:THR:OG1	2.18	0.42
2:D:311:HIS:HB3	2:D:313:PHE:CE2	2.54	0.42
1:A:292:LEU:HD23	1:A:295:GLY:HA3	2.01	0.42
1:A:371:GLN:HG2	1:A:389:ASN:HA	2.00	0.42
1:A:218:PHE:O	1:A:220:PRO:HD3	2.20	0.42
1:A:82:LEU:O	1:A:87:VAL:HG13	2.20	0.42
1:A:341:LEU:O	1:A:345:VAL:HG23	2.19	0.42
2:D:190:ILE:HG23	2:D:197:TRP:HB2	2.02	0.42
1:A:379:ASN:O	1:A:380:ARG:HD3	2.20	0.41
2:D:380:LYS:C	2:D:382:LYS:H	2.23	0.41
2:D:379:TRP:HE3	2:D:384:LEU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:O	1:A:80:GLU:HG3	2.20	0.41
2:D:337:ARG:O	2:D:340:ILE:HG22	2.21	0.41
1:A:309:VAL:HG12	1:A:313:ILE:HG13	2.02	0.41
1:A:255:SER:O	1:A:259:LEU:HG	2.20	0.41
2:D:129:GLY:HA2	2:D:132:MET:HG3	2.03	0.41
2:D:340:ILE:HD11	2:D:353:GLU:N	2.36	0.41
2:D:123:ILE:O	2:D:143:PHE:HA	2.20	0.41
2:D:124:LEU:HA	2:D:124:LEU:HD23	1.84	0.41
2:D:366:LEU:HB2	2:D:376:VAL:CG2	2.47	0.41
1:A:25:LYS:O	1:A:59:GLN:N	2.53	0.40
1:A:103:THR:O	1:A:105:THR:N	2.54	0.40
1:A:219:GLU:O	1:A:222:THR:OG1	2.26	0.40
2:D:106:GLU:N	2:D:106:GLU:CD	2.74	0.40
2:D:287:TYR:OH	2:D:295:ASP:OD2	2.31	0.40
2:D:314:ILE:HD13	2:D:314:ILE:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	348/383 (91%)	320 (92%)	27 (8%)	1 (0%)	44	79
2	D	349/362 (96%)	299 (86%)	49 (14%)	1 (0%)	44	79
All	All	697/745 (94%)	619 (89%)	76 (11%)	2 (0%)	44	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	299	ILE
1	A	104	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/329 (71%)	206 (88%)	29 (12%)	5	23
2	D	211/325 (65%)	182 (86%)	29 (14%)	4	19
All	All	446/654 (68%)	388 (87%)	58 (13%)	5	21

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	54	PHE
1	A	59	GLN
1	A	63	THR
1	A	77	SER
1	A	84	SER
1	A	92	VAL
1	A	123	THR
1	A	133	ILE
1	A	138	LEU
1	A	139	ARG
1	A	146	HIS
1	A	149	LEU
1	A	165	LEU
1	A	217	GLN
1	A	225	LEU
1	A	247	ASP
1	A	258	MET
1	A	285	ASP
1	A	299	SER
1	A	303	SER
1	A	323	THR
1	A	335	ILE
1	A	344	ARG
1	A	347	MET
1	A	364	ASP
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	382	LEU
1	A	383	VAL
2	D	34	SER
2	D	47	GLU
2	D	71	VAL
2	D	73	MET
2	D	83	THR
2	D	103	THR
2	D	106	GLU
2	D	136	ASP
2	D	140	SER
2	D	141	SER
2	D	161	MET
2	D	165	ASP
2	D	189	THR
2	D	192	ASN
2	D	207	MET
2	D	211	ASP
2	D	233	THR
2	D	235	GLU
2	D	238	THR
2	D	278	ILE
2	D	282	TYR
2	D	321	CYS
2	D	332	SER
2	D	342	VAL
2	D	343	THR
2	D	345	GLU
2	D	350	SER
2	D	371	ARG
2	D	387	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	A	501	1	14,14,15	0.46	0	15,19,21	0.93	1 (6%)
3	NAG	A	502	1	14,14,15	0.54	0	15,19,21	0.40	0
3	NAG	A	503	1	14,14,15	0.36	0	15,19,21	0.54	0
3	NAG	D	401	2	14,14,15	0.90	1 (7%)	15,19,21	1.01	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
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	D	401	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAG	C1-C2	2.97	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	NAG	C1-O5-C5	2.94	116.22	112.17
3	A	501	NAG	C1-O5-C5	2.95	116.23	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	NAG	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	354/383 (92%)	-0.25	1 (0%)	93	86	55, 81, 104, 120	0
2	D	352/362 (97%)	-0.19	1 (0%)	93	86	57, 88, 120, 139	0
All	All	706/745 (94%)	-0.22	2 (0%)	93	86	55, 84, 114, 139	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	ILE	2.7
2	D	254	TYR	2.4

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

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

6.3   Carbohydrates (i)

There are no carbohydrates in this entry.

6.4   Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	D	401	14/15	0.79	0.32	1.57	100,115,121,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	501	14/15	0.60	0.29	-	100,110,121,130	0
3	NAG	A	502	14/15	0.71	0.26	-	121,136,143,144	0
3	NAG	A	503	14/15	0.74	0.19	-	121,132,140,143	0

6.5 Other polymers (i)

There are no such residues in this entry.