



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 10:29 PM EDT

PDB ID : 5TQ2  
Title : Crystal structure of amino terminal domains of the NMDA receptor subunit GluN1 and GluN2A in complex with zinc at GluN1 and GluN2A  
Authors : Romero-Hernandez, A.; Simorowski, N.; Karakas, E.; Furukawa, H.  
Deposited on : unknown  
Resolution : 3.29 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](mailto: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.

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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 : rb-20029824  
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) : rb-20029824

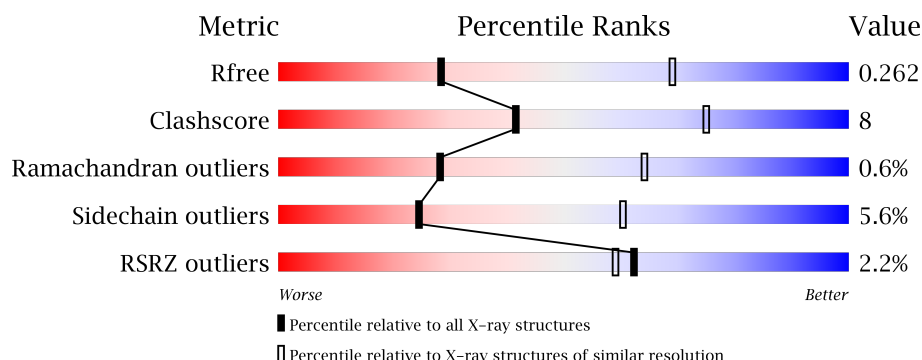
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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	1006 (3.34-3.22)
Clashscore	112137	1070 (3.34-3.22)
Ramachandran outliers	110173	1050 (3.34-3.22)
Sidechain outliers	110143	1049 (3.34-3.22)
RSRZ outliers	101464	1011 (3.34-3.22)

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  $\geq 3$ , 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	389	
2	B	360	
3	H	221	
4	L	214	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7999 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	365	Total	C	N	O	S	0	0	0
			2671	1697	458	506	10			

There are 6 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	GLY	-	expression tag	UNP Q91977
A	410	THR	-	expression tag	UNP Q91977
A	411	LEU	-	expression tag	UNP Q91977
A	412	VAL	-	expression tag	UNP Q91977

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	335	Total	C	N	O	S	0	0	0
			2396	1541	387	456	12			

- Molecule 3 is a protein called FAB, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	205	Total	C	N	O	S	0	0	0
			1444	927	232	279	6			

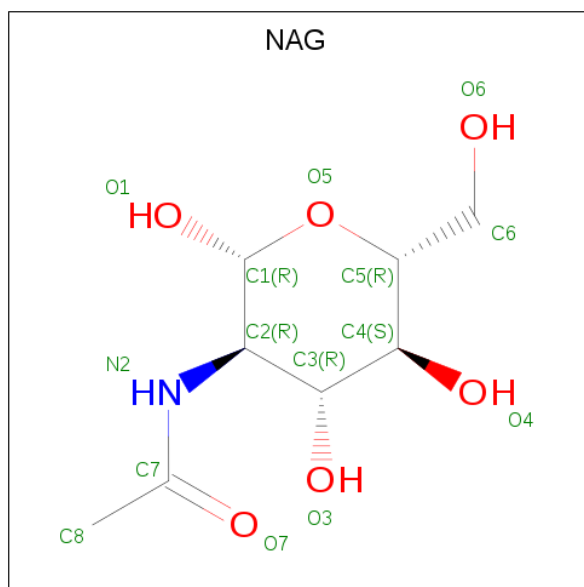
- Molecule 4 is a protein called FAB, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	202	Total	C	N	O	S	0	0	0
			1415	895	238	275	7			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

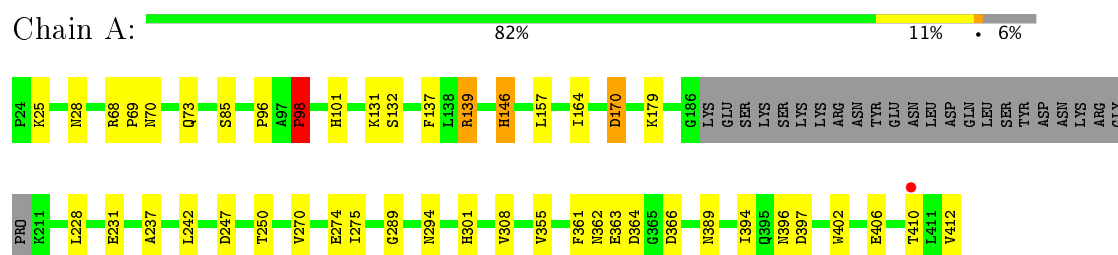
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total	O	0	0
			5	5		
9	B	5	Total	O	0	0
			5	5		
9	H	1	Total	O	0	0
			1	1		

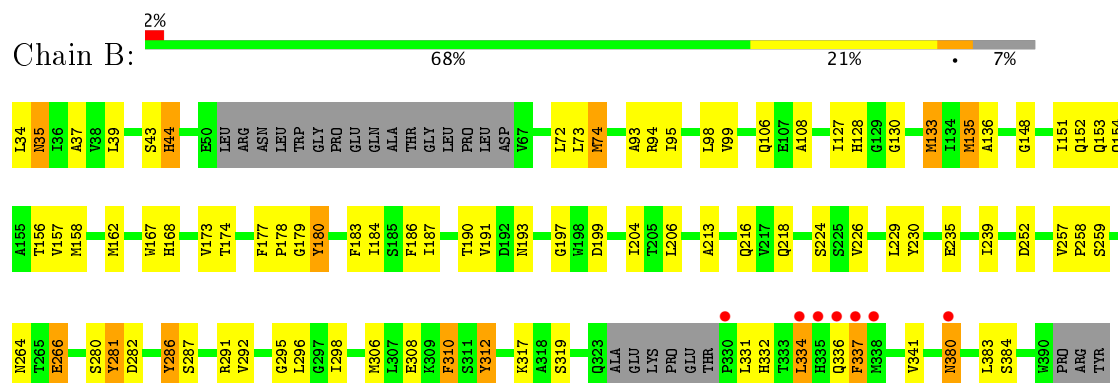
### 3 Residue-property plots [i](#)

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

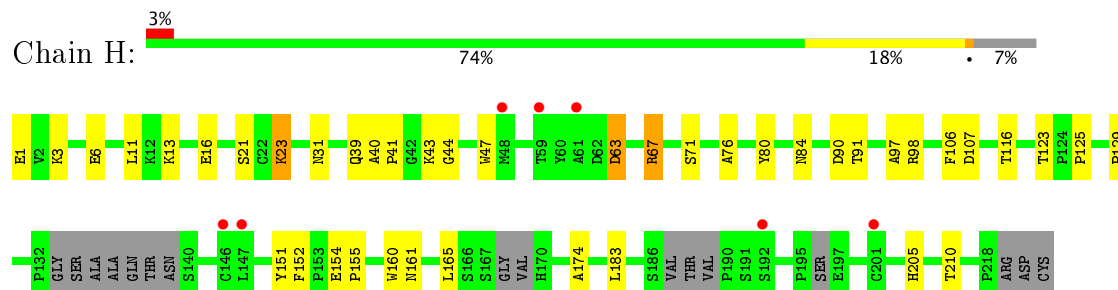
- Molecule 1: NMDA glutamate receptor subunit



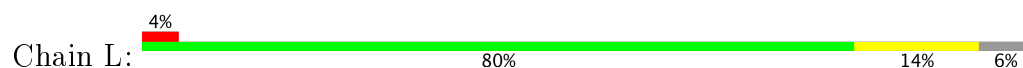
- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

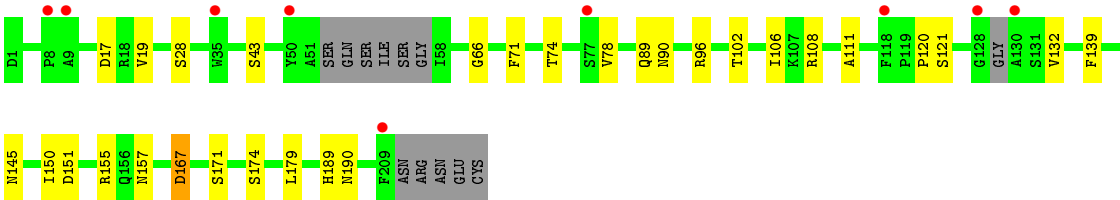


- Molecule 3: FAB, HEAVY CHAIN



- Molecule 4: FAB, LIGHT CHAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.16Å 117.83Å 158.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 3.29 48.33 – 3.29	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.33-3.29) 96.9 (48.33-3.29)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.10 _2155	Depositor
R, $R_{free}$	0.224 , 0.261 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	2210 reflections (9.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	103.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NAG, SO4

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	0.26	0/2727	0.44	0/3730
2	B	0.28	0/2449	0.50	1/3355 (0.0%)
3	H	0.28	0/1486	0.49	0/2046
4	L	0.26	0/1450	0.45	0/1990
All	All	0.27	0/8112	0.47	1/11121 (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
1	A	0	1
2	B	0	1
3	H	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	GLU	OE1-CD-OE2	-7.78	113.96	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	PRO	Peptide
2	B	380	ASN	Peptide

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Mol	Chain	Res	Type	Group
3	H	165	LEU	Peptide

## 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	2671	0	2489	25	0
2	B	2396	0	2122	63	0
3	H	1444	0	1221	21	0
4	L	1415	0	1201	15	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	26	0	0
7	A	15	0	0	0	0
7	B	5	0	0	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	5	0	0	0	0
9	B	5	0	0	1	0
9	H	1	0	0	0	0
All	All	7999	0	7075	120	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 8.

All (120) 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:130:GLY:HA2	2:B:133:MET:HG3	1.60	0.81
3:H:71:SER:HB3	3:H:80:TYR:HB2	1.62	0.80
2:B:128:HIS:CD2	2:B:282:ASP:OD1	2.34	0.79
2:B:213:ALA:HA	2:B:216:GLN:HB2	1.71	0.73
1:A:362:ASN:OD1	1:A:363:GLU:N	2.23	0.70
2:B:44:HIS:CE1	2:B:128:HIS:CE1	2.80	0.70
1:A:170:ASP:OD1	1:A:170:ASP:N	2.26	0.67
2:B:298:ILE:HA	2:B:341:VAL:HG11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:THR:HG22	2:B:230:TYR:HB3	1.75	0.67
2:B:306:MET:HA	2:B:337:PHE:CE2	2.31	0.66
2:B:308:GLU:N	2:B:308:GLU:OE1	2.29	0.66
3:H:11:LEU:HD11	3:H:152:PHE:HE1	1.59	0.65
2:B:43:SER:HB2	2:B:44:HIS:ND1	2.13	0.64
2:B:334:LEU:HD12	2:B:334:LEU:H	1.64	0.62
2:B:93:ALA:O	2:B:95:ILE:N	2.34	0.61
2:B:154:GLN:HE22	2:B:259:SER:HB3	1.65	0.60
2:B:230:TYR:HD1	2:B:258:PRO:HG3	1.67	0.59
3:H:174:ALA:HB2	3:H:183:LEU:HD23	1.83	0.59
2:B:264:ASN:HB3	2:B:266:GLU:HG2	1.84	0.59
2:B:336:GLN:HB2	2:B:337:PHE:CD1	2.38	0.58
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.86	0.57
3:H:91:THR:HG23	3:H:116:THR:HA	1.85	0.57
2:B:37:ALA:HB2	2:B:95:ILE:HG21	1.87	0.56
2:B:128:HIS:CE1	2:B:266:GLU:OE2	2.58	0.56
1:A:362:ASN:N	1:A:366:ASP:O	2.36	0.56
3:H:97:ALA:HB1	3:H:106:PHE:HB3	1.87	0.55
2:B:286:TYR:CE1	2:B:291:ARG:HG2	2.42	0.55
1:A:28:ASN:ND2	1:A:85:SER:O	2.41	0.54
2:B:158:MET:O	2:B:162:MET:HG3	2.09	0.53
2:B:187:ILE:O	2:B:191:VAL:HG22	2.08	0.53
3:H:11:LEU:HD11	3:H:152:PHE:CE1	2.41	0.53
2:B:180:TYR:O	2:B:184:ILE:HD12	2.08	0.53
2:B:173:VAL:HA	2:B:204:ILE:O	2.09	0.53
2:B:287:SER:O	2:B:291:ARG:HG3	2.09	0.53
1:A:131:LYS:NZ	1:A:137:PHE:O	2.43	0.52
2:B:317:LYS:NZ	2:B:319:SER:O	2.38	0.52
2:B:152:GLN:O	2:B:156:THR:HG23	2.10	0.52
2:B:312:TYR:HD1	2:B:312:TYR:H	1.58	0.52
1:A:274:GLU:N	1:A:274:GLU:OE2	2.43	0.52
2:B:135:MET:HG2	2:B:136:ALA:O	2.11	0.51
2:B:331:LEU:O	2:B:332:HIS:ND1	2.43	0.51
2:B:128:HIS:HD2	2:B:291:ARG:HH12	1.57	0.50
2:B:154:GLN:NE2	2:B:259:SER:HB3	2.26	0.50
4:L:155:ARG:HD3	4:L:157:ASN:H	1.76	0.50
2:B:337:PHE:N	2:B:337:PHE:HD1	2.09	0.50
1:A:132:SER:HA	2:B:178:PRO:HG3	1.93	0.50
2:B:337:PHE:N	2:B:337:PHE:CD1	2.79	0.50
2:B:230:TYR:CD1	2:B:258:PRO:HG3	2.47	0.49
2:B:336:GLN:HB2	2:B:337:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD13	1:A:289:GLY:HA3	1.95	0.49
3:H:23:LYS:HE3	3:H:76:ALA:O	2.13	0.49
2:B:35:ASN:OD1	2:B:35:ASN:N	2.44	0.49
1:A:68:ARG:NH1	3:H:31:ASN:OD1	2.46	0.49
2:B:252:ASP:OD2	9:B:501:HOH:O	2.20	0.48
4:L:108:ARG:HH21	4:L:111:ALA:HB2	1.78	0.48
3:H:63:ASP:OD1	3:H:63:ASP:N	2.46	0.48
1:A:396:ASN:OD1	1:A:397:ASP:N	2.47	0.48
1:A:164:ILE:HG12	1:A:237:ALA:HB3	1.96	0.48
2:B:167:TRP:HB3	2:B:226:VAL:HG21	1.96	0.47
2:B:72:LEU:HD12	2:B:73:LEU:H	1.79	0.47
4:L:190:ASN:O	4:L:190:ASN:ND2	2.47	0.47
2:B:306:MET:HA	2:B:337:PHE:HE2	1.77	0.47
1:A:157:LEU:HD21	1:A:410:THR:HG23	1.96	0.46
1:A:308:VAL:HG11	1:A:361:PHE:HE2	1.80	0.46
2:B:44:HIS:N	2:B:44:HIS:ND1	2.63	0.46
2:B:179:GLY:HA3	2:B:230:TYR:OH	2.16	0.46
4:L:150:ILE:HD11	4:L:179:LEU:HD21	1.97	0.46
2:B:168:HIS:HB3	2:B:197:GLY:O	2.15	0.46
3:H:125:PRO:HD2	3:H:205:HIS:CE1	2.51	0.46
1:A:389:ASN:HB2	1:A:394:ILE:HG13	1.99	0.45
3:H:39:GLN:HG3	3:H:44:GLY:O	2.16	0.45
1:A:69:PRO:HA	1:A:98:PRO:HG2	1.97	0.45
2:B:99:VAL:HG13	2:B:127:ILE:HD13	1.99	0.45
2:B:336:GLN:HB2	2:B:337:PHE:CE1	2.52	0.45
2:B:177:PHE:CG	2:B:178:PRO:HD2	2.52	0.44
1:A:146:HIS:CE1	1:A:179:LYS:HE3	2.52	0.44
1:A:70:ASN:HB3	1:A:73:GLN:HB3	1.99	0.44
1:A:294:ASN:O	1:A:301:HIS:NE2	2.50	0.44
2:B:306:MET:O	2:B:310:PHE:O	2.35	0.44
3:H:13:LYS:N	3:H:16:GLU:OE1	2.51	0.44
4:L:167:ASP:HB3	4:L:171:SER:H	1.82	0.44
4:L:19:VAL:HG23	4:L:78:VAL:HG21	2.00	0.44
2:B:186:PHE:O	2:B:190:THR:HG22	2.19	0.43
1:A:137:PHE:CE2	1:A:139:ARG:HG3	2.53	0.43
4:L:139:PHE:HE1	4:L:174:SER:HA	1.83	0.43
2:B:235:GLU:O	2:B:239:ILE:HG12	2.18	0.43
3:H:174:ALA:HA	3:H:183:LEU:HB3	2.01	0.43
3:H:6:GLU:HA	3:H:21:SER:O	2.19	0.43
4:L:120:PRO:HD3	4:L:132:VAL:HG22	2.00	0.43
3:H:154:GLU:N	3:H:155:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:VAL:O	2:B:296:LEU:N	2.41	0.43
2:B:148:GLY:HA2	2:B:281:TYR:CD2	2.54	0.42
2:B:43:SER:HB2	2:B:44:HIS:CE1	2.54	0.42
2:B:151:ILE:HD11	2:B:183:PHE:CD1	2.54	0.42
2:B:39:LEU:HD12	2:B:74:MET:HB2	2.02	0.42
4:L:151:ASP:CG	4:L:189:HIS:HB3	2.40	0.42
2:B:106:GLN:HG3	2:B:108:ALA:H	1.84	0.42
4:L:106:ILE:HD11	4:L:171:SER:OG	2.19	0.42
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.51	0.42
2:B:259:SER:HB2	2:B:280:SER:HA	2.02	0.42
4:L:89:GLN:HE21	4:L:96:ARG:HD2	1.84	0.42
2:B:229:LEU:HB3	2:B:257:VAL:HG12	2.02	0.42
3:H:40:ALA:HB3	3:H:43:LYS:CB	2.50	0.42
3:H:47:TRP:CD2	4:L:96:ARG:HB2	2.55	0.41
1:A:402:TRP:HB2	1:A:406:GLU:HG3	2.02	0.41
4:L:17:ASP:O	4:L:78:VAL:HG23	2.20	0.41
1:A:410:THR:O	1:A:410:THR:HG22	2.20	0.41
1:A:25:LYS:HB2	1:A:25:LYS:HE3	1.84	0.41
4:L:66:GLY:HA3	4:L:71:PHE:HA	2.02	0.41
2:B:252:ASP:OD1	2:B:252:ASP:N	2.54	0.41
3:H:98:ARG:NH2	3:H:107:ASP:OD2	2.35	0.41
3:H:129:PRO:O	4:L:121:SER:OG	2.30	0.40
1:A:247:ASP:O	1:A:250:THR:OG1	2.31	0.40
2:B:187:ILE:HA	2:B:190:THR:HG22	2.03	0.40
2:B:312:TYR:CD1	2:B:312:TYR:N	2.89	0.40
1:A:228:LEU:O	1:A:231:GLU:HB3	2.21	0.40
1:A:242:LEU:HB3	1:A:270:VAL:HG12	2.02	0.40
2:B:98:LEU:HD12	2:B:99:VAL:N	2.36	0.40
2:B:153:GLN:O	2:B:157:VAL:HG23	2.22	0.40
2:B:291:ARG:O	2:B:295:GLY:N	2.52	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	361/389 (93%)	340 (94%)	19 (5%)	2 (1%)	28	64
2	B	329/360 (91%)	299 (91%)	26 (8%)	4 (1%)	15	50
3	H	195/221 (88%)	181 (93%)	13 (7%)	1 (0%)	32	67
4	L	196/214 (92%)	182 (93%)	14 (7%)	0	100	100
All	All	1081/1184 (91%)	1002 (93%)	72 (7%)	7 (1%)	28	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
2	B	310	PHE
2	B	94	ARG
2	B	383	LEU
1	A	96	PRO
2	B	380	ASN
3	H	41	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	262/334 (78%)	255 (97%)	7 (3%)	50	77
2	B	225/318 (71%)	207 (92%)	18 (8%)	14	45
3	H	130/188 (69%)	120 (92%)	10 (8%)	15	47
4	L	129/188 (69%)	122 (95%)	7 (5%)	26	61
All	All	746/1028 (73%)	704 (94%)	42 (6%)	25	60

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	HIS

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Mol	Chain	Res	Type
1	A	139	ARG
1	A	146	HIS
1	A	170	ASP
1	A	355	VAL
1	A	364	ASP
1	A	412	VAL
2	B	34	LEU
2	B	35	ASN
2	B	44	HIS
2	B	74	MET
2	B	133	MET
2	B	135	MET
2	B	180	TYR
2	B	193	ASN
2	B	199	ASP
2	B	206	LEU
2	B	218	GLN
2	B	224	SER
2	B	281	TYR
2	B	286	TYR
2	B	312	TYR
2	B	334	LEU
2	B	337	PHE
2	B	384	SER
3	H	1	GLU
3	H	3	LYS
3	H	23	LYS
3	H	63	ASP
3	H	67	ARG
3	H	84	ASN
3	H	123	THR
3	H	160	TRP
3	H	161	ASN
3	H	210	THR
4	L	28	SER
4	L	43	SER
4	L	74	THR
4	L	90	ASN
4	L	102	THR
4	L	145	ASN
4	L	167	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
4	L	190	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](#)

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	$\# Z  > 2$
6	NAG	A	502	1	14,14,15	0.68	1 (7%)	15,19,21	1.16	1 (6%)
6	NAG	A	503	1	14,14,15	0.23	0	15,19,21	0.80	0
7	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.07	0
7	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.07	0
7	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.07	0
8	GOL	A	507	-	5,5,5	0.35	0	5,5,5	0.21	0
7	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.09	0
8	GOL	B	403	-	5,5,5	0.35	0	5,5,5	0.23	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
6	NAG	A	502	1	-	0/6/23/26	0/1/1/1
6	NAG	A	503	1	-	0/6/23/26	0/1/1/1
7	SO4	A	504	-	-	0/0/0/0	0/0/0/0
7	SO4	A	505	-	-	0/0/0/0	0/0/0/0
7	SO4	A	506	-	-	0/0/0/0	0/0/0/0
8	GOL	A	507	-	-	0/4/4/4	0/0/0/0
7	SO4	B	402	-	-	0/0/0/0	0/0/0/0
8	GOL	B	403	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	502	NAG	C1-C2	2.45	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	502	NAG	C1-O5-C5	3.79	117.39	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	365/389 (93%)	-0.12	1 (0%) 93 93	51, 75, 104, 139	0
2	B	335/360 (93%)	0.05	7 (2%) 64 60	57, 94, 126, 159	0
3	H	205/221 (92%)	0.15	7 (3%) 46 41	67, 100, 139, 156	0
4	L	202/214 (94%)	0.22	9 (4%) 34 31	71, 96, 121, 138	0
All	All	1107/1184 (93%)	0.04	24 (2%) 62 59	51, 90, 127, 159	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	337	PHE	3.9
3	H	59	THR	3.6
2	B	335	HIS	3.2
4	L	209	PHE	3.1
2	B	380	ASN	2.7
3	H	146	CYS	2.7
1	A	410	THR	2.7
4	L	128	GLY	2.6
4	L	9	ALA	2.5
4	L	118	PHE	2.5
3	H	61	ALA	2.4
3	H	201	CYS	2.4
3	H	192	SER	2.4
2	B	334	LEU	2.3
3	H	147	LEU	2.3
4	L	77	SER	2.2
2	B	330	PRO	2.2
2	B	336	GLN	2.2
4	L	50	TYR	2.1
4	L	35	TRP	2.1
4	L	8	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	338	MET	2.1
4	L	130	ALA	2.0
3	H	48	MET	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	NAG	A	502	14/15	0.86	0.26	0.06	90,112,122,123	0
7	SO4	A	506	5/5	0.86	0.24	-0.46	102,116,127,135	0
7	SO4	A	505	5/5	0.96	0.16	-1.26	66,78,86,93	0
5	ZN	B	401	1/1	0.97	0.08	-1.68	167,167,167,167	0
7	SO4	B	402	5/5	0.97	0.10	-3.64	74,78,85,87	0
6	NAG	A	503	14/15	0.78	0.19	-	92,101,109,110	0
8	GOL	A	507	6/6	0.81	0.23	-	79,94,95,102	0
5	ZN	A	501	1/1	0.85	0.12	-	119,119,119,119	0
7	SO4	A	504	5/5	0.95	0.11	-	90,92,106,109	0
8	GOL	B	403	6/6	0.84	0.15	-	95,109,121,124	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.