Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 04:53 AM EDT

PDB ID	:	5TPW
Title	:	Crystal structure of amino terminal domains of the NMDA receptor subunit GluN1 and GluN2A in complex with zinc at the GluN2A
Authors	:	Romero-Hernandez, A.; Simorowski, N.; Karakas, E.; Furukawa, H.
Deposited on	:	2016-10-21
Resolution	:	2.91 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

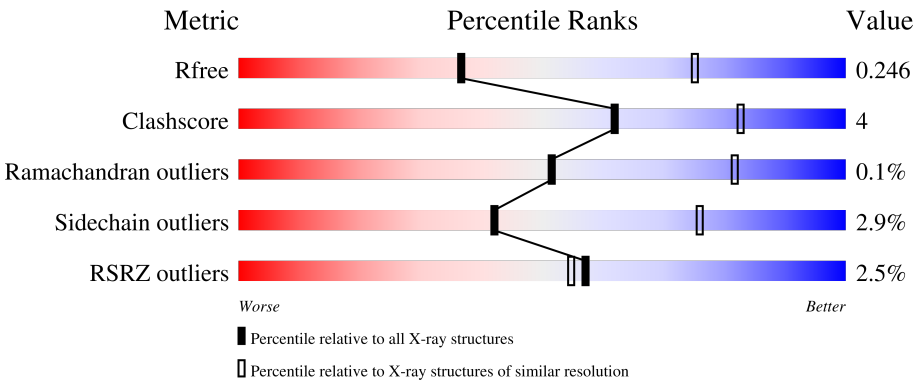
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	389	.% 81% 11% • 7%
2	B	360	4% 81% 11% 8%
3	H	221	.% 80% 15% • 5%
4	L	214	4% 86% 9% •

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8358 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
			Total	C	N	O	S			
1	A	362	2734	1745	467	511	11	0	0	0

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
			Total	C	N	O	S			
2	B	331	2472	1586	405	469	12	0	0	0

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

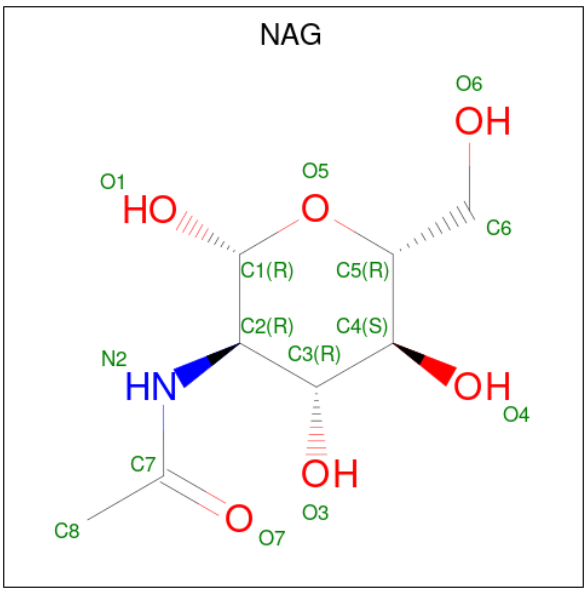
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	211	1542	993	244	298	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	206	1500	945	258	290	7	0	0	0

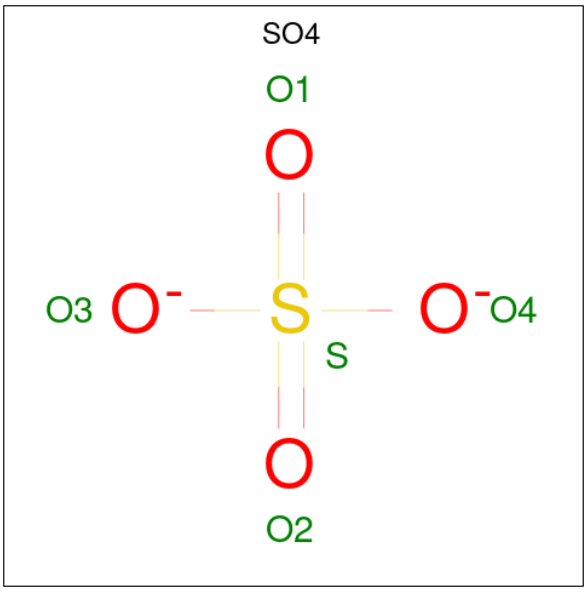
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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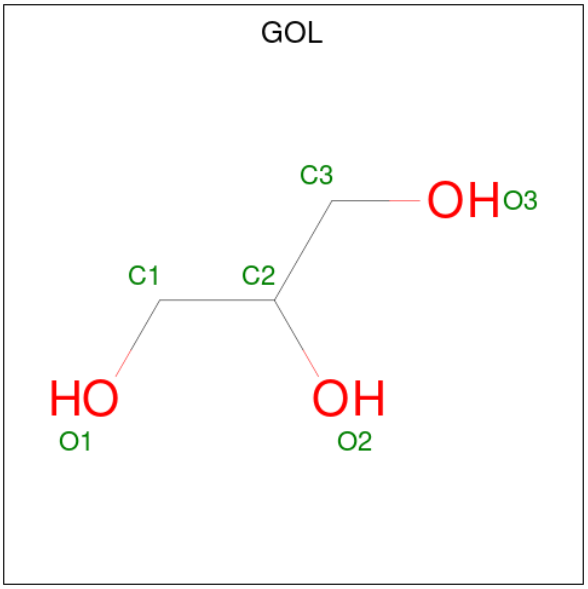
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Zn 1 1	0	0

- Molecule 9 is water.

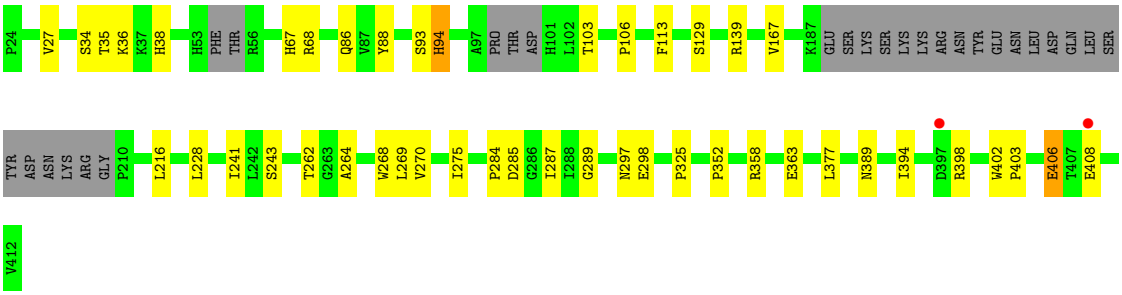
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	19	19	19	0	0
			Total	O		
9	B	7	7	7	0	0
			Total	O		
9	H	5	5	5	0	0
			Total	O		
9	L	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

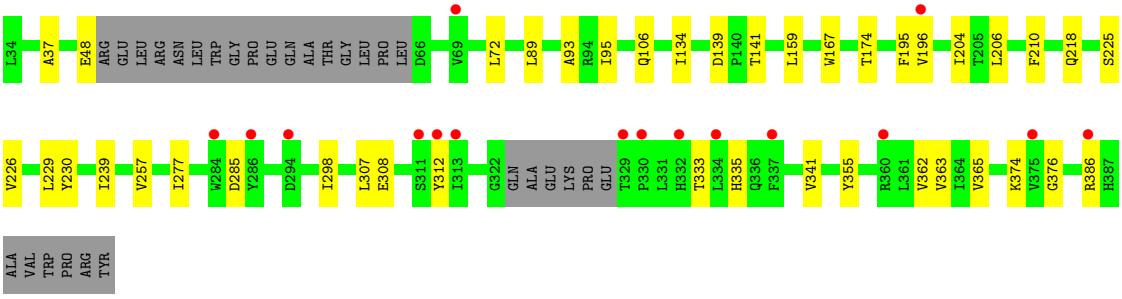
• Molecule 1: NMDA glutamate receptor subunit

Chain A:



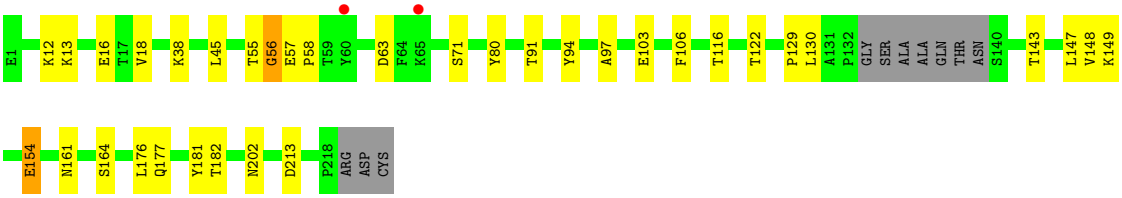
• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:



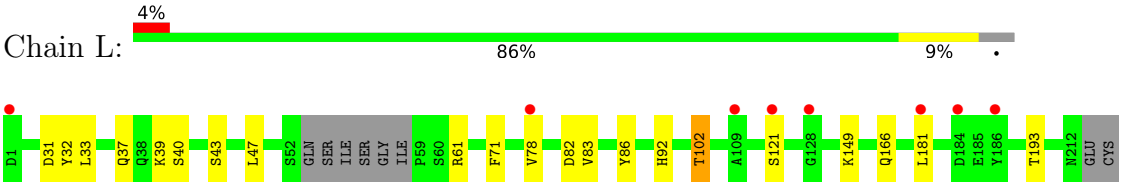
• Molecule 3: FAB, HEAVY CHAIN

Chain H:



• Molecule 4: FAB, LIGHT CHAIN

Chain L:


4%
86%
9%
D1
D31
Y32
L33
Q37
Q38
K39
S40
S43
L47
S52
GLN
SER
ILE
SER
GLY
ILE
P59
S60
R61
F71
V78
D82
V83
Y86
H92
T102
A109
S121
G128
K149
Q166
L181
D184
E185
Y186
T193
N212
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.56Å 118.40Å 155.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 2.91 47.56 – 2.91	Depositor EDS
% Data completeness (in resolution range)	88.5 (47.56-2.91) 94.4 (47.56-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.200 , 0.245 0.200 , 0.246	Depositor DCC
R_{free} test set	3180 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8358	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN, SO4, NAG, GOL

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	0.25	0/2787	0.42	0/3791
2	B	0.24	0/2527	0.43	0/3447
3	H	0.26	0/1590	0.47	0/2188
4	L	0.25	0/1536	0.47	0/2096
All	All	0.25	0/8440	0.44	0/11522

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
3	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	148	VAL	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	2734	0	2683	29	1
2	B	2472	0	2285	19	1
3	H	1542	0	1376	16	0
4	L	1500	0	1341	10	0
5	A	28	0	26	2	0
6	A	15	0	0	1	0
6	B	15	0	0	1	0
7	A	12	0	16	3	0
8	B	1	0	0	0	0
9	A	19	0	0	1	0
9	B	7	0	0	0	0
9	H	5	0	0	0	0
9	L	8	0	0	0	0
All	All	8358	0	7727	71	1

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 (71) 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)
3:H:71:SER:HB3	3:H:80:TYR:HB2	1.64	0.79
3:H:149:LYS:O	3:H:182:THR:OG1	2.05	0.71
2:B:174:THR:HG22	2:B:230:TYR:HB3	1.75	0.67
2:B:159:LEU:HB3	2:B:196:VAL:HG11	1.78	0.64
3:H:12:LYS:HG3	3:H:18:VAL:HG22	1.80	0.63
1:A:38:HIS:NE2	6:A:504:SO4:O1	2.27	0.63
3:H:149:LYS:HA	3:H:182:THR:HG23	1.82	0.61
2:B:167:TRP:HB3	2:B:226:VAL:HG21	1.82	0.60
1:A:389:ASN:OD1	5:A:502:NAG:N2	2.35	0.60
1:A:67:HIS:CE1	1:A:93:SER:O	2.55	0.59
3:H:91:THR:HG23	3:H:116:THR:HA	1.85	0.58
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.84	0.58
1:A:262:THR:HG23	1:A:284:PRO:HB3	1.86	0.58
1:A:389:ASN:HB2	1:A:394:ILE:HG13	1.85	0.58
3:H:38:LYS:NZ	3:H:94:TYR:OH	2.36	0.57
1:A:216:LEU:HB3	1:A:228:LEU:HD11	1.88	0.56
1:A:297:ASN:OD1	5:A:501:NAG:H83	2.05	0.56
3:H:161:ASN:HB3	3:H:164:SER:HB3	1.87	0.56
2:B:134:ILE:HG12	2:B:355:TYR:HB3	1.88	0.55
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.40	0.55
2:B:308:GLU:OE1	2:B:308:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH2	9:A:603:HOH:O	2.38	0.54
1:A:36:LYS:H	7:A:506:GOL:H32	1.72	0.53
1:A:275:ILE:HD13	1:A:289:GLY:HA3	1.90	0.52
2:B:89:LEU:HB3	2:B:95:ILE:HD12	1.92	0.52
1:A:36:LYS:HE2	3:H:103:GLU:HB2	1.91	0.51
3:H:129:PRO:O	4:L:121:SER:OG	2.23	0.50
1:A:35:THR:HB	7:A:506:GOL:H32	1.93	0.49
1:A:129:SER:OG	1:A:139:ARG:NH2	2.46	0.49
3:H:154:GLU:HG2	3:H:181:TYR:CZ	2.48	0.49
2:B:139:ASP:OD1	2:B:141:THR:OG1	2.25	0.48
3:H:202:ASN:ND2	3:H:213:ASP:OD2	2.40	0.48
2:B:277:ILE:HG12	2:B:365:VAL:HG12	1.95	0.48
3:H:55:THR:O	3:H:57:GLU:N	2.45	0.48
3:H:130:LEU:HD21	3:H:147:LEU:HB2	1.95	0.47
3:H:97:ALA:HB1	3:H:106:PHE:HB3	1.97	0.47
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.97	0.46
4:L:149:LYS:HB2	4:L:193:THR:OG1	2.15	0.46
2:B:298:ILE:HA	2:B:341:VAL:HG11	1.96	0.46
1:A:86:GLN:HB3	1:A:325:PRO:HG2	1.97	0.46
4:L:33:LEU:HG	4:L:71:PHE:CD1	2.49	0.46
1:A:287:ILE:HG22	1:A:377:LEU:HB3	1.98	0.46
2:B:333:THR:OG1	6:B:404:SO4:O3	2.34	0.45
1:A:67:HIS:HE1	1:A:93:SER:O	2.00	0.45
1:A:34:SER:HB3	1:A:94:HIS:O	2.16	0.44
3:H:13:LYS:N	3:H:16:GLU:OE1	2.45	0.44
4:L:83:VAL:HG11	4:L:166:GLN:HB3	2.00	0.44
2:B:307:LEU:HD23	2:B:307:LEU:HA	1.75	0.44
2:B:206:LEU:HD13	2:B:239:ILE:HD12	2.00	0.44
2:B:285:ASP:OD2	2:B:374:LYS:NZ	2.32	0.44
1:A:352:PRO:HA	1:A:358:ARG:HA	1.99	0.43
1:A:363:GLU:H	1:A:363:GLU:CD	2.21	0.43
1:A:298:GLU:O	1:A:298:GLU:HG2	2.18	0.43
1:A:264:ALA:HA	1:A:403:PRO:O	2.19	0.43
2:B:229:LEU:HB3	2:B:257:VAL:HG12	2.00	0.42
4:L:86:TYR:HB2	4:L:102:THR:HG23	2.01	0.42
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.54	0.42
1:A:36:LYS:HG3	7:A:506:GOL:H12	2.00	0.42
2:B:37:ALA:HB2	2:B:95:ILE:HD13	2.01	0.42
4:L:32:TYR:HB2	4:L:92:HIS:HB2	2.00	0.42
1:A:113:PHE:CZ	2:B:106:GLN:HG2	2.54	0.42
1:A:103:THR:O	1:A:106:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ALA:O	2:B:95:ILE:HG13	2.20	0.42
2:B:363:VAL:HB	2:B:376:GLY:HA3	2.02	0.42
2:B:204:ILE:HG23	2:B:218:GLN:HG3	2.02	0.41
1:A:268:TRP:HB3	1:A:287:ILE:HG13	2.03	0.41
4:L:31:ASP:OD1	4:L:31:ASP:N	2.53	0.41
1:A:241:ILE:HA	1:A:269:LEU:O	2.21	0.41
1:A:402:TRP:HE1	1:A:408:GLU:CB	2.34	0.40
4:L:39:LYS:HB3	4:L:40:SER:H	1.79	0.40
3:H:56:GLY:O	3:H:58:PRO:HD3	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:OE1	2:B:225:SER:OG[3_454]	2.17	0.03

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	354/389 (91%)	338 (96%)	16 (4%)	0	100	100
2	B	325/360 (90%)	311 (96%)	14 (4%)	0	100	100
3	H	207/221 (94%)	193 (93%)	13 (6%)	1 (0%)	29	61
4	L	202/214 (94%)	192 (95%)	10 (5%)	0	100	100
All	All	1088/1184 (92%)	1034 (95%)	53 (5%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	56	GLY

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	285/334 (85%)	280 (98%)	5 (2%)	59	85
2	B	251/318 (79%)	243 (97%)	8 (3%)	39	73
3	H	151/188 (80%)	144 (95%)	7 (5%)	27	60
4	L	146/188 (78%)	142 (97%)	4 (3%)	44	77
All	All	833/1028 (81%)	809 (97%)	24 (3%)	42	76

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	270	VAL
1	A	285	ASP
1	A	398	ARG
1	A	406	GLU
2	B	48	GLU
2	B	72	LEU
2	B	195	PHE
2	B	210	PHE
2	B	312	TYR
2	B	335	HIS
2	B	362	VAL
2	B	386	ARG
3	H	45	LEU
3	H	63	ASP
3	H	122	THR
3	H	143	THR
3	H	154	GLU
3	H	176	LEU
3	H	177	GLN
4	L	43	SER
4	L	78	VAL
4	L	102	THR
4	L	181	LEU

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

Mol	Chain	Res	Type
1	A	67	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	SO4	A	504	-	4,4,4	0.26	0	6,6,6	0.20	0
6	SO4	B	404	-	4,4,4	0.15	0	6,6,6	0.05	0
5	NAG	A	502	1	14,14,15	0.46	0	17,19,21	0.47	0
5	NAG	A	501	1	14,14,15	0.72	1 (7%)	17,19,21	1.22	1 (5%)
6	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.08	0
6	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.06	0
7	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.21	0
7	GOL	A	506	-	5,5,5	0.37	0	5,5,5	0.31	0
6	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.06	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
5	NAG	A	501	1	-	4/6/23/26	0/1/1/1
7	GOL	A	507	-	-	2/4/4/4	-
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
7	GOL	A	506	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	NAG	C1-C2	2.52	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	NAG	C1-O5-C5	4.32	118.04	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	506	GOL	O1-C1-C2-C3
5	A	502	NAG	O5-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	A	502	NAG	C4-C5-C6-O6
5	A	501	NAG	C8-C7-N2-C2
5	A	501	NAG	O7-C7-N2-C2
7	A	506	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	SO4	1	0
6	B	404	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	NAG	1	0
5	A	501	NAG	1	0
7	A	506	GOL	3	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	362/389 (93%)	-0.17	2 (0%)	89	89	12, 34, 69, 98	0
2	B	331/360 (91%)	0.30	16 (4%)	30	27	22, 56, 89, 104	0
3	H	211/221 (95%)	-0.01	2 (0%)	84	84	24, 52, 78, 94	0
4	L	206/214 (96%)	0.30	8 (3%)	39	35	23, 51, 80, 100	0
All	All	1110/1184 (93%)	0.09	28 (2%)	57	55	12, 48, 82, 104	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	312	TYR	4.8
2	B	337	PHE	3.8
4	L	1	ASP	3.7
2	B	196	VAL	3.5
2	B	284	TRP	3.1
2	B	286	TYR	2.9
2	B	332	HIS	2.9
2	B	330	PRO	2.9
2	B	313	ILE	2.8
2	B	386	ARG	2.8
4	L	109	ALA	2.8
1	A	408	GLU	2.8
2	B	360	ARG	2.6
4	L	121	SER	2.6
2	B	334	LEU	2.6
1	A	397	ASP	2.5
4	L	128	GLY	2.4
2	B	329	THR	2.4
2	B	69	VAL	2.3
2	B	311	SER	2.2
4	L	181	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	L	184	ASP	2.2
4	L	78	VAL	2.2
4	L	186	TYR	2.2
3	H	60	TYR	2.1
2	B	294	ASP	2.1
2	B	375	VAL	2.1
3	H	65	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
8	ZN	B	401	1/1	0.83	0.07	58,58,58,58	1
7	GOL	A	507	6/6	0.84	0.20	43,57,77,88	0
5	NAG	A	502	14/15	0.89	0.20	70,86,101,103	0
5	NAG	A	501	14/15	0.90	0.22	63,77,93,93	0
7	GOL	A	506	6/6	0.91	0.15	41,55,60,63	0
6	SO4	B	404	5/5	0.92	0.29	83,85,103,106	0
6	SO4	A	505	5/5	0.93	0.10	65,74,100,106	0
6	SO4	B	402	5/5	0.95	0.19	39,71,78,83	0
6	SO4	A	504	5/5	0.96	0.15	36,39,60,73	0
6	SO4	A	503	5/5	0.97	0.11	61,67,71,81	0
6	SO4	B	403	5/5	0.97	0.15	44,46,56,67	0

6.5 Other polymers (i)

There are no such residues in this entry.