



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 01:24 PM EDT

PDB ID : 3H6H
Title : Crystal structure of the GluR6 amino terminal domain dimer assembly MPD form
Authors : Kumar, J.; Mayer, M.L.
Deposited on : 2009-04-23
Resolution : 2.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.17.1
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) : 2.17.1

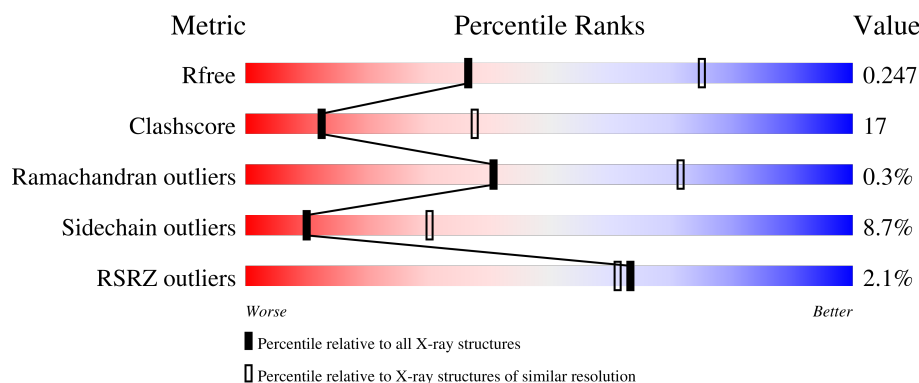
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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 $\leq 5\%$. 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	395	 2% 66% 28% . .
1	B	395	 3% 65% 28% . .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	396	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6186 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 Glutamate receptor, ionotropic kainate 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3051	1947	519	568	17			
1	B	379	Total	C	N	O	S	0	0	0
			3021	1927	513	564	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LEU	-	expression tag	UNP P42260
A	391	GLU	-	expression tag	UNP P42260
A	392	LEU	-	expression tag	UNP P42260
A	393	VAL	-	expression tag	UNP P42260
A	394	PRO	-	expression tag	UNP P42260
A	395	ARG	-	expression tag	UNP P42260
B	390	LEU	-	expression tag	UNP P42260
B	391	GLU	-	expression tag	UNP P42260
B	392	LEU	-	expression tag	UNP P42260
B	393	VAL	-	expression tag	UNP P42260
B	394	PRO	-	expression tag	UNP P42260
B	395	ARG	-	expression tag	UNP P42260

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

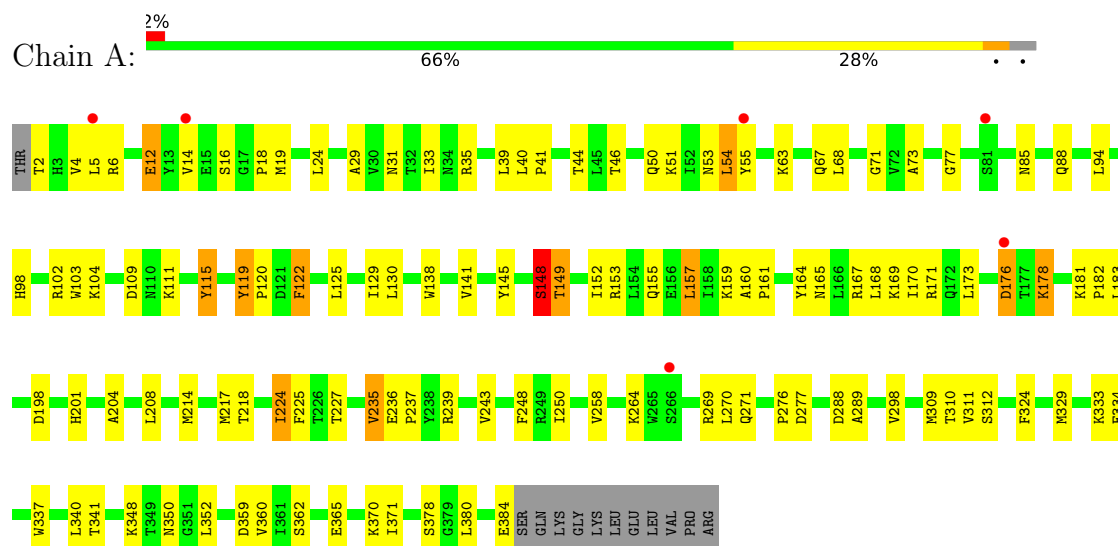
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

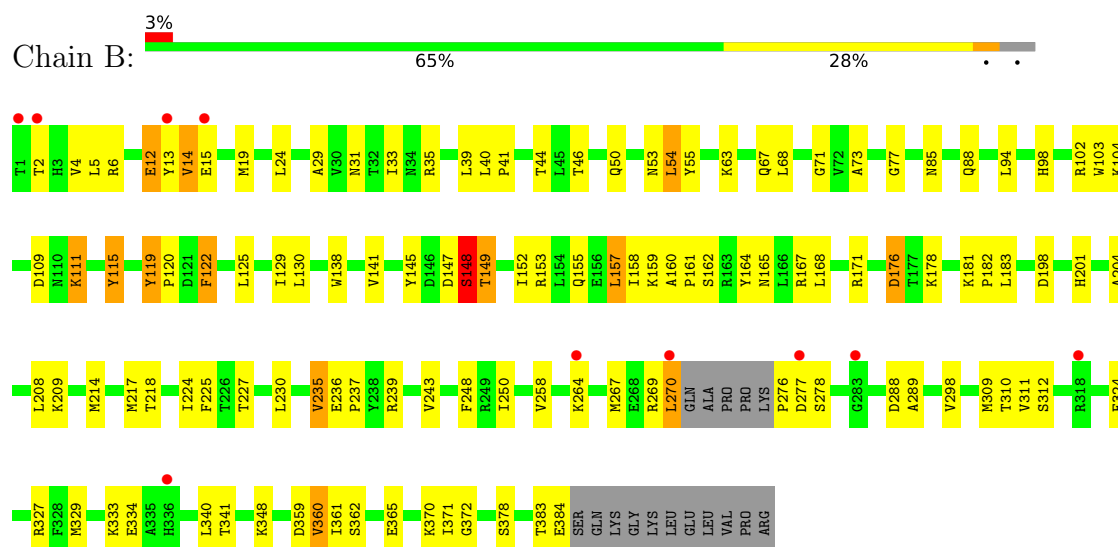
3 Residue-property plots [i](#)

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: Glutamate receptor, ionotropic kainate 2



- Molecule 1: Glutamate receptor, ionotropic kainate 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	177.25Å 177.25Å 81.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.31 – 2.90 44.31 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.31-2.90) 98.6 (44.31-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.254 0.208 , 0.247	Depositor DCC
R_{free} test set	1623 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6186	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.36	2/3121 (0.1%)	0.57	4/4226 (0.1%)
1	B	0.36	2/3088 (0.1%)	0.56	3/4178 (0.1%)
All	All	0.36	4/6209 (0.1%)	0.57	7/8404 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ARG	CZ-NH1	-7.37	1.23	1.33
1	B	167	ARG	CZ-NH2	-7.27	1.23	1.33
1	B	167	ARG	CZ-NH1	-7.01	1.24	1.33
1	A	167	ARG	CZ-NH2	-6.97	1.24	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ARG	NE-CZ-NH2	10.95	125.77	120.30
1	B	167	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	B	167	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	B	167	ARG	NH1-CZ-NH2	-8.69	109.84	119.40
1	A	167	ARG	NH1-CZ-NH2	-8.49	110.06	119.40
1	A	167	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	51	LYS	CD-CE-NZ	5.65	124.69	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3051	0	3020	106	0
1	B	3021	0	2991	110	0
2	A	56	0	52	4	0
2	B	56	0	52	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	6186	0	6115	206	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 17.

All (206) 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:B:122:PHE:CZ	1:B:153:ARG:CG	2.60	0.84
1:B:270:LEU:HD23	1:B:270:LEU:H	1.43	0.84
1:A:122:PHE:CZ	1:A:153:ARG:CG	2.61	0.83
1:B:122:PHE:CE1	1:B:153:ARG:HG2	2.14	0.82
1:A:122:PHE:CE1	1:A:153:ARG:CG	2.63	0.82
1:A:122:PHE:CE1	1:A:153:ARG:HG2	2.15	0.81
1:B:122:PHE:CE1	1:B:153:ARG:CG	2.62	0.81
1:A:122:PHE:CZ	1:A:153:ARG:HG2	2.18	0.79
1:B:122:PHE:CZ	1:B:153:ARG:HG2	2.16	0.79
1:A:122:PHE:HB3	1:A:125:LEU:HB2	1.66	0.78
1:A:39:LEU:HB2	2:A:396:NAG:H82	1.67	0.75
1:B:122:PHE:HB3	1:B:125:LEU:HB2	1.68	0.74
1:B:122:PHE:CZ	1:B:153:ARG:HD2	2.23	0.74
1:A:122:PHE:CZ	1:A:153:ARG:HD2	2.23	0.73
1:B:270:LEU:HD23	1:B:270:LEU:N	2.03	0.73
1:A:103:TRP:NE1	1:A:122:PHE:CE1	2.59	0.71
1:A:122:PHE:CE1	1:A:153:ARG:HG3	2.27	0.69
1:A:362:SER:HB2	1:A:371:ILE:HD13	1.73	0.69
1:B:103:TRP:NE1	1:B:122:PHE:CE1	2.60	0.69
1:B:122:PHE:CE1	1:B:153:ARG:HG3	2.27	0.69
1:B:68:LEU:HD13	1:B:94:LEU:HD22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:SER:HB2	1:B:371:ILE:HD13	1.73	0.68
1:A:68:LEU:HD13	1:A:94:LEU:HD22	1.75	0.67
1:A:130:LEU:HD13	1:A:157:LEU:HD23	1.77	0.66
1:A:103:TRP:NE1	1:A:122:PHE:HE1	1.93	0.65
1:B:85:ASN:OD1	1:B:104:LYS:HE3	1.98	0.64
1:A:276:PRO:O	1:A:277:ASP:HB3	1.97	0.63
1:B:13:TYR:CE2	1:B:15:GLU:HB3	2.33	0.63
1:B:103:TRP:NE1	1:B:122:PHE:HE1	1.95	0.63
1:B:130:LEU:HD13	1:B:157:LEU:HD23	1.79	0.63
1:B:63:LYS:O	1:B:67:GLN:HG3	1.98	0.63
1:A:63:LYS:O	1:A:67:GLN:HG3	1.99	0.62
1:B:122:PHE:CZ	1:B:153:ARG:CD	2.82	0.62
1:A:103:TRP:CD1	1:A:122:PHE:CZ	2.88	0.62
1:B:103:TRP:CG	1:B:122:PHE:CZ	2.88	0.61
1:A:85:ASN:OD1	1:A:104:LYS:HE3	1.99	0.61
1:B:103:TRP:CD1	1:B:122:PHE:CZ	2.88	0.61
1:A:122:PHE:CZ	1:A:153:ARG:CD	2.83	0.61
1:A:217:MET:HA	1:A:243:VAL:CG1	2.31	0.61
1:A:103:TRP:CG	1:A:122:PHE:CZ	2.88	0.60
1:A:103:TRP:CD1	1:A:122:PHE:CE1	2.89	0.60
1:B:71:GLY:C	1:B:311:VAL:HG11	2.22	0.60
1:A:71:GLY:C	1:A:311:VAL:HG11	2.23	0.59
1:A:103:TRP:CE2	1:A:122:PHE:HE1	2.20	0.59
1:B:217:MET:HA	1:B:243:VAL:CG1	2.32	0.59
1:B:103:TRP:CD1	1:B:122:PHE:CE1	2.90	0.59
1:B:103:TRP:CE2	1:B:122:PHE:HE1	2.21	0.59
1:A:276:PRO:O	1:A:277:ASP:CB	2.51	0.58
1:B:103:TRP:CG	1:B:122:PHE:HZ	2.21	0.58
1:A:359:ASP:OD1	1:A:370:LYS:HE3	2.04	0.58
1:A:103:TRP:CG	1:A:122:PHE:HZ	2.22	0.57
1:B:239:ARG:HD2	1:B:365:GLU:O	2.05	0.57
1:B:359:ASP:OD1	1:B:370:LYS:HE3	2.04	0.57
2:B:396:NAG:O3	2:B:396:NAG:H83	2.05	0.56
1:A:217:MET:HE1	1:A:243:VAL:HG21	1.87	0.56
1:B:181:LYS:HB3	1:B:214:MET:HE3	1.88	0.56
1:A:103:TRP:CE2	1:A:122:PHE:CE1	2.94	0.55
1:A:148:SER:HB2	1:B:152:ILE:HG23	1.87	0.55
1:A:29:ALA:O	1:A:33:ILE:HG13	2.06	0.55
1:B:103:TRP:CE2	1:B:122:PHE:CE1	2.95	0.55
1:B:217:MET:HA	1:B:243:VAL:HG11	1.89	0.55
1:A:119:TYR:CD2	1:A:120:PRO:HD2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:HG13	1:B:340:LEU:HD22	1.88	0.55
1:A:239:ARG:HD2	1:A:365:GLU:O	2.06	0.54
1:A:217:MET:HA	1:A:243:VAL:HG11	1.89	0.54
1:A:155:GLN:NE2	1:B:148:SER:HB3	2.22	0.54
1:B:119:TYR:CD2	1:B:120:PRO:HD2	2.42	0.54
1:A:258:VAL:HG13	1:A:340:LEU:HD22	1.89	0.54
1:B:29:ALA:O	1:B:33:ILE:HG13	2.07	0.54
1:B:33:ILE:HG23	1:B:39:LEU:HD23	1.90	0.54
1:A:33:ILE:HG23	1:A:39:LEU:HD23	1.90	0.53
1:B:236:GLU:N	1:B:237:PRO:CD	2.71	0.53
1:A:122:PHE:HA	1:A:125:LEU:H	1.72	0.53
1:B:122:PHE:HA	1:B:125:LEU:HB2	1.91	0.53
1:A:362:SER:CB	1:A:371:ILE:HD13	2.38	0.53
1:A:122:PHE:HA	1:A:125:LEU:HB2	1.91	0.53
1:B:168:LEU:HD12	1:B:168:LEU:O	2.08	0.52
1:A:159:LYS:HE2	1:B:145:TYR:OH	2.10	0.52
1:B:12:GLU:HB2	1:B:54:LEU:HD23	1.90	0.52
1:A:122:PHE:CB	1:A:125:LEU:HB2	2.39	0.52
1:A:12:GLU:HB2	1:A:54:LEU:HD23	1.90	0.52
1:A:337:TRP:CH2	2:A:396:NAG:H83	2.45	0.52
1:A:236:GLU:N	1:A:237:PRO:CD	2.73	0.51
1:B:77:GLY:HA3	1:B:98:HIS:NE2	2.25	0.51
1:B:362:SER:CB	1:B:371:ILE:HD13	2.40	0.51
1:A:115:TYR:CD1	1:A:115:TYR:C	2.84	0.51
1:A:160:ALA:N	1:A:161:PRO:CD	2.72	0.51
1:B:13:TYR:CZ	1:B:15:GLU:HB3	2.45	0.51
1:B:160:ALA:N	1:B:161:PRO:CD	2.73	0.51
1:B:115:TYR:CD1	1:B:115:TYR:C	2.84	0.51
1:B:122:PHE:HA	1:B:125:LEU:H	1.74	0.51
1:A:168:LEU:HD12	1:A:168:LEU:O	2.11	0.50
1:B:171:ARG:HB3	1:B:183:LEU:HD11	1.94	0.50
1:A:217:MET:CE	1:A:243:VAL:HG21	2.41	0.50
1:A:71:GLY:C	1:A:311:VAL:CG1	2.80	0.50
1:A:77:GLY:HA3	1:A:98:HIS:NE2	2.26	0.50
1:B:12:GLU:HB2	1:B:54:LEU:CD2	2.42	0.50
1:B:270:LEU:N	1:B:270:LEU:CD2	2.70	0.50
1:B:288:ASP:OD1	1:B:289:ALA:N	2.44	0.50
1:A:5:LEU:HD11	1:A:73:ALA:HB2	1.94	0.50
1:B:5:LEU:HD11	1:B:73:ALA:HB2	1.94	0.50
1:B:88:GLN:OE1	1:B:115:TYR:CE2	2.64	0.50
1:A:171:ARG:HB3	1:A:183:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:HB2	1:A:54:LEU:CD2	2.43	0.49
1:A:88:GLN:OE1	1:A:115:TYR:CE2	2.65	0.49
1:A:362:SER:HB2	1:A:371:ILE:CD1	2.42	0.49
1:B:71:GLY:C	1:B:311:VAL:CG1	2.81	0.49
1:A:288:ASP:OD1	1:A:289:ALA:N	2.45	0.49
1:A:181:LYS:HB2	1:A:182:PRO:HD3	1.95	0.49
1:B:208:LEU:HD21	1:B:225:PHE:HZ	1.78	0.48
1:B:217:MET:HE3	1:B:243:VAL:HG11	1.96	0.48
1:A:170:ILE:HG13	1:B:158:ILE:HG22	1.96	0.48
1:B:217:MET:CE	1:B:243:VAL:HG21	2.43	0.48
1:A:169:LYS:HB3	1:B:162:SER:OG	2.13	0.48
1:A:350:ASN:ND2	2:A:398:NAG:C7	2.76	0.48
1:A:155:GLN:HE22	1:B:148:SER:HB3	1.78	0.48
1:A:152:ILE:HG23	1:B:148:SER:HB2	1.96	0.48
1:B:53:ASN:OD1	1:B:53:ASN:C	2.53	0.48
1:B:103:TRP:CD2	1:B:122:PHE:HZ	2.32	0.47
1:B:122:PHE:CB	1:B:125:LEU:HB2	2.40	0.47
1:B:235:VAL:O	1:B:235:VAL:CG1	2.62	0.47
1:B:209:LYS:HE3	1:B:277:ASP:O	2.14	0.47
1:A:50:GLN:HB3	1:A:63:LYS:HD2	1.97	0.47
1:A:337:TRP:HH2	2:A:396:NAG:H83	1.80	0.47
1:B:383:THR:HG22	2:B:399:NAG:O6	2.15	0.47
1:A:145:TYR:OH	1:B:159:LYS:HE2	2.15	0.46
1:A:208:LEU:HD21	1:A:225:PHE:HZ	1.81	0.46
1:B:88:GLN:OE1	1:B:115:TYR:CD2	2.68	0.46
1:A:181:LYS:HB3	1:A:214:MET:HE3	1.96	0.46
1:A:235:VAL:CG1	1:A:235:VAL:O	2.63	0.46
1:A:138:TRP:CH2	1:A:224:ILE:HG13	2.50	0.46
1:B:4:VAL:HG12	1:B:4:VAL:O	2.15	0.46
1:B:164:TYR:CG	1:B:165:ASN:N	2.84	0.46
1:B:218:THR:O	1:B:243:VAL:HA	2.15	0.46
1:A:164:TYR:CG	1:A:165:ASN:N	2.84	0.46
1:B:138:TRP:CH2	1:B:224:ILE:HG13	2.51	0.46
1:A:14:VAL:O	1:A:16:SER:HA	2.16	0.46
1:A:53:ASN:OD1	1:A:53:ASN:C	2.53	0.46
1:A:88:GLN:OE1	1:A:115:TYR:CD2	2.69	0.46
1:B:311:VAL:HG12	1:B:312:SER:N	2.31	0.46
1:A:4:VAL:HG12	1:A:4:VAL:O	2.15	0.45
1:A:148:SER:HB3	1:B:155:GLN:NE2	2.30	0.45
1:A:103:TRP:CD2	1:A:122:PHE:HZ	2.33	0.45
1:A:176:ASP:O	1:A:176:ASP:OD2	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:CD1	1:B:153:ARG:HG2	2.50	0.45
1:B:181:LYS:HB2	1:B:182:PRO:HD3	1.98	0.45
1:A:141:VAL:O	1:A:168:LEU:HA	2.17	0.45
1:B:14:VAL:HG22	1:B:14:VAL:O	2.17	0.45
1:A:311:VAL:HG12	1:A:312:SER:N	2.31	0.44
1:B:141:VAL:O	1:B:168:LEU:HA	2.18	0.44
1:B:176:ASP:O	1:B:176:ASP:OD2	2.36	0.44
1:A:53:ASN:OD1	1:A:55:TYR:CD1	2.70	0.44
1:A:218:THR:O	1:A:243:VAL:HA	2.17	0.44
1:B:31:ASN:O	1:B:35:ARG:HG3	2.18	0.44
1:B:53:ASN:OD1	1:B:55:TYR:CD1	2.71	0.44
1:A:119:TYR:HD2	1:A:120:PRO:N	2.16	0.43
1:A:122:PHE:CD1	1:A:153:ARG:HG2	2.51	0.43
1:A:204:ALA:O	1:A:208:LEU:HG	2.18	0.43
1:B:119:TYR:HD2	1:B:120:PRO:N	2.15	0.43
1:B:217:MET:HE1	1:B:243:VAL:HG21	2.01	0.43
1:B:250:ILE:HG13	1:B:341:THR:HB	2.00	0.43
1:B:269:ARG:HB3	1:B:270:LEU:H	1.63	0.43
1:B:267:MET:C	1:B:269:ARG:H	2.22	0.43
1:B:334:GLU:OE2	1:B:348:LYS:HD2	2.19	0.43
1:B:147:ASP:O	1:B:149:THR:N	2.51	0.43
1:B:276:PRO:C	1:B:278:SER:H	2.22	0.43
1:B:50:GLN:HB3	1:B:63:LYS:HD2	1.99	0.43
1:A:102:ARG:HA	1:A:119:TYR:HD1	1.84	0.43
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.85	0.43
1:A:31:ASN:O	1:A:35:ARG:HG3	2.19	0.43
1:A:40:LEU:N	1:A:41:PRO:HD3	2.34	0.43
1:A:334:GLU:OE2	1:A:348:LYS:HD2	2.19	0.43
1:A:225:PHE:HB3	1:A:227:THR:HG22	2.01	0.42
1:A:178:LYS:HA	1:A:178:LYS:HD3	1.71	0.42
1:B:85:ASN:OD1	1:B:104:LYS:CE	2.67	0.42
1:A:53:ASN:OD1	1:A:55:TYR:CE1	2.72	0.42
1:A:324:PHE:CD2	1:A:324:PHE:N	2.87	0.42
1:A:329:MET:HE3	1:A:329:MET:HA	2.00	0.42
1:B:329:MET:O	1:B:333:LYS:HG3	2.19	0.42
1:A:153:ARG:NH2	1:A:198:ASP:OD1	2.53	0.42
1:B:40:LEU:N	1:B:41:PRO:HD3	2.35	0.42
1:A:149:THR:HG23	1:A:153:ARG:NH1	2.34	0.42
1:A:329:MET:O	1:A:333:LYS:HG3	2.20	0.42
1:B:324:PHE:CD2	1:B:324:PHE:N	2.87	0.42
1:A:129:ILE:HD13	1:A:248:PHE:HE2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:O	1:B:129:ILE:HG12	2.20	0.41
1:A:18:PRO:HG2	1:A:271:GLN:HG2	2.02	0.41
1:B:204:ALA:O	1:B:208:LEU:HG	2.21	0.41
1:B:102:ARG:HA	1:B:119:TYR:HD1	1.85	0.41
1:B:309:MET:HG2	1:B:310:THR:N	2.35	0.41
1:B:360:VAL:HG12	1:B:372:GLY:C	2.41	0.41
1:A:350:ASN:HB3	1:A:352:LEU:HG	2.02	0.41
1:A:141:VAL:CG1	1:A:168:LEU:HB3	2.50	0.41
1:A:250:ILE:HG13	1:A:341:THR:HB	2.02	0.41
1:A:309:MET:HG2	1:A:310:THR:N	2.34	0.41
1:B:230:LEU:HB3	1:B:361:ILE:HD11	2.02	0.41
1:B:149:THR:HG23	1:B:153:ARG:NH1	2.36	0.41
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.84	0.40
1:B:129:ILE:HD13	1:B:248:PHE:HE2	1.86	0.40
1:B:141:VAL:CG1	1:B:168:LEU:HB3	2.51	0.40
1:A:55:TYR:OH	1:B:111:LYS:HG3	2.22	0.40
1:A:148:SER:HB3	1:B:155:GLN:HE22	1.87	0.40
1:B:153:ARG:NH2	1:B:198:ASP:OD1	2.54	0.40
1:A:94:LEU:N	1:A:94:LEU:HD12	2.36	0.40
1:B:103:TRP:CD2	1:B:122:PHE:CZ	3.09	0.40
1:B:225:PHE:HB3	1:B:227:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/395 (96%)	361 (95%)	19 (5%)	1 (0%)	41	71
1	B	375/395 (95%)	353 (94%)	21 (6%)	1 (0%)	41	71
All	All	756/790 (96%)	714 (94%)	40 (5%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	SER
1	A	148	SER

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	335/346 (97%)	305 (91%)	30 (9%)	9	29
1	B	332/346 (96%)	304 (92%)	28 (8%)	11	31
All	All	667/692 (96%)	609 (91%)	58 (9%)	10	30

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	6	ARG
1	A	12	GLU
1	A	19	MET
1	A	24	LEU
1	A	44	THR
1	A	46	THR
1	A	54	LEU
1	A	109	ASP
1	A	111	LYS
1	A	115	TYR
1	A	119	TYR
1	A	122	PHE
1	A	148	SER
1	A	149	THR
1	A	157	LEU
1	A	173	LEU
1	A	176	ASP
1	A	178	LYS
1	A	201	HIS
1	A	224	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	VAL
1	A	264	LYS
1	A	269	ARG
1	A	270	LEU
1	A	298	VAL
1	A	360	VAL
1	A	378	SER
1	A	380	LEU
1	A	384	GLU
1	B	2	THR
1	B	6	ARG
1	B	12	GLU
1	B	14	VAL
1	B	19	MET
1	B	24	LEU
1	B	44	THR
1	B	46	THR
1	B	54	LEU
1	B	109	ASP
1	B	111	LYS
1	B	115	TYR
1	B	119	TYR
1	B	122	PHE
1	B	148	SER
1	B	149	THR
1	B	157	LEU
1	B	176	ASP
1	B	178	LYS
1	B	201	HIS
1	B	235	VAL
1	B	264	LYS
1	B	270	LEU
1	B	298	VAL
1	B	327	ARG
1	B	360	VAL
1	B	378	SER
1	B	384	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	HIS
1	A	134	GLN
1	A	155	GLN
1	A	319	HIS
1	B	3	HIS
1	B	80	HIS
1	B	134	GLN
1	B	155	GLN
1	B	319	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 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	$\# Z > 2$
2	NAG	A	398	1	14,14,15	0.79	1 (7%)	17,19,21	1.77	3 (17%)
2	NAG	A	397	1	14,14,15	0.44	0	17,19,21	1.64	2 (11%)
2	NAG	B	399	1	14,14,15	0.59	0	17,19,21	0.94	0
2	NAG	B	396	1	14,14,15	0.58	0	17,19,21	1.68	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	398	1	14,14,15	0.44	0	17,19,21	1.52	2 (11%)
2	NAG	A	399	1	14,14,15	0.59	0	17,19,21	0.61	0
2	NAG	B	397	1	14,14,15	0.47	0	17,19,21	1.42	1 (5%)
2	NAG	A	396	1	14,14,15	0.71	0	17,19,21	2.45	6 (35%)

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
2	NAG	A	398	1	-	5/6/23/26	0/1/1/1
2	NAG	A	397	1	-	0/6/23/26	0/1/1/1
2	NAG	B	399	1	-	4/6/23/26	0/1/1/1
2	NAG	B	396	1	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	B	398	1	-	0/6/23/26	0/1/1/1
2	NAG	A	399	1	-	2/6/23/26	0/1/1/1
2	NAG	B	397	1	-	2/6/23/26	0/1/1/1
2	NAG	A	396	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	398	NAG	O5-C1	-2.33	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	396	NAG	O5-C1-C2	-6.67	100.76	111.29
2	A	397	NAG	C1-O5-C5	5.35	119.44	112.19
2	A	396	NAG	C1-O5-C5	-5.02	105.39	112.19
2	A	398	NAG	O5-C1-C2	-4.95	103.47	111.29
2	B	396	NAG	O5-C1-C2	-4.95	103.47	111.29
2	B	397	NAG	C1-O5-C5	4.93	118.87	112.19
2	B	398	NAG	C1-O5-C5	4.57	118.38	112.19
2	A	398	NAG	C1-O5-C5	-4.12	106.61	112.19
2	A	396	NAG	C2-N2-C7	-2.98	118.66	122.90
2	B	396	NAG	O5-C5-C6	2.81	111.61	107.20
2	B	398	NAG	O5-C1-C2	2.45	115.16	111.29
2	A	398	NAG	C3-C4-C5	2.40	114.52	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	396	NAG	O5-C5-C6	2.27	110.77	107.20
2	A	397	NAG	C4-C3-C2	-2.24	107.74	111.02
2	B	396	NAG	C2-N2-C7	-2.09	119.92	122.90
2	A	396	NAG	C1-C2-N2	2.06	114.00	110.49
2	A	396	NAG	O5-C5-C4	-2.05	105.83	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	396	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	398	NAG	C3-C2-N2-C7
2	A	399	NAG	C8-C7-N2-C2
2	A	399	NAG	O7-C7-N2-C2
2	B	396	NAG	C8-C7-N2-C2
2	B	396	NAG	O7-C7-N2-C2
2	A	398	NAG	O7-C7-N2-C2
2	A	398	NAG	C8-C7-N2-C2
2	B	399	NAG	C8-C7-N2-C2
2	B	399	NAG	O7-C7-N2-C2
2	B	399	NAG	O5-C5-C6-O6
2	A	396	NAG	C8-C7-N2-C2
2	B	399	NAG	C4-C5-C6-O6
2	A	396	NAG	O7-C7-N2-C2
2	A	398	NAG	O5-C5-C6-O6
2	B	397	NAG	C4-C5-C6-O6
2	A	398	NAG	C1-C2-N2-C7
2	B	396	NAG	C1-C2-N2-C7
2	B	397	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	398	NAG	1	0
2	B	399	NAG	1	0
2	B	396	NAG	1	0
2	A	396	NAG	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	383/395 (96%)	-0.08	6 (1%) 72 71	49, 91, 151, 192	0
1	B	379/395 (95%)	-0.01	10 (2%) 56 52	51, 91, 160, 223	0
All	All	762/790 (96%)	-0.05	16 (2%) 63 61	49, 91, 156, 223	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	ASP	6.4
1	B	2	THR	3.2
1	B	1	THR	3.2
1	B	283	GLY	3.1
1	A	266	SER	3.1
1	B	15	GLU	2.9
1	A	5	LEU	2.8
1	B	264	LYS	2.7
1	B	13	TYR	2.4
1	B	318	ARG	2.4
1	A	55	TYR	2.3
1	A	14	VAL	2.2
1	A	81	SER	2.1
1	A	176	ASP	2.1
1	B	270	LEU	2.0
1	B	336	HIS	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
2	NAG	B	399	14/15	0.75	0.27	110,160,183,192	0
2	NAG	A	399	14/15	0.81	0.35	111,162,186,190	0
3	CA	A	400	1/1	0.86	0.27	157,157,157,157	0
2	NAG	A	396	14/15	0.87	0.22	112,157,183,189	0
2	NAG	B	397	14/15	0.88	0.26	97,144,152,166	0
2	NAG	A	397	14/15	0.89	0.20	88,152,178,184	0
2	NAG	B	396	14/15	0.90	0.16	118,158,179,184	0
2	NAG	A	398	14/15	0.94	0.25	91,120,156,165	0
2	NAG	B	398	14/15	0.94	0.23	78,104,117,117	0
3	CA	B	400	1/1	0.94	0.12	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.