



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:06 PM UTC

PDB ID : 3H6G / pdb_00003h6g
Title : Crystal structure of the GluR6 amino terminal domain dimer assembly
Authors : Kumar, J.; Mayer, M.L.
Deposited on : 2009-04-23
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

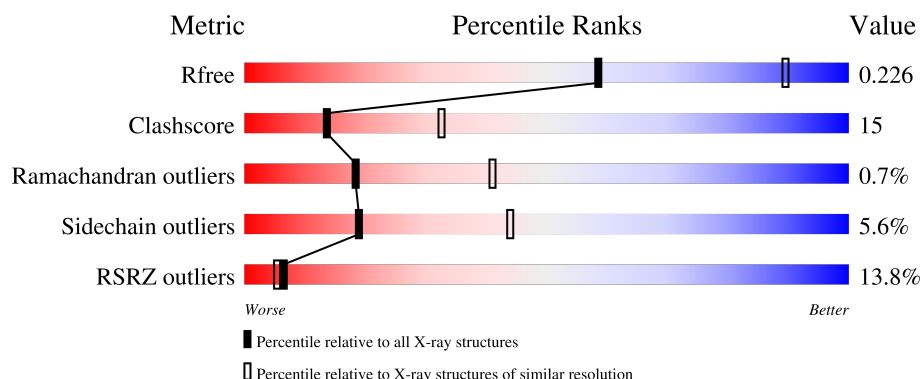
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	13% 72% 19% • 5%
1	B	395	13% 70% 22% • •

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	A	396	X	-	-	-
2	NAG	A	397	X	-	-	-
2	NAG	A	398	X	-	-	-
2	NAG	B	396	X	-	-	-
2	NAG	B	398	X	-	-	-
3	TLA	A	401	-	X	-	-
3	TLA	B	399	X	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6233 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.

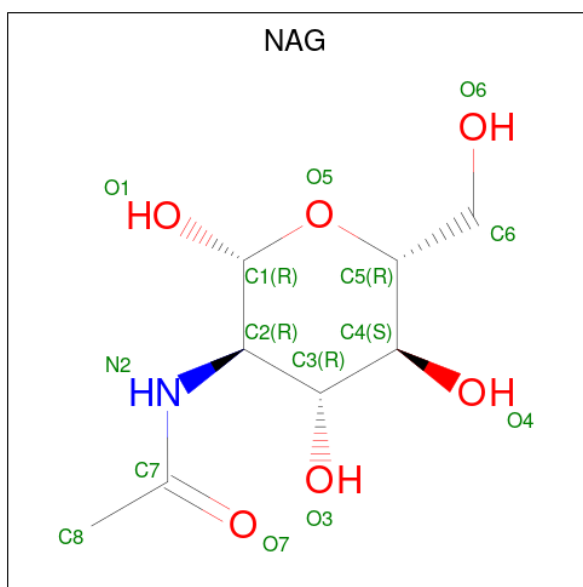
- Molecule 1 is a protein called Glutamate receptor, ionotropic kainate 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3004	1917	509	561	17			
1	B	383	Total	C	N	O	S	0	0	0
			3051	1947	519	568	17			

There are 12 discrepancies between the modelled and reference sequences:

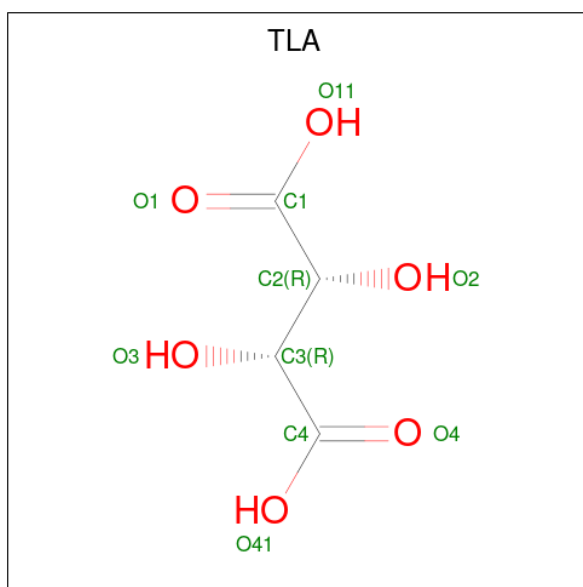
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LEU	-	expression tag	UNP P42260
A	391	GLU	-	expression tag	UNP P42260
A	392	LEU	-	expression tag	UNP P42260
A	393	VAL	-	expression tag	UNP P42260
A	394	PRO	-	expression tag	UNP P42260
A	395	ARG	-	expression tag	UNP P42260
B	390	LEU	-	expression tag	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 (CCD ID: 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	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 L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

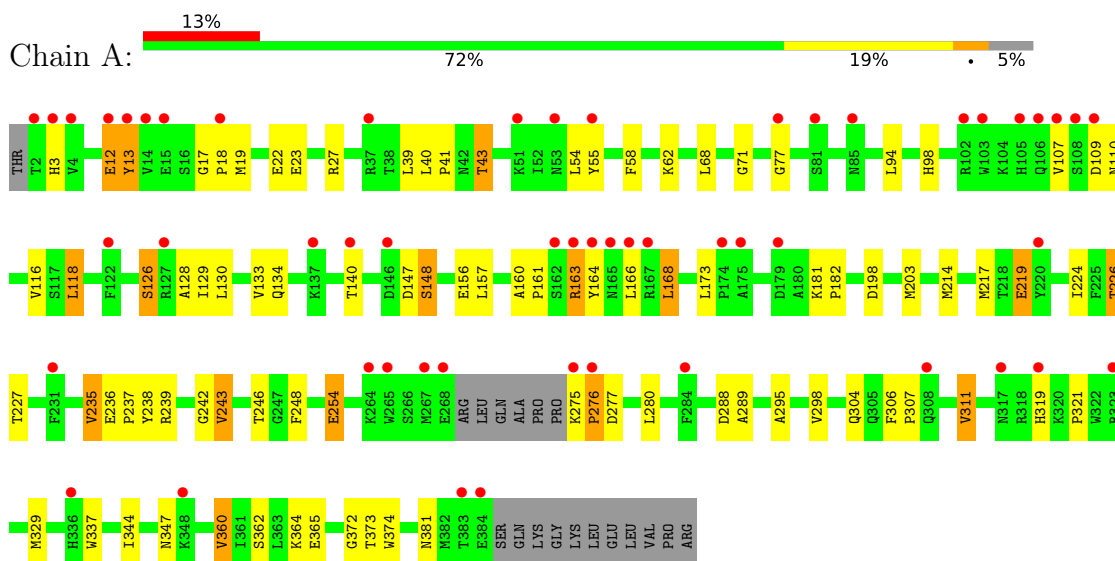
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	22	Total	O	0	0
			22	22		

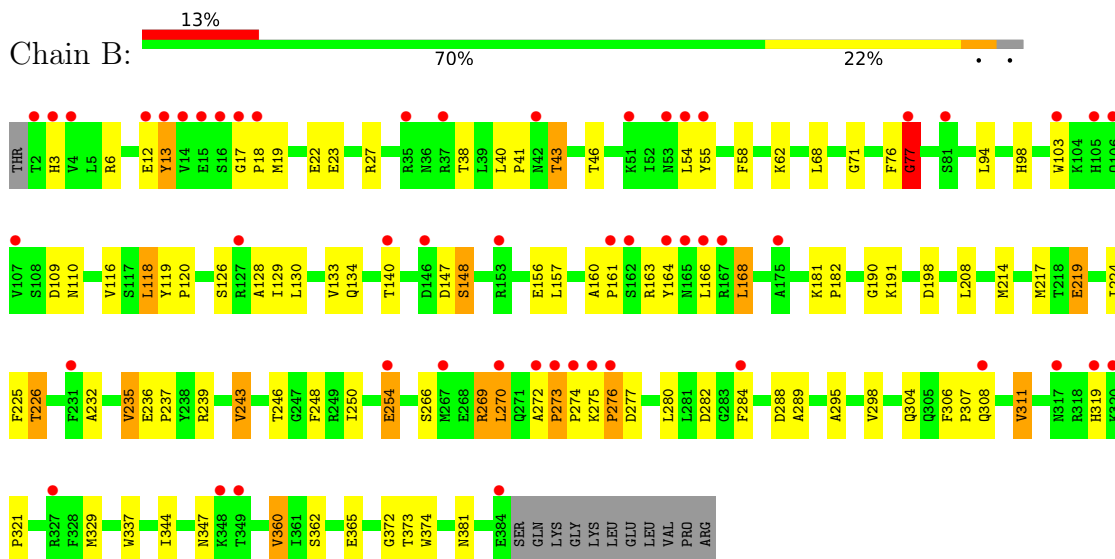
3 Residue-property plots [i](#)

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	172.07 Å 172.07 Å 111.55 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.80 – 2.70 46.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.80-2.70) 97.8 (46.80-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.69 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.227 0.209 , 0.226	Depositor DCC
R_{free} test set	2571 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: NAG, TLA, CA

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	0.51	0/3071	0.79	1/4155 (0.0%)
1	B	0.51	0/3121	0.80	4/4226 (0.1%)
All	All	0.51	0/6192	0.80	5/8381 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	VAL	CB-CA-C	-6.13	103.34	111.13
1	B	273	PRO	N-CA-C	5.96	117.97	110.70
1	A	243	VAL	CB-CA-C	-5.86	103.69	111.13
1	B	77	GLY	CA-C-N	5.08	125.09	120.21
1	B	77	GLY	C-N-CA	5.08	125.09	120.21

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	3004	0	2968	89	0
1	B	3051	0	3022	97	0
2	A	70	0	65	7	0
2	B	42	0	39	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	4	1	0
3	B	10	0	4	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	22	0	0	0	0
5	B	22	0	0	0	0
All	All	6233	0	6102	180	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 15.

All (180) 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:19:MET:HE1	1:B:27:ARG:HD2	1.61	0.82
1:B:54:LEU:HG	1:B:55:TYR:CD2	2.15	0.82
1:A:19:MET:HE1	1:A:27:ARG:HD2	1.62	0.81
1:A:54:LEU:HG	1:A:55:TYR:CD2	2.16	0.80
1:B:272:ALA:HB1	1:B:273:PRO:CD	2.11	0.79
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.65	0.78
1:B:54:LEU:HG	1:B:55:TYR:CE2	2.24	0.73
1:B:19:MET:CE	1:B:23:GLU:HG2	2.19	0.72
1:A:54:LEU:HG	1:A:55:TYR:CE2	2.24	0.72
1:A:39:LEU:HB2	2:A:396:NAG:H82	1.69	0.72
1:A:227:THR:OG1	3:A:401:TLA:H3	1.89	0.72
1:B:118:LEU:HD13	1:B:295:ALA:HB2	1.73	0.71
1:B:181:LYS:HG2	1:B:214:MET:HE3	1.72	0.71
1:B:134:GLN:OE1	1:B:164:TYR:CE2	2.45	0.69
1:A:134:GLN:OE1	1:A:164:TYR:CE2	2.45	0.68
1:A:19:MET:CE	1:A:23:GLU:HG2	2.22	0.68
1:A:19:MET:HE3	1:A:23:GLU:HG2	1.75	0.68
1:A:19:MET:HE3	1:A:23:GLU:CD	2.20	0.68
1:B:19:MET:HE3	1:B:23:GLU:HG2	1.73	0.67
1:B:168:LEU:HD12	1:B:168:LEU:C	2.19	0.67
1:B:12:GLU:HG2	1:B:54:LEU:HA	1.75	0.67
1:A:118:LEU:HD13	1:A:295:ALA:HB2	1.78	0.66
1:B:19:MET:HE3	1:B:23:GLU:CD	2.20	0.66
1:B:347:ASN:OD1	2:B:398:NAG:N2	2.27	0.66
1:B:168:LEU:HD12	1:B:168:LEU:O	1.96	0.65
1:A:12:GLU:HG2	1:A:54:LEU:HA	1.77	0.65
1:A:19:MET:HE3	1:A:23:GLU:CG	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:HE3	1:B:23:GLU:CG	2.27	0.64
1:B:360:VAL:HG12	1:B:372:GLY:C	2.22	0.64
1:A:168:LEU:C	1:A:168:LEU:HD12	2.22	0.64
1:A:217:MET:HA	1:A:243:VAL:CG1	2.28	0.64
1:A:181:LYS:HG2	1:A:214:MET:HE3	1.78	0.63
1:A:360:VAL:HG12	1:A:372:GLY:C	2.23	0.63
1:B:217:MET:HA	1:B:243:VAL:CG1	2.29	0.62
1:A:168:LEU:HD12	1:A:168:LEU:O	1.99	0.62
1:B:181:LYS:CG	1:B:214:MET:HE3	2.31	0.61
1:B:272:ALA:CB	1:B:273:PRO:HD2	2.32	0.60
1:A:68:LEU:HD13	1:A:94:LEU:HD22	1.83	0.59
1:B:272:ALA:CB	1:B:273:PRO:CD	2.81	0.59
1:B:38:THR:HG21	2:B:396:NAG:O7	2.03	0.58
1:B:77:GLY:HA3	1:B:98:HIS:NE2	2.19	0.57
1:B:347:ASN:OD1	2:B:398:NAG:C7	2.52	0.57
1:B:266:SER:O	1:B:270:LEU:HB2	2.05	0.57
1:A:298:VAL:HG21	1:A:344:ILE:HG21	1.85	0.57
1:B:68:LEU:HD13	1:B:94:LEU:HD22	1.85	0.57
1:B:128:ALA:HB2	1:B:374:TRP:CE2	2.40	0.57
1:A:217:MET:HA	1:A:243:VAL:HG11	1.85	0.56
1:B:298:VAL:HG21	1:B:344:ILE:HG21	1.87	0.56
1:B:217:MET:HA	1:B:243:VAL:HG11	1.87	0.56
1:A:55:TYR:HB3	1:B:110:ASN:HD22	1.71	0.55
1:B:118:LEU:HD13	1:B:295:ALA:CB	2.37	0.55
1:A:110:ASN:HD22	1:B:55:TYR:HB3	1.72	0.54
1:A:337:TRP:CH2	2:A:396:NAG:H83	2.42	0.54
1:A:360:VAL:CG1	1:A:372:GLY:C	2.80	0.54
1:A:288:ASP:OD1	1:A:289:ALA:N	2.41	0.54
1:A:71:GLY:HA3	1:A:311:VAL:CG1	2.38	0.54
1:A:128:ALA:HB2	1:A:374:TRP:CE2	2.44	0.54
1:A:181:LYS:CG	1:A:214:MET:HE3	2.38	0.54
1:A:217:MET:CA	1:A:243:VAL:CG1	2.86	0.54
1:B:298:VAL:HG22	1:B:337:TRP:HB3	1.90	0.53
1:A:77:GLY:HA3	1:A:98:HIS:NE2	2.23	0.53
1:B:360:VAL:CG1	1:B:372:GLY:C	2.82	0.53
1:B:54:LEU:HG	1:B:55:TYR:CG	2.43	0.53
1:A:298:VAL:HG22	1:A:337:TRP:HB3	1.91	0.53
1:B:217:MET:CA	1:B:243:VAL:CG1	2.87	0.53
1:A:41:PRO:HD3	1:A:304:GLN:HE21	1.74	0.52
1:B:129:ILE:HD13	1:B:248:PHE:HE2	1.74	0.52
1:B:71:GLY:HA3	1:B:311:VAL:CG1	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASN:OD1	2:A:399:NAG:O5	2.24	0.52
1:A:54:LEU:HG	1:A:55:TYR:CG	2.44	0.52
1:A:3:HIS:ND1	1:A:43:THR:HG23	2.24	0.51
1:B:288:ASP:OD1	1:B:289:ALA:N	2.44	0.51
1:B:181:LYS:HB3	1:B:214:MET:HE3	1.92	0.51
1:B:3:HIS:ND1	1:B:43:THR:HG23	2.24	0.51
1:B:41:PRO:HD3	1:B:304:GLN:HE21	1.74	0.51
1:B:181:LYS:CB	1:B:214:MET:HE3	2.41	0.51
1:A:68:LEU:HD13	1:A:94:LEU:CD2	2.41	0.50
1:B:54:LEU:HD21	1:B:55:TYR:CZ	2.46	0.50
1:B:71:GLY:C	1:B:311:VAL:HG11	2.37	0.50
1:A:55:TYR:CE2	1:B:109:ASP:HB2	2.47	0.49
1:A:118:LEU:HD13	1:A:295:ALA:CB	2.42	0.49
1:B:168:LEU:C	1:B:168:LEU:CD1	2.84	0.49
1:A:129:ILE:HD13	1:A:248:PHE:HE2	1.76	0.49
1:B:269:ARG:HG3	1:B:270:LEU:N	2.22	0.48
1:A:168:LEU:C	1:A:168:LEU:CD1	2.87	0.48
1:A:242:GLY:HA2	2:A:398:NAG:H82	1.96	0.48
1:B:76:PHE:O	1:B:77:GLY:O	2.32	0.48
1:A:160:ALA:N	1:A:161:PRO:CD	2.77	0.48
1:B:13:TYR:CD1	1:B:13:TYR:C	2.92	0.48
1:A:306:PHE:N	1:A:307:PRO:HD3	2.29	0.47
1:A:337:TRP:HH2	2:A:396:NAG:H83	1.79	0.47
1:A:198:ASP:HA	1:A:226:THR:HB	1.96	0.47
1:A:54:LEU:HD21	1:A:55:TYR:CZ	2.49	0.47
1:A:236:GLU:HB3	1:A:237:PRO:HD3	1.96	0.47
1:A:71:GLY:C	1:A:311:VAL:HG11	2.39	0.47
1:B:130:LEU:HD21	1:B:164:TYR:HE2	1.79	0.47
1:A:364:LYS:HZ2	2:A:398:NAG:H62	1.80	0.47
1:B:71:GLY:C	1:B:311:VAL:CG1	2.88	0.47
1:B:58:PHE:CZ	1:B:62:LYS:HE3	2.50	0.47
1:A:13:TYR:C	1:A:13:TYR:CD1	2.91	0.46
1:A:235:VAL:O	1:A:235:VAL:HG13	2.14	0.46
1:B:219:GLU:H	1:B:219:GLU:CD	2.22	0.46
1:A:58:PHE:CZ	1:A:62:LYS:HE3	2.51	0.46
1:B:54:LEU:O	1:B:55:TYR:HB2	2.16	0.46
1:A:17:GLY:HA2	1:A:18:PRO:O	2.16	0.46
1:A:181:LYS:N	1:A:182:PRO:CD	2.78	0.46
1:A:19:MET:CE	1:A:23:GLU:CG	2.91	0.46
1:B:181:LYS:N	1:B:182:PRO:CD	2.78	0.46
1:B:217:MET:HE3	1:B:243:VAL:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:HA	1:B:226:THR:HB	1.97	0.45
1:B:17:GLY:HA2	1:B:18:PRO:O	2.16	0.45
1:B:306:PHE:N	1:B:307:PRO:HD3	2.32	0.45
1:A:130:LEU:HD21	1:A:164:TYR:HE2	1.81	0.45
1:A:147:ASP:O	1:A:148:SER:C	2.59	0.45
1:A:254:GLU:HA	1:A:254:GLU:OE1	2.16	0.45
1:A:173:LEU:HD13	1:A:203:MET:HE3	1.99	0.45
1:A:364:LYS:NZ	2:A:398:NAG:H62	2.32	0.45
1:B:236:GLU:HB3	1:B:237:PRO:HD3	1.98	0.45
1:B:160:ALA:N	1:B:161:PRO:CD	2.79	0.45
1:B:254:GLU:HA	1:B:254:GLU:OE1	2.16	0.45
1:A:217:MET:HE3	1:A:243:VAL:HG21	1.98	0.45
1:B:129:ILE:HD13	1:B:248:PHE:CE2	2.52	0.45
1:B:133:VAL:HG11	1:B:166:LEU:HD21	1.99	0.44
1:A:71:GLY:C	1:A:311:VAL:CG1	2.90	0.44
1:A:157:LEU:O	1:A:157:LEU:HD23	2.18	0.44
1:A:217:MET:C	1:A:243:VAL:CG1	2.91	0.44
1:A:116:VAL:HG13	1:A:329:MET:CE	2.48	0.44
1:B:12:GLU:CG	1:B:54:LEU:HA	2.45	0.44
1:B:269:ARG:CG	1:B:270:LEU:N	2.80	0.44
1:A:181:LYS:HB3	1:A:214:MET:HE3	1.99	0.44
1:B:68:LEU:HD13	1:B:94:LEU:CD2	2.47	0.44
1:A:129:ILE:HD13	1:A:248:PHE:CE2	2.53	0.44
1:B:147:ASP:O	1:B:148:SER:C	2.61	0.44
1:B:232:ALA:HB2	1:B:284:PHE:CD2	2.54	0.43
1:B:235:VAL:O	1:B:235:VAL:HG13	2.17	0.43
1:A:54:LEU:O	1:A:55:TYR:HB2	2.18	0.43
1:A:254:GLU:OE1	1:A:254:GLU:CA	2.66	0.43
1:B:274:PRO:HB3	1:B:282:ASP:CG	2.43	0.43
1:A:239:ARG:HD2	1:A:365:GLU:O	2.19	0.43
1:A:71:GLY:CA	1:A:311:VAL:CG1	2.96	0.43
1:A:219:GLU:H	1:A:219:GLU:CD	2.24	0.43
1:B:71:GLY:CA	1:B:311:VAL:CG1	2.96	0.43
1:B:217:MET:C	1:B:243:VAL:CG1	2.92	0.43
1:A:133:VAL:HG11	1:A:166:LEU:HD21	2.01	0.43
1:B:224:ILE:HA	1:B:246:THR:O	2.19	0.43
1:B:266:SER:O	1:B:270:LEU:CB	2.67	0.43
1:A:224:ILE:HA	1:A:246:THR:O	2.19	0.42
1:A:235:VAL:O	1:A:235:VAL:CG1	2.66	0.42
1:A:163:ARG:H	1:A:163:ARG:HG3	1.68	0.42
1:A:181:LYS:CB	1:A:214:MET:HE3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:OG1	1:B:381:ASN:HB2	2.19	0.42
1:B:41:PRO:HD3	1:B:304:GLN:NE2	2.34	0.42
1:B:254:GLU:OE1	1:B:254:GLU:CA	2.67	0.42
1:B:276:PRO:HD2	1:B:277:ASP:H	1.84	0.42
1:A:13:TYR:C	1:A:13:TYR:HD1	2.28	0.42
1:B:103:TRP:HB2	1:B:119:TYR:CD2	2.55	0.42
1:B:239:ARG:HD2	1:B:365:GLU:O	2.20	0.42
1:B:157:LEU:HD23	1:B:157:LEU:O	2.19	0.42
1:A:12:GLU:CG	1:A:54:LEU:HA	2.47	0.41
1:A:55:TYR:HE2	1:B:109:ASP:CB	2.33	0.41
1:B:40:LEU:N	1:B:41:PRO:HD3	2.35	0.41
1:B:190:GLY:O	1:B:191:LYS:HB2	2.20	0.41
1:A:319:HIS:O	1:A:321:PRO:HD3	2.21	0.41
1:B:235:VAL:O	1:B:235:VAL:CG1	2.68	0.41
1:B:19:MET:CE	1:B:23:GLU:CG	2.89	0.41
1:B:307:PRO:HD2	1:B:308:GLN:OE1	2.21	0.41
1:A:109:ASP:HB2	1:B:55:TYR:CE2	2.56	0.41
1:B:6:ARG:HG3	1:B:46:THR:HG23	2.03	0.41
1:A:55:TYR:CE2	1:B:109:ASP:CB	3.04	0.41
1:A:126:SER:OG	1:A:156:GLU:HB2	2.20	0.41
1:A:276:PRO:HD2	1:A:277:ASP:H	1.84	0.41
1:A:373:THR:OG1	1:A:381:ASN:HB2	2.21	0.41
1:B:120:PRO:HG3	1:B:250:ILE:CD1	2.51	0.41
1:B:126:SER:OG	1:B:156:GLU:HB2	2.20	0.41
1:B:319:HIS:O	1:B:321:PRO:HD3	2.21	0.41
1:A:217:MET:HE2	1:A:238:TYR:CD1	2.56	0.41
1:A:41:PRO:HD3	1:A:304:GLN:NE2	2.35	0.40
1:A:40:LEU:N	1:A:41:PRO:HD3	2.36	0.40
1:B:208:LEU:HD21	1:B:225:PHE:HZ	1.87	0.40
1:B:116:VAL:HG13	1:B:329:MET:CE	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	373/395 (94%)	354 (95%)	17 (5%)	2 (0%)	24	48
1	B	381/395 (96%)	356 (93%)	22 (6%)	3 (1%)	16	37
All	All	754/790 (95%)	710 (94%)	39 (5%)	5 (1%)	18	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	PRO
1	B	276	PRO
1	A	148	SER
1	B	77	GLY
1	B	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	330/346 (95%)	311 (94%)	19 (6%)	18	42
1	B	335/346 (97%)	317 (95%)	18 (5%)	20	45
All	All	665/692 (96%)	628 (94%)	37 (6%)	19	44

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	13	TYR
1	A	22	GLU
1	A	43	THR
1	A	107	VAL
1	A	118	LEU
1	A	126	SER
1	A	140	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	163	ARG
1	A	168	LEU
1	A	219	GLU
1	A	226	THR
1	A	235	VAL
1	A	254	GLU
1	A	275	LYS
1	A	280	LEU
1	A	311	VAL
1	A	360	VAL
1	A	362	SER
1	B	13	TYR
1	B	22	GLU
1	B	43	THR
1	B	118	LEU
1	B	140	THR
1	B	163	ARG
1	B	168	LEU
1	B	219	GLU
1	B	226	THR
1	B	235	VAL
1	B	254	GLU
1	B	269	ARG
1	B	270	LEU
1	B	275	LYS
1	B	280	LEU
1	B	311	VAL
1	B	360	VAL
1	B	362	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	110	ASN
1	A	134	GLN
1	A	304	GLN
1	B	106	GLN
1	B	110	ASN
1	B	134	GLN
1	B	304	GLN
1	B	315	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are 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$
2	NAG	B	398	1	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
3	TLA	B	399	-	9,9,9	2.71	4 (44%)	12,12,12	3.08	7 (58%)
2	NAG	A	397	1	14,14,15	0.56	0	17,19,21	1.66	1 (5%)
2	NAG	A	399	1	14,14,15	0.87	0	17,19,21	1.77	4 (23%)
2	NAG	A	396	1	14,14,15	0.63	0	17,19,21	2.28	1 (5%)
2	NAG	B	396	1	14,14,15	0.79	0	17,19,21	1.96	4 (23%)
2	NAG	A	400	1	14,14,15	0.59	0	17,19,21	1.59	2 (11%)
3	TLA	A	401	-	9,9,9	2.76	4 (44%)	12,12,12	2.85	5 (41%)
2	NAG	A	398	1	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
2	NAG	B	397	1	14,14,15	0.57	0	17,19,21	1.09	1 (5%)

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	B	398	1	1/1/5/7	0/6/23/26	0/1/1/1
3	TLA	B	399	-	1/1/4/4	6/12/12/12	-
2	NAG	A	397	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	399	1	-	2/6/23/26	0/1/1/1
2	NAG	A	396	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	396	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	400	1	-	2/6/23/26	0/1/1/1
3	TLA	A	401	-	-	10/12/12/12	-
2	NAG	A	398	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	397	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	399	TLA	O4-C4	4.82	1.36	1.22
3	B	399	TLA	O1-C1	4.77	1.36	1.22
3	A	401	TLA	O4-C4	4.61	1.35	1.22
3	A	401	TLA	O1-C1	4.59	1.35	1.22
3	A	401	TLA	O41-C4	-3.17	1.20	1.30
3	B	399	TLA	O41-C4	-2.93	1.21	1.30
3	A	401	TLA	O11-C1	-2.73	1.21	1.30
3	B	399	TLA	O11-C1	-2.48	1.22	1.30

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	396	NAG	C1-O5-C5	8.36	123.39	112.19
3	A	401	TLA	O41-C4-O4	-5.86	110.79	124.08
2	A	397	NAG	O5-C1-C2	-5.74	102.41	111.29
3	B	399	TLA	O41-C4-O4	-5.61	111.35	124.08
2	B	396	NAG	C1-O5-C5	5.34	119.35	112.19
3	A	401	TLA	O11-C1-C2	4.88	126.88	113.31
3	B	399	TLA	O11-C1-C2	4.40	125.54	113.31
2	A	400	NAG	C1-O5-C5	4.34	118.00	112.19
3	A	401	TLA	O41-C4-C3	3.93	124.23	113.31
3	B	399	TLA	O11-C1-O1	-3.83	115.39	124.08
3	B	399	TLA	C3-C2-C1	-3.72	101.59	109.82
3	B	399	TLA	O1-C1-C2	-3.64	111.93	121.62
2	A	399	NAG	C1-O5-C5	-3.59	107.37	112.19
2	B	397	NAG	C1-O5-C5	3.54	116.93	112.19
2	B	396	NAG	O5-C1-C2	-3.47	105.92	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	399	NAG	O5-C5-C4	-3.38	102.61	110.83
2	A	399	NAG	O5-C1-C2	-3.11	106.48	111.29
2	A	399	NAG	C4-C3-C2	3.05	115.49	111.02
3	A	401	TLA	O11-C1-O1	-3.04	117.17	124.08
2	B	398	NAG	O5-C5-C6	2.78	113.07	107.66
2	B	396	NAG	C1-C2-N2	2.77	114.80	110.43
3	B	399	TLA	O41-C4-C3	2.72	120.88	113.31
2	B	398	NAG	C1-O5-C5	2.61	115.69	112.19
2	A	400	NAG	C1-C2-N2	2.52	114.41	110.43
2	B	396	NAG	C2-N2-C7	-2.40	119.68	122.90
3	B	399	TLA	O2-C2-C3	-2.31	105.46	110.17
2	A	398	NAG	C2-N2-C7	-2.28	119.84	122.90
3	A	401	TLA	O1-C1-C2	-2.23	115.67	121.62

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	396	NAG	C1
2	A	397	NAG	C1
2	A	398	NAG	C1
2	B	396	NAG	C1
2	B	398	NAG	C1
3	B	399	TLA	C3

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	398	NAG	C8-C7-N2-C2
2	A	398	NAG	O7-C7-N2-C2
3	B	399	TLA	C2-C3-C4-O41
3	B	399	TLA	O3-C3-C4-O4
3	B	399	TLA	O3-C3-C4-O41
3	A	401	TLA	O3-C3-C4-O41
2	B	397	NAG	C8-C7-N2-C2
2	B	397	NAG	O7-C7-N2-C2
3	A	401	TLA	C1-C2-C3-C4
3	A	401	TLA	C1-C2-C3-O3
3	B	399	TLA	O1-C1-C2-O2
2	A	396	NAG	O5-C5-C6-O6
2	A	400	NAG	O5-C5-C6-O6
2	B	396	NAG	O5-C5-C6-O6
3	A	401	TLA	O2-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	396	NAG	C8-C7-N2-C2
2	A	396	NAG	C4-C5-C6-O6
2	A	399	NAG	O5-C5-C6-O6
3	A	401	TLA	O2-C2-C3-O3
2	A	399	NAG	C4-C5-C6-O6
2	B	396	NAG	C4-C5-C6-O6
2	B	396	NAG	O7-C7-N2-C2
3	A	401	TLA	O1-C1-C2-O2
3	A	401	TLA	O3-C3-C4-O4
2	A	400	NAG	C4-C5-C6-O6
3	A	401	TLA	C2-C3-C4-O4
3	B	399	TLA	O2-C2-C3-O3
3	A	401	TLA	O11-C1-C2-C3
3	A	401	TLA	O11-C1-C2-O2
2	A	398	NAG	C4-C5-C6-O6
2	A	398	NAG	O5-C5-C6-O6
3	B	399	TLA	O11-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	398	NAG	2	0
2	A	399	NAG	1	0
2	A	396	NAG	3	0
2	B	396	NAG	1	0
3	A	401	TLA	1	0
2	A	398	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/395 (95%)	0.77	53 (14%) 6 5	52, 78, 149, 215	0
1	B	383/395 (96%)	0.86	52 (13%) 7 6	52, 78, 161, 220	0
All	All	760/790 (96%)	0.81	105 (13%) 6 5	52, 78, 155, 220	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	6.8
1	B	13	TYR	6.1
1	B	53	ASN	6.0
1	B	348	LYS	5.6
1	B	18	PRO	5.3
1	B	3	HIS	5.2
1	B	272	ALA	4.9
1	A	14	VAL	4.8
1	B	107	VAL	4.8
1	B	270	LEU	4.7
1	A	13	TYR	4.7
1	A	348	LYS	4.7
1	B	14	VAL	4.6
1	A	162	SER	4.4
1	A	18	PRO	4.4
1	A	275	LYS	4.4
1	A	3	HIS	4.3
1	B	273	PRO	4.2
1	A	175	ALA	4.1
1	A	167	ARG	4.1
1	B	175	ALA	4.1
1	B	162	SER	4.0
1	A	107	VAL	3.8
1	A	12	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	166	LEU	3.6
1	B	167	ARG	3.6
1	B	77	GLY	3.5
1	A	2	THR	3.5
1	A	268	GLU	3.5
1	A	103	TRP	3.5
1	A	164	TYR	3.4
1	A	105	HIS	3.4
1	A	140	THR	3.4
1	B	164	TYR	3.3
1	A	166	LEU	3.3
1	B	308	GLN	3.3
1	B	4	VAL	3.3
1	B	284	PHE	3.2
1	B	17	GLY	3.2
1	B	275	LYS	3.1
1	B	106	GLN	3.1
1	A	37	ARG	3.1
1	B	105	HIS	3.0
1	A	4	VAL	3.0
1	A	319	HIS	2.9
1	B	317	ASN	2.8
1	A	146	ASP	2.8
1	A	317	ASN	2.8
1	B	349	THR	2.8
1	B	274	PRO	2.7
1	A	267	MET	2.7
1	B	319	HIS	2.7
1	B	51	LYS	2.7
1	B	327	ARG	2.7
1	A	15	GLU	2.7
1	B	55	TYR	2.6
1	A	53	ASN	2.6
1	A	77	GLY	2.6
1	B	276	PRO	2.6
1	B	267	MET	2.5
1	A	383	THR	2.5
1	A	108	SER	2.5
1	A	165	ASN	2.4
1	B	54	LEU	2.4
1	B	103	TRP	2.4
1	A	276	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	2.4
1	B	146	ASP	2.4
1	A	308	GLN	2.4
1	A	163	ARG	2.4
1	B	165	ASN	2.4
1	B	231	PHE	2.4
1	B	254	GLU	2.4
1	A	264	LYS	2.4
1	B	161	PRO	2.4
1	A	323	ARG	2.4
1	A	336	HIS	2.3
1	B	12	GLU	2.3
1	B	16	SER	2.3
1	A	109	ASP	2.3
1	A	102	ARG	2.3
1	B	81	SER	2.3
1	A	231	PHE	2.3
1	B	35	ARG	2.2
1	B	127	ARG	2.2
1	A	81	SER	2.2
1	A	265	TRP	2.2
1	A	384	GLU	2.2
1	B	140	THR	2.2
1	A	55	TYR	2.2
1	A	106	GLN	2.2
1	A	179	ASP	2.2
1	B	320	LYS	2.2
1	A	51	LYS	2.1
1	B	37	ARG	2.1
1	B	153	ARG	2.1
1	A	137	LYS	2.1
1	A	122	PHE	2.1
1	A	220	TYR	2.1
1	B	15	GLU	2.0
1	B	384	GLU	2.0
1	A	174	PRO	2.0
1	A	85	ASN	2.0
1	B	42	ASN	2.0
1	A	127	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	A	397	14/15	0.59	0.19	145,173,192,193	0
2	NAG	A	400	14/15	0.72	0.17	76,187,212,218	0
2	NAG	B	396	14/15	0.80	0.19	120,148,173,182	0
2	NAG	B	398	14/15	0.80	0.18	109,125,179,213	0
2	NAG	A	399	14/15	0.82	0.17	96,118,131,135	0
2	NAG	A	398	14/15	0.85	0.20	94,153,179,181	0
2	NAG	A	396	14/15	0.86	0.18	122,141,157,171	0
2	NAG	B	397	14/15	0.89	0.16	93,126,152,157	0
3	TLA	A	401	10/10	0.89	0.12	60,78,130,133	0
3	TLA	B	399	10/10	0.91	0.11	65,87,94,104	0
4	CA	A	402	1/1	0.94	0.09	114,114,114,114	0
4	CA	B	400	1/1	0.94	0.08	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.