



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 AM UTC

PDB ID : 6FPJ / pdb_00006fpj
Title : Structure of the AMPAR GluA3 N-terminal domain bound to phosphate
Authors : Herguedas, B.; Garcia-Nafria, J.; Greger, I.
Deposited on : 2018-02-09
Resolution : 1.96 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

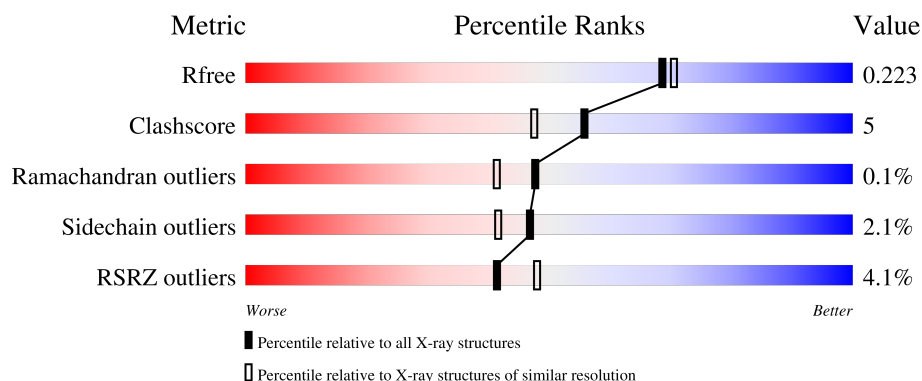
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	390	4% 86% 9% • •
1	B	390	3% 91% 5% • •
1	C	390	5% 86% 7% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10060 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	11	0
			3095	1978	537	561	19			
1	B	379	Total	C	N	O	S	0	9	0
			3118	1987	545	568	18			
1	C	365	Total	C	N	O	S	0	8	0
			3013	1929	515	550	19			

There are 27 discrepancies between the modelled and reference sequences:

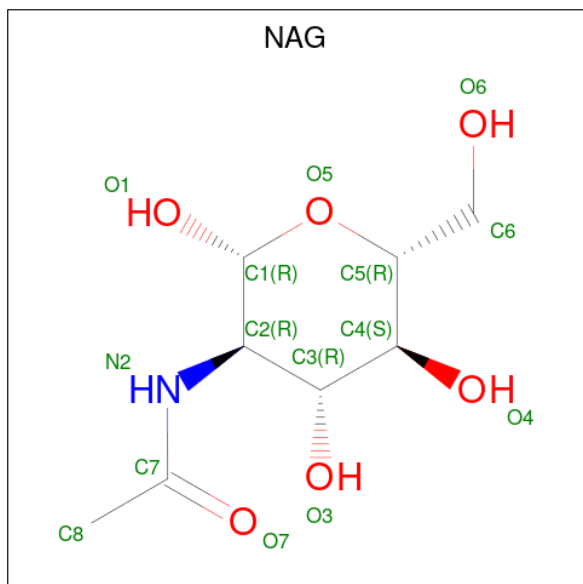
Chain	Residue	Modelled	Actual	Comment	Reference
A	382	GLY	-	expression tag	UNP P19492
A	383	THR	-	expression tag	UNP P19492
A	384	LYS	-	expression tag	UNP P19492
A	385	HIS	-	expression tag	UNP P19492
A	386	HIS	-	expression tag	UNP P19492
A	387	HIS	-	expression tag	UNP P19492
A	388	HIS	-	expression tag	UNP P19492
A	389	HIS	-	expression tag	UNP P19492
A	390	HIS	-	expression tag	UNP P19492
B	382	GLY	-	expression tag	UNP P19492
B	383	THR	-	expression tag	UNP P19492
B	384	LYS	-	expression tag	UNP P19492
B	385	HIS	-	expression tag	UNP P19492
B	386	HIS	-	expression tag	UNP P19492
B	387	HIS	-	expression tag	UNP P19492
B	388	HIS	-	expression tag	UNP P19492
B	389	HIS	-	expression tag	UNP P19492
B	390	HIS	-	expression tag	UNP P19492
C	382	GLY	-	expression tag	UNP P19492
C	383	THR	-	expression tag	UNP P19492
C	384	LYS	-	expression tag	UNP P19492
C	385	HIS	-	expression tag	UNP P19492
C	386	HIS	-	expression tag	UNP P19492

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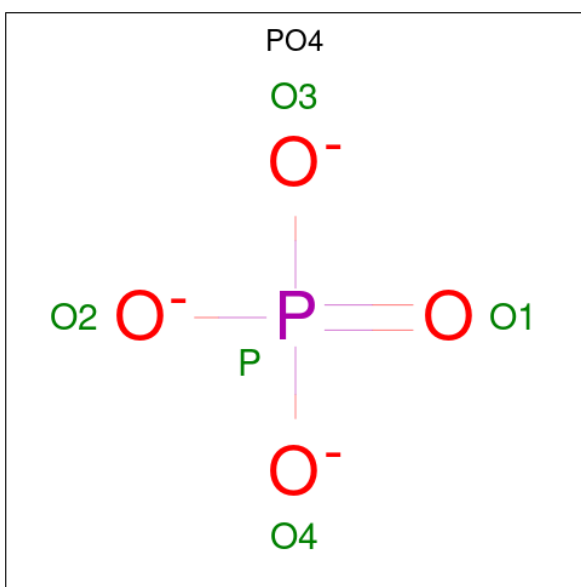
Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP P19492
C	388	HIS	-	expression tag	UNP P19492
C	389	HIS	-	expression tag	UNP P19492
C	390	HIS	-	expression tag	UNP P19492

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



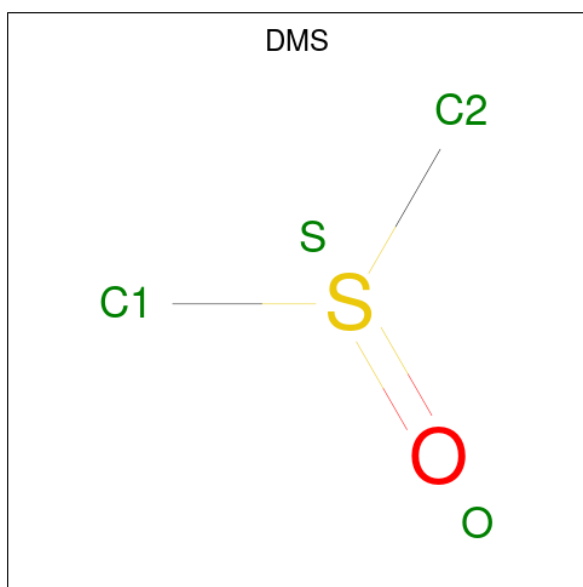
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



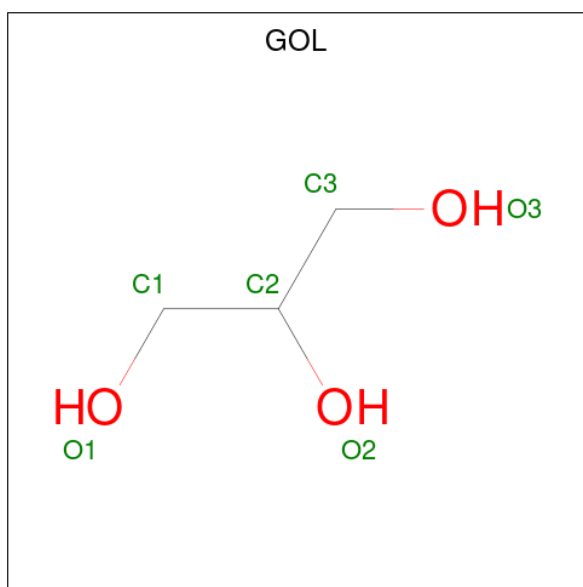
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

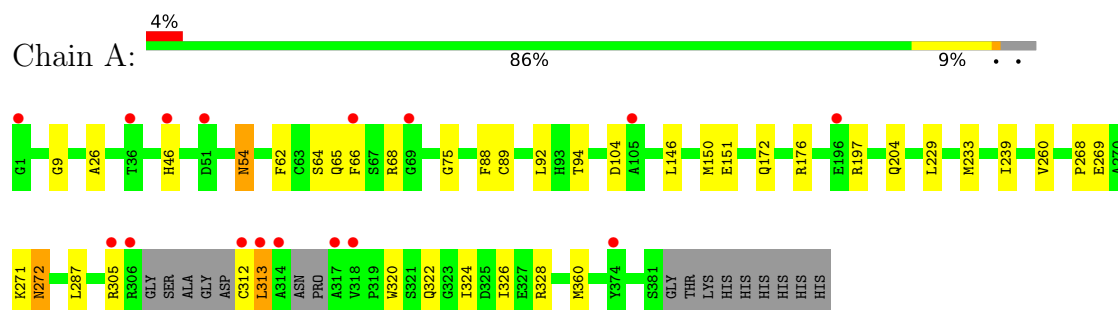
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total	O	0	0
			221	221		
6	B	253	Total	O	0	0
			253	253		
6	C	179	Total	O	0	0
			179	179		

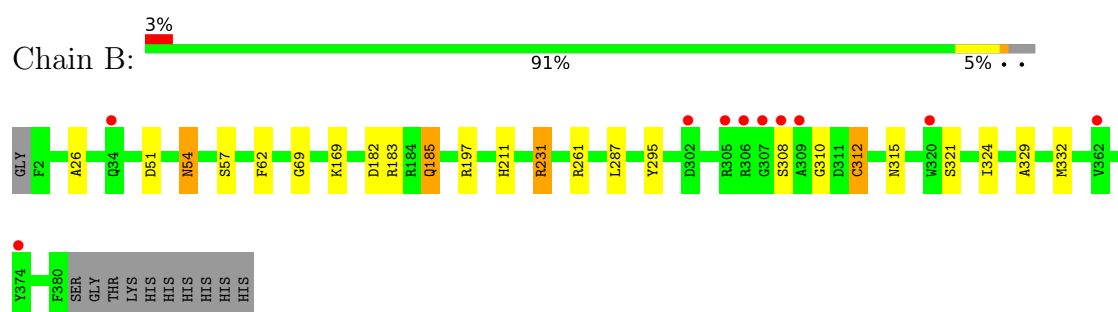
3 Residue-property plots [i](#)

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.

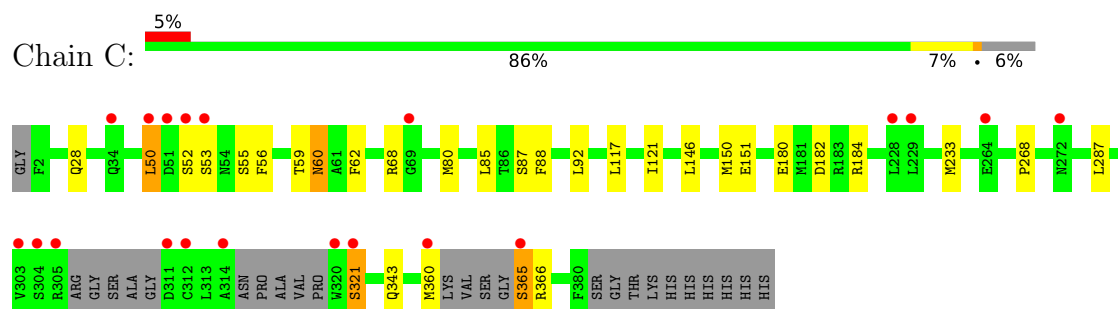
• Molecule 1: Glutamate receptor 3



• Molecule 1: Glutamate receptor 3



• Molecule 1: Glutamate receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.15Å 164.77Å 63.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.00 – 1.96 91.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.8 (91.00-1.96) 98.8 (91.00-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.179 , 0.219 0.188 , 0.223	Depositor DCC
R_{free} test set	4119 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10060	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DMS, 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	1.05	3/3197 (0.1%)	0.97	5/4320 (0.1%)
1	B	1.09	2/3212 (0.1%)	0.98	6/4347 (0.1%)
1	C	0.99	2/3099 (0.1%)	0.96	2/4191 (0.0%)
All	All	1.04	7/9508 (0.1%)	0.97	13/12858 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197[A]	ARG	CA-C	8.29	1.63	1.52
1	A	197[B]	ARG	CA-C	8.29	1.63	1.52
1	B	185[A]	GLN	CA-C	7.92	1.64	1.53
1	B	185[B]	GLN	CA-C	7.92	1.64	1.53
1	A	268	PRO	C-O	5.87	1.30	1.23
1	C	321	SER	N-CA	5.58	1.53	1.46
1	C	268	PRO	C-O	5.37	1.29	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197[A]	ARG	CA-C-O	8.68	129.75	120.55
1	A	197[B]	ARG	CA-C-O	8.68	129.75	120.55
1	C	50	LEU	N-CA-C	6.32	118.78	109.24
1	B	185[A]	GLN	CA-C-O	6.27	128.92	121.08
1	B	185[B]	GLN	CA-C-O	6.27	128.92	121.08
1	B	312	CYS	CB-CA-C	-5.69	101.34	110.79
1	B	185[A]	GLN	N-CA-C	5.51	119.17	111.90
1	B	185[B]	GLN	N-CA-C	5.51	119.17	111.90
1	A	197[A]	ARG	N-CA-C	5.44	117.21	111.28
1	A	197[B]	ARG	N-CA-C	5.44	117.21	111.28
1	C	52	SER	N-CA-C	5.30	117.13	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	GLY	N-CA-C	5.26	119.28	111.76
1	A	75	GLY	N-CA-C	5.18	117.58	110.69

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	3095	0	3040	43	0
1	B	3118	0	3034	27	0
1	C	3013	0	2916	27	0
2	A	42	0	39	0	0
2	B	42	0	39	0	0
2	C	28	0	26	2	0
3	A	5	0	0	0	0
3	B	25	0	0	1	0
3	C	5	0	0	0	0
4	A	12	0	18	4	0
4	B	8	0	12	3	0
4	C	8	0	12	1	0
5	B	6	0	8	0	0
6	A	221	0	0	4	0
6	B	253	0	0	5	0
6	C	179	0	0	1	0
All	All	10060	0	9144	87	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 5.

All (87) 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:231:ARG:HH21	1:B:231:ARG:HG2	1.21	1.02
1:B:295:TYR:CE1	1:B:332[A]:MET:HE1	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:CD1	1:B:332[A]:MET:HE1	2.09	0.88
1:B:324:ILE:HG22	6:B:501:HOH:O	1.73	0.87
1:B:295:TYR:CZ	1:B:332[A]:MET:HE1	2.16	0.81
1:A:92:LEU:HD11	1:C:56:PHE:HZ	1.46	0.80
1:A:269:GLU:HA	1:A:272:ASN:HD21	1.47	0.79
1:A:146:LEU:HD21	1:C:146:LEU:HD21	1.69	0.74
1:A:229:LEU:HD22	1:A:360:MET:HE1	1.70	0.74
1:A:269:GLU:HA	1:A:272:ASN:ND2	2.04	0.72
1:C:50:LEU:C	1:C:50:LEU:HD12	2.18	0.67
1:B:295:TYR:CD1	1:B:332[A]:MET:CE	2.76	0.67
1:A:46:HIS:HB3	1:A:68:ARG:HH11	1.58	0.67
1:B:332[A]:MET:HE3	6:B:568:HOH:O	1.93	0.67
1:B:332[B]:MET:SD	3:B:407:PO4:O4	2.53	0.66
1:A:172:GLN:HG3	1:A:176:ARG:NH2	2.11	0.66
1:B:231:ARG:HG2	1:B:231:ARG:NH2	1.94	0.65
1:A:92:LEU:HD11	1:C:56:PHE:CZ	2.30	0.65
1:A:146:LEU:CD2	1:C:146:LEU:HD21	2.29	0.62
1:A:66:PHE:CE1	1:A:92:LEU:HD13	2.34	0.62
1:A:287:LEU:HD23	4:A:406:DMS:S	2.40	0.61
1:B:287:LEU:HD12	4:B:410:DMS:S	2.41	0.61
1:C:59:THR:HG22	1:C:88:PHE:HE2	1.67	0.60
1:C:343:GLN:HE22	2:C:402:NAG:H83	1.66	0.60
1:A:146:LEU:HD21	1:C:146:LEU:CD2	2.32	0.59
1:B:183:ARG:O	1:B:185[B]:GLN:NE2	2.34	0.59
1:B:332[A]:MET:CE	6:B:568:HOH:O	2.50	0.59
1:C:233:MET:HE2	1:C:360:MET:SD	2.42	0.59
1:A:233[B]:MET:HE2	1:A:360:MET:SD	2.45	0.56
1:B:329:ALA:HA	1:B:332[A]:MET:HE2	1.87	0.56
1:A:272:ASN:HD22	1:A:272:ASN:H	1.51	0.55
1:A:229:LEU:HD13	1:A:360:MET:HE1	1.90	0.54
1:A:229:LEU:CD2	1:A:360:MET:HE1	2.37	0.54
1:B:295:TYR:CG	1:B:332[A]:MET:HE1	2.42	0.53
1:B:295:TYR:CG	1:B:332[A]:MET:CE	2.91	0.53
1:A:233[A]:MET:SD	1:A:239:ILE:HD12	2.50	0.52
1:B:332[B]:MET:HG2	6:B:600:HOH:O	2.09	0.52
1:A:260:VAL:O	1:A:271:LYS:HG2	2.09	0.51
1:A:313:LEU:H	1:C:56:PHE:HE2	1.60	0.50
1:A:172:GLN:CG	1:A:176:ARG:NH2	2.75	0.49
1:B:54:ASN:ND2	1:B:57:SER:OG	2.45	0.49
1:B:321:SER:O	6:B:501:HOH:O	2.19	0.49
1:A:229:LEU:HD22	1:A:360:MET:CE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:SER:O	1:A:68:ARG:HG3	2.13	0.49
1:A:328[B]:ARG:CZ	1:A:328[B]:ARG:HB3	2.36	0.48
1:C:55:SER:O	1:C:59:THR:HG23	2.14	0.48
1:B:295:TYR:CE2	1:B:332[A]:MET:HE1	2.48	0.47
1:C:117:LEU:HG	1:C:121:ILE:HD11	1.96	0.47
1:A:104:ASP:HB2	4:A:407:DMS:H11	1.95	0.47
1:A:150:MET:HG3	1:C:150[A]:MET:SD	2.53	0.47
1:A:322:GLN:HG3	6:A:677:HOH:O	2.13	0.47
1:C:343:GLN:HE22	2:C:402:NAG:C8	2.27	0.47
1:A:62:PHE:CZ	1:A:92:LEU:HD12	2.51	0.46
1:C:287:LEU:HD23	4:C:405:DMS:S	2.56	0.46
1:A:62:PHE:HZ	1:A:92:LEU:HD12	1.81	0.46
1:A:320:TRP:CH2	1:A:326:ILE:HD12	2.50	0.46
1:B:182:ASP:CG	1:B:211:HIS:HE2	2.24	0.46
1:C:28:GLN:NE2	6:C:501:HOH:O	2.29	0.46
1:C:360:MET:HG2	1:C:365:SER:HA	1.98	0.46
1:C:62:PHE:CZ	1:C:92:LEU:HD12	2.51	0.46
1:B:26:ALA:O	4:B:410:DMS:H23	2.16	0.45
1:A:233[A]:MET:HE2	1:A:360:MET:HB3	1.98	0.45
1:C:53:SER:HA	1:C:80[B]:MET:HG2	1.98	0.45
1:B:62:PHE:CD1	1:B:62:PHE:C	2.95	0.45
1:A:104:ASP:H	4:A:407:DMS:H21	1.82	0.45
1:A:324:ILE:HG13	6:A:611:HOH:O	2.17	0.44
1:C:50:LEU:C	1:C:50:LEU:CD1	2.88	0.43
1:A:54:ASN:HB2	1:C:87[B]:SER:OG	2.18	0.43
1:A:233[A]:MET:CG	1:A:360:MET:HE3	2.47	0.43
1:C:62:PHE:CE2	1:C:92:LEU:HD12	2.53	0.43
1:A:233[A]:MET:SD	1:A:360:MET:HE3	2.58	0.43
1:A:204:GLN:NE2	6:A:514:HOH:O	2.51	0.43
1:B:197[B]:ARG:HB2	1:B:197[B]:ARG:NH1	2.34	0.43
1:A:26:ALA:O	4:A:406:DMS:H23	2.19	0.42
1:A:89:CYS:HB3	1:A:94:THR:O	2.19	0.42
1:A:146:LEU:CD2	1:C:146:LEU:CD2	2.96	0.42
1:A:9:GLY:HA3	1:A:65:GLN:OE1	2.20	0.41
1:A:66:PHE:CD1	1:A:92:LEU:HD13	2.55	0.41
1:A:88:PHE:HD1	1:C:56:PHE:CE1	2.39	0.41
1:B:287:LEU:CD1	4:B:410:DMS:S	3.08	0.41
1:B:295:TYR:CD2	1:B:332[A]:MET:HE1	2.57	0.40
1:C:56:PHE:O	1:C:60:ASN:HB2	2.22	0.40
1:C:180:GLU:OE2	1:C:184:ARG:NH2	2.54	0.40
1:A:172:GLN:HG3	1:A:176:ARG:CZ	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:524:HOH:O	1:C:151:GLU:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/390 (97%)	369 (97%)	9 (2%)	1 (0%)	36	28
1	B	386/390 (99%)	379 (98%)	7 (2%)	0	100	100
1	C	365/390 (94%)	359 (98%)	6 (2%)	0	100	100
All	All	1130/1170 (97%)	1107 (98%)	22 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	ARG

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	336/341 (98%)	331 (98%)	5 (2%)	57	54
1	B	336/341 (98%)	326 (97%)	10 (3%)	36	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	324/341 (95%)	317 (98%)	7 (2%)	45	40
All	All	996/1023 (97%)	974 (98%)	22 (2%)	47	40

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	151	GLU
1	A	272	ASN
1	A	312	CYS
1	A	313	LEU
1	B	51	ASP
1	B	54	ASN
1	B	169	LYS
1	B	231	ARG
1	B	261[A]	ARG
1	B	261[B]	ARG
1	B	308[A]	SER
1	B	308[B]	SER
1	B	312	CYS
1	B	315	ASN
1	C	60	ASN
1	C	68	ARG
1	C	85	LEU
1	C	182	ASP
1	C	321	SER
1	C	365	SER
1	C	366	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	147	GLN
1	A	156	ASN
1	A	204	GLN
1	A	243	GLN
1	A	272	ASN
1	A	336	GLN
1	A	341	ASN
1	B	155	GLN

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Mol	Chain	Res	Type
1	B	172	GLN
1	B	272	ASN
1	B	336	GLN
1	C	46	HIS
1	C	49	HIS
1	C	65	GLN
1	C	83	ASN
1	C	108	GLN
1	C	156	ASN
1	C	336	GLN
1	C	341	ASN

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 ⓘ

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	402	1	14,14,15	0.44	0	17,19,21	1.11	2 (11%)
3	PO4	B	406	-	4,4,4	0.89	0	6,6,6	0.83	0
3	PO4	B	407	-	4,4,4	1.10	0	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	402	1	14,14,15	0.50	0	17,19,21	1.69	4 (23%)
3	PO4	B	408	-	4,4,4	0.81	0	6,6,6	0.51	0
2	NAG	B	402	1	14,14,15	0.70	0	17,19,21	1.06	2 (11%)
4	DMS	A	407	-	3,3,3	0.55	0	3,3,3	0.59	0
4	DMS	B	409	-	3,3,3	0.54	0	3,3,3	0.34	0
2	NAG	C	401	1	14,14,15	0.45	0	17,19,21	0.88	0
3	PO4	B	405	-	4,4,4	0.87	0	6,6,6	0.64	0
2	NAG	B	403	1	14,14,15	0.39	0	17,19,21	1.03	1 (5%)
2	NAG	B	401	1	14,14,15	0.59	0	17,19,21	1.05	2 (11%)
2	NAG	A	401	1	14,14,15	0.44	0	17,19,21	0.96	2 (11%)
3	PO4	A	404	-	4,4,4	0.92	0	6,6,6	1.34	0
4	DMS	B	410	-	3,3,3	0.46	0	3,3,3	0.99	0
5	GOL	B	411	-	5,5,5	0.41	0	5,5,5	1.05	0
3	PO4	B	404	-	4,4,4	1.19	0	6,6,6	0.60	0
4	DMS	C	405	-	3,3,3	0.69	0	3,3,3	0.46	0
4	DMS	A	405	-	3,3,3	0.53	0	3,3,3	0.21	0
4	DMS	A	406	-	3,3,3	0.52	0	3,3,3	0.92	0
3	PO4	C	403	-	4,4,4	0.91	0	6,6,6	0.42	0
4	DMS	C	404	-	3,3,3	0.45	0	3,3,3	0.61	0
2	NAG	A	403	1	14,14,15	0.53	0	17,19,21	1.39	2 (11%)

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	402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	402	1	-	3/6/23/26	0/1/1/1
2	NAG	B	403	1	-	2/6/23/26	0/1/1/1
2	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	GOL	B	411	-	-	2/4/4/4	-
2	NAG	A	403	1	-	0/6/23/26	0/1/1/1
2	NAG	C	401	1	-	1/6/23/26	0/1/1/1
2	NAG	B	402	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	NAG	C1-C2-N2	-4.06	104.04	110.43
2	A	403	NAG	C1-C2-N2	-3.77	104.50	110.43
2	A	403	NAG	C1-O5-C5	3.17	116.44	112.19
2	C	402	NAG	C2-N2-C7	3.09	127.04	122.90
2	A	402	NAG	C1-O5-C5	2.90	116.07	112.19
2	B	402	NAG	O5-C5-C6	2.78	113.07	107.66
2	B	401	NAG	O5-C1-C2	-2.66	107.18	111.29
2	C	402	NAG	C1-O5-C5	2.64	115.73	112.19
2	C	402	NAG	C8-C7-N2	2.44	120.16	116.12
2	B	401	NAG	C4-C3-C2	-2.27	107.69	111.02
2	B	402	NAG	C4-C3-C2	2.21	114.26	111.02
2	B	403	NAG	C1-O5-C5	2.20	115.13	112.19
2	A	402	NAG	C6-C5-C4	-2.18	107.68	113.02
2	A	401	NAG	O5-C5-C6	2.08	111.71	107.66
2	A	401	NAG	O5-C5-C4	-2.06	105.82	110.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	NAG	C4-C5-C6-O6
2	B	402	NAG	O5-C5-C6-O6
2	B	403	NAG	C4-C5-C6-O6
2	C	402	NAG	C8-C7-N2-C2
2	C	402	NAG	O7-C7-N2-C2
2	B	403	NAG	O5-C5-C6-O6
5	B	411	GOL	C1-C2-C3-O3
5	B	411	GOL	O2-C2-C3-O3
2	C	401	NAG	O5-C5-C6-O6
2	B	402	NAG	C1-C2-N2-C7
2	C	402	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	407	PO4	1	0
2	C	402	NAG	2	0
4	A	407	DMS	2	0
4	B	410	DMS	3	0
4	C	405	DMS	1	0
4	A	406	DMS	2	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	374/390 (95%)	0.12	16 (4%)	40 46	9, 25, 47, 86	11 (2%)
1	B	379/390 (97%)	0.09	10 (2%)	57 64	11, 24, 46, 56	9 (2%)
1	C	365/390 (93%)	0.31	20 (5%)	30 36	12, 29, 53, 76	8 (2%)
All	All	1118/1170 (95%)	0.17	46 (4%)	41 48	9, 26, 48, 86	28 (2%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	TRP	6.6
1	A	314	ALA	6.5
1	A	318	VAL	4.6
1	B	308[A]	SER	4.1
1	A	306	ARG	4.0
1	A	51	ASP	3.9
1	C	312	CYS	3.9
1	A	374	TYR	3.8
1	A	69	GLY	3.7
1	C	321	SER	3.6
1	C	303	VAL	3.4
1	B	374	TYR	3.3
1	C	314	ALA	3.3
1	A	66	PHE	3.2
1	A	312	CYS	3.1
1	A	317	ALA	3.1
1	A	313	LEU	3.0
1	A	305	ARG	3.0
1	C	365	SER	2.9
1	C	304	SER	2.9
1	C	50	LEU	2.9
1	A	105	ALA	2.8
1	C	51[A]	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	53	SER	2.8
1	C	311	ASP	2.7
1	C	360	MET	2.6
1	B	305	ARG	2.6
1	C	272	ASN	2.6
1	B	306	ARG	2.5
1	C	69	GLY	2.5
1	C	229	LEU	2.5
1	C	264	GLU	2.5
1	C	305	ARG	2.4
1	B	309	ALA	2.4
1	C	34	GLN	2.3
1	A	36	THR	2.3
1	B	362	VAL	2.3
1	A	1	GLY	2.2
1	B	302	ASP	2.2
1	B	307	GLY	2.2
1	B	320	TRP	2.1
1	C	228	LEU	2.1
1	B	34	GLN	2.1
1	A	196	GLU	2.1
1	A	46	HIS	2.1
1	C	52	SER	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	401	14/15	0.62	0.14	56,65,69,73	0
2	NAG	B	402	14/15	0.71	0.16	45,53,59,59	0
3	PO4	B	408	5/5	0.71	0.12	76,81,82,84	0
2	NAG	B	403	14/15	0.73	0.15	62,69,75,81	0
2	NAG	C	402	14/15	0.81	0.12	35,41,45,46	0
4	DMS	A	407	4/4	0.82	0.23	44,54,58,58	0
2	NAG	C	401	14/15	0.83	0.10	39,43,51,54	0
4	DMS	C	405	4/4	0.83	0.19	65,68,69,73	0
4	DMS	A	406	4/4	0.85	0.20	60,64,64,70	0
5	GOL	B	411	6/6	0.85	0.15	44,45,46,47	0
2	NAG	A	403	14/15	0.86	0.11	29,36,39,42	0
4	DMS	B	410	4/4	0.86	0.17	49,49,52,54	0
3	PO4	C	403	5/5	0.87	0.10	59,59,66,67	0
3	PO4	B	407	5/5	0.89	0.11	53,60,64,65	0
3	PO4	B	406	5/5	0.89	0.11	46,49,58,64	0
2	NAG	A	402	14/15	0.90	0.08	27,31,34,37	0
3	PO4	A	404	5/5	0.91	0.15	42,47,50,50	0
3	PO4	B	405	5/5	0.93	0.11	45,45,50,51	0
2	NAG	B	401	14/15	0.95	0.06	18,21,24,28	0
4	DMS	C	404	4/4	0.98	0.11	23,26,27,28	0
4	DMS	B	409	4/4	0.98	0.07	19,20,21,21	0
3	PO4	B	404	5/5	0.98	0.06	30,30,32,32	5
4	DMS	A	405	4/4	0.99	0.07	20,20,21,24	0

6.5 Other polymers

There are no such residues in this entry.