



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 3PD8 / pdb_00003pd8
Title : X-ray structure of the ligand-binding core of GluA2 in complex with (S)-7-HPCA at 2.5 Å resolution
Authors : Frydenvang, K.; Kastrup, J.S.
Deposited on : 2010-10-22
Resolution : 2.48 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

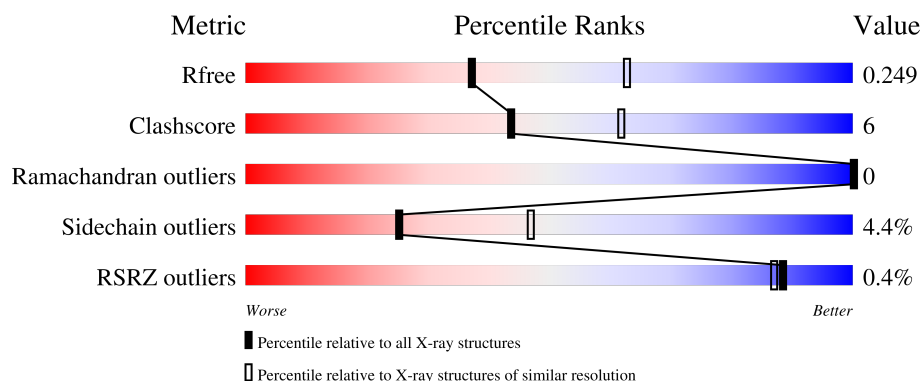
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

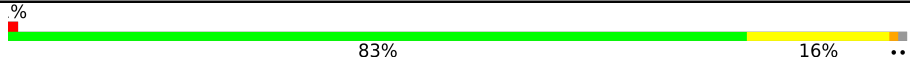
The reported resolution of this entry is 2.48 Å.

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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	261	 83% 16% 1% 0%
1	B	261	 82% 16% 2% 0%
1	C	261	 84% 13% 3% 0%

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
5	ACY	A	263	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6551 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2022	1288	337	383	14			
1	B	261	Total	C	N	O	S	0	0	0
			2035	1295	340	386	14			
1	C	260	Total	C	N	O	S	0	1	0
			2039	1299	340	386	14			

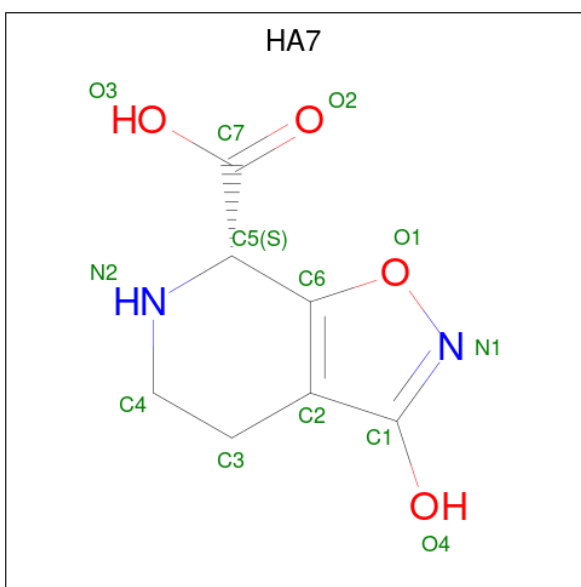
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P19491
A	115	GLY	-	linker	UNP P19491
A	116	THR	-	linker	UNP P19491
B	-1	ALA	-	expression tag	UNP P19491
B	115	GLY	-	linker	UNP P19491
B	116	THR	-	linker	UNP P19491
C	-1	ALA	-	expression tag	UNP P19491
C	115	GLY	-	linker	UNP P19491
C	116	THR	-	linker	UNP P19491

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

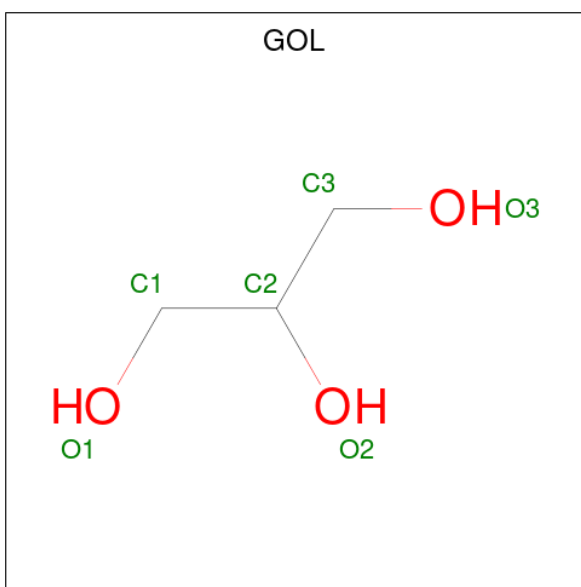
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (7S)-3-hydroxy-4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridine-7-carboxylic acid (CCD ID: HA7) (formula: C₇H₈N₂O₄).



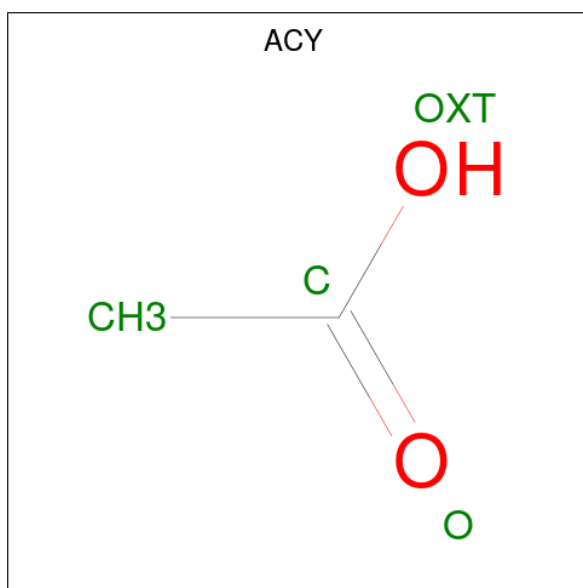
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	7	2	4		
3	B	1	Total	C	N	O	0	0
			13	7	2	4		
3	C	1	Total	C	N	O	0	0
			13	7	2	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



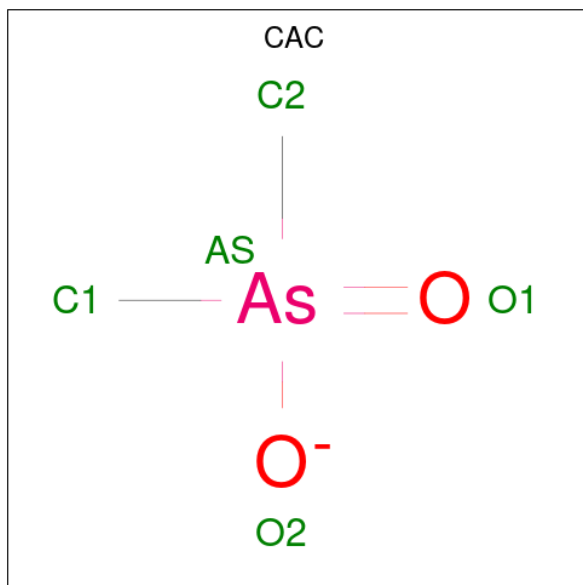
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 6 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).

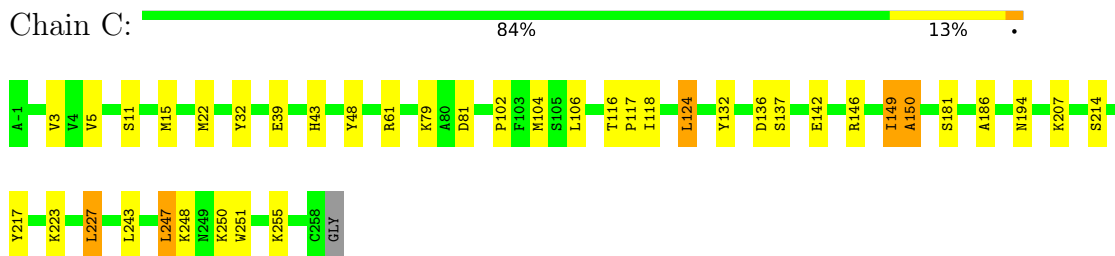
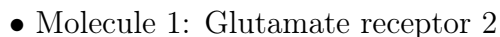
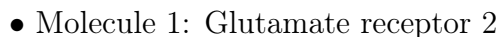


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total 102	O 102	0	0
7	B	120	Total 120	O 120	0	0
7	C	174	Total 174	O 174	0	0

- Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.62Å 164.00Å 47.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 2.48 29.32 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.32-2.48) 97.8 (29.32-2.48)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.175 , 0.261 0.164 , 0.249	Depositor DCC
R_{free} test set	1641 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% 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: ZN, ACY, HA7, CAC, 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	0.36	0/2058	0.78	0/2767
1	B	0.40	0/2071	0.76	0/2785
1	C	0.41	0/2075	0.75	1/2791 (0.0%)
All	All	0.39	0/6204	0.76	1/8343 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	ALA	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

There are no planarity outliers.

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	2022	0	2056	26	0
1	B	2035	0	2067	25	0
1	C	2039	0	2074	25	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	13	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	6	1	0
3	C	13	0	6	0	0
4	A	6	0	8	0	0
5	A	4	0	3	2	0
6	C	5	0	0	0	0
7	A	102	0	0	1	0
7	B	120	0	0	1	0
7	C	174	0	0	1	0
All	All	6551	0	6226	75	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 6.

All (75) 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:A:61:ARG:HD3	1:A:66:LYS:HA	1.63	0.81
1:A:19:ASN:HD22	1:A:22:MET:HE3	1.48	0.78
1:C:11:SER:OG	1:C:15:MET:HE3	1.91	0.69
1:B:133:GLY:HA3	1:B:166:VAL:O	1.99	0.63
1:B:40:ILE:HD12	1:B:219:ILE:HD12	1.80	0.63
1:C:104:MET:HE2	1:C:248:LYS:HD3	1.79	0.63
1:C:251:TRP:CZ3	1:C:255:LYS:HE3	2.34	0.62
1:A:134:THR:HG22	1:A:188:LEU:HB2	1.80	0.62
1:C:102:PRO:HA	1:C:217:TYR:O	2.01	0.61
1:B:177:ARG:HA	1:B:180:LYS:HE2	1.85	0.59
1:B:61:ARG:NH2	1:B:68:TRP:HE1	2.03	0.56
1:C:136:ASP:O	1:C:137:SER:HB2	2.06	0.56
1:C:149:ILE:HD12	1:C:150:ALA:N	2.21	0.55
1:B:102:PRO:HA	1:B:217:TYR:O	2.07	0.54
1:A:106:LEU:C	1:A:106:LEU:HD22	2.33	0.54
1:B:237:LYS:O	1:B:241:GLN:HG2	2.08	0.54
1:A:5:VAL:HG22	1:A:82:ILE:CG2	2.38	0.53
1:B:147:SER:OG	1:B:149:ILE:HG23	2.07	0.53
1:A:43:HIS:HD1	5:A:263:ACY:C	2.21	0.53
1:A:106:LEU:HD23	1:A:190:GLU:HB3	1.90	0.53
1:A:201:LYS:HE2	1:A:257:GLU:HB2	1.91	0.52
1:A:102:PRO:HA	1:A:217:TYR:O	2.09	0.51
1:A:201:LYS:HG3	1:A:257:GLU:HG3	1.92	0.51
1:B:149:ILE:HD12	1:B:150:ALA:N	2.26	0.51
1:A:177:ARG:HA	1:A:180:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:O	1:C:146:ARG:HG2	2.12	0.49
1:C:61:ARG:HH11	1:C:61:ARG:HG3	1.77	0.48
1:A:237:LYS:O	1:A:241:GLN:HG3	2.14	0.48
1:C:11:SER:CB	1:C:15:MET:HE3	2.43	0.48
1:B:177:ARG:HA	1:B:180:LYS:HG2	1.97	0.47
1:B:206:MET:HE2	1:B:208:VAL:CG1	2.45	0.47
1:C:61:ARG:HG3	1:C:61:ARG:NH1	2.30	0.47
1:A:43:HIS:ND1	5:A:263:ACY:OXT	2.42	0.47
1:A:36:LEU:HD21	1:A:219:ILE:HD11	1.96	0.47
1:A:131:ALA:O	1:A:185:TYR:HA	2.15	0.46
1:B:193:MET:HG2	7:B:302:HOH:O	2.15	0.46
1:C:181:SER:HB2	7:C:434:HOH:O	2.16	0.45
1:A:88:THR:OG1	3:A:261:HA7:H5	2.15	0.45
1:A:101:LYS:HE3	1:B:100:SER:O	2.17	0.45
1:C:118:ILE:HD12	1:C:124:LEU:HD13	1.98	0.45
1:B:156:TRP:NE1	1:B:160:ARG:HD3	2.32	0.44
1:B:19:ASN:OD1	1:B:19:ASN:N	2.49	0.44
1:A:148:LYS:HA	1:A:153:ASP:HB2	2.00	0.44
1:B:5:VAL:HG22	1:B:82:ILE:CG2	2.48	0.44
1:A:148:LYS:HD2	1:A:148:LYS:H	1.83	0.44
1:B:132:TYR:HA	1:B:186:ALA:O	2.18	0.44
1:C:5:VAL:HG23	1:C:48:TYR:HB2	2.00	0.44
1:B:58:TYR:CZ	3:B:262:HA7:H4	2.52	0.44
1:C:39:GLU:O	1:C:43:HIS:HD2	2.01	0.43
1:A:239:ASN:HA	1:A:244:LEU:HG	2.00	0.43
1:B:163:GLU:HA	1:B:164:PRO:C	2.44	0.43
1:B:40:ILE:CD1	1:B:219:ILE:HD12	2.47	0.42
1:B:120:SER:O	1:B:123:ASP:HB2	2.18	0.42
1:C:250:LYS:HE2	1:C:251:TRP:CE2	2.55	0.42
1:C:223:LYS:HA	1:C:223:LYS:HD3	1.86	0.42
1:B:32:TYR:CZ	1:B:104:MET:HE3	2.54	0.42
1:C:3:VAL:HG13	1:C:81:ASP:HB2	2.01	0.42
1:C:243:LEU:C	1:C:243:LEU:HD13	2.45	0.42
1:A:15:MET:HG2	7:A:340:HOH:O	2.19	0.42
1:C:227:LEU:HD12	1:C:227:LEU:HA	1.83	0.42
1:B:171:THR:O	1:B:175:VAL:HG23	2.20	0.42
1:B:239:ASN:HB2	1:B:244:LEU:HD12	2.03	0.41
1:A:177:ARG:HG2	1:A:185:TYR:CD2	2.56	0.41
1:B:61:ARG:HH21	1:B:68:TRP:HE1	1.67	0.41
1:A:19:ASN:HB2	1:A:22:MET:HE2	2.03	0.41
1:C:32:TYR:CE2	1:C:247:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ASN:ND2	1:C:207:LYS:HG3	2.36	0.41
1:A:163:GLU:HA	1:A:164:PRO:C	2.45	0.41
1:C:116:THR:HA	1:C:117:PRO:HD2	1.92	0.41
1:A:32:TYR:CD1	1:A:32:TYR:C	2.98	0.41
1:A:116:THR:HA	1:A:117:PRO:HD2	1.94	0.40
1:B:18:LYS:HG3	1:B:19:ASN:N	2.36	0.40
1:C:22:MET:HE3	1:C:22:MET:HB2	1.94	0.40
1:C:132:TYR:HA	1:C:186:ALA:O	2.21	0.40
1:C:149:ILE:HD12	1:C:149:ILE:C	2.47	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	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
1	B	259/261 (99%)	253 (98%)	6 (2%)	0	100	100
1	C	259/261 (99%)	252 (97%)	7 (3%)	0	100	100
All	All	775/783 (99%)	754 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	217/218 (100%)	207 (95%)	10 (5%)	24	45
1	B	218/218 (100%)	206 (94%)	12 (6%)	19	37
1	C	219/218 (100%)	212 (97%)	7 (3%)	34	58
All	All	654/654 (100%)	625 (96%)	29 (4%)	25	47

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	A	106	LEU
1	A	124	LEU
1	A	148	LYS
1	A	149	ILE
1	A	160	ARG
1	A	223	LYS
1	A	225	SER
1	A	243	LEU
1	A	247	LEU
1	B	40	ILE
1	B	42	LYS
1	B	106	LEU
1	B	124	LEU
1	B	128	THR
1	B	129	GLU
1	B	149	ILE
1	B	193	MET
1	B	212	LEU
1	B	219	ILE
1	B	243	LEU
1	B	247	LEU
1	C	79	LYS
1	C	106	LEU
1	C	124	LEU
1	C	149	ILE
1	C	214	SER
1	C	227	LEU
1	C	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	C	19	ASN
1	C	194	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 ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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
4	GOL	A	262	-	5,5,5	0.33	0	5,5,5	0.23	0
3	HA7	B	262	-	12,14,14	2.05	5 (41%)	11,20,20	1.54	2 (18%)
3	HA7	A	261	-	12,14,14	2.16	5 (41%)	11,20,20	1.71	3 (27%)
3	HA7	C	262	-	12,14,14	2.33	5 (41%)	11,20,20	1.81	3 (27%)
5	ACY	A	263	-	3,3,3	0.83	0	3,3,3	0.78	0
6	CAC	C	263	2	2,4,4	2.98	2 (100%)	4,6,6	1.64	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
3	HA7	B	262	-	-	1/3/14/14	0/2/2/2
3	HA7	C	262	-	-	1/3/14/14	0/2/2/2
4	GOL	A	262	-	-	0/4/4/4	-
3	HA7	A	261	-	-	1/3/14/14	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	262	HA7	C2-C6	4.33	1.39	1.34
3	A	261	HA7	C2-C6	4.07	1.39	1.34
3	B	262	HA7	C2-C6	3.97	1.39	1.34
3	C	262	HA7	O4-C1	-3.48	1.23	1.33
3	A	261	HA7	O4-C1	-3.46	1.23	1.33
3	B	262	HA7	O4-C1	-3.41	1.23	1.33
3	A	261	HA7	C2-C1	-3.11	1.38	1.42
3	C	262	HA7	O1-C6	3.06	1.38	1.34
6	C	263	CAC	AS-C1	3.01	1.97	1.90
3	C	262	HA7	C1-N1	2.98	1.33	1.31
6	C	263	CAC	AS-C2	2.96	1.97	1.90
3	C	262	HA7	C2-C1	-2.92	1.38	1.42
3	B	262	HA7	C2-C1	-2.60	1.39	1.42
3	A	261	HA7	C1-N1	2.47	1.33	1.31
3	A	261	HA7	O1-C6	2.43	1.37	1.34
3	B	262	HA7	O1-C6	2.31	1.37	1.34
3	B	262	HA7	C1-N1	2.12	1.33	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	262	HA7	C3-C2-C6	3.70	124.73	121.73
3	A	261	HA7	C3-C2-C6	3.58	124.63	121.73
3	B	262	HA7	C3-C2-C6	3.41	124.49	121.73
3	C	262	HA7	C6-O1-N1	-2.99	106.99	109.45
3	B	262	HA7	O1-C6-C2	-2.94	107.33	110.15
3	A	261	HA7	O1-C6-C2	-2.87	107.40	110.15
3	C	262	HA7	O1-C6-C2	-2.34	107.91	110.15
3	A	261	HA7	C6-O1-N1	-2.15	107.69	109.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	262	HA7	N2-C5-C7-O2
3	A	261	HA7	N2-C5-C7-O2
3	B	262	HA7	N2-C5-C7-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	262	HA7	1	0
3	A	261	HA7	1	0
5	A	263	ACY	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 [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	259/261 (99%)	-0.48	2 (0%) 82 80	14, 33, 71, 100	0
1	B	261/261 (100%)	-0.59	1 (0%) 88 87	13, 29, 63, 98	0
1	C	260/261 (99%)	-0.72	0 100 100	9, 24, 56, 127	1 (0%)
All	All	780/783 (99%)	-0.60	3 (0%) 88 87	9, 28, 65, 127	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	2.9
1	B	-1	ALA	2.9
1	A	147	SER	2.2

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(Å ²)	Q<0.9
5	ACY	A	263	4/4	0.86	0.12	32,44,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	262	6/6	0.93	0.11	42,60,69,82	0
3	HA7	C	262	13/13	0.96	0.07	15,22,40,48	0
3	HA7	A	261	13/13	0.98	0.05	15,25,39,45	0
3	HA7	B	262	13/13	0.98	0.05	10,22,38,41	0
2	ZN	A	260	1/1	0.98	0.04	71,71,71,71	0
2	ZN	B	261	1/1	0.98	0.03	45,45,45,45	0
2	ZN	C	261	1/1	0.98	0.03	27,27,27,27	0
6	CAC	C	263	5/5	0.98	0.08	6,45,55,55	0
2	ZN	C	260	1/1	0.99	0.03	29,29,29,29	0
2	ZN	B	260	1/1	0.99	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.