



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:25 AM UTC

PDB ID : 1M5E / pdb_00001m5e
Title : X-RAY STRUCTURE OF THE GLUR2 LIGAND BINDING CORE (S1S2J)
IN COMPLEX WITH ACPA AT 1.46 Å RESOLUTION
Authors : Hogner, A.; Kastrup, J.S.; Jin, R.; Liljefors, T.; Mayer, M.L.; Egebjerg, J.;
Larsen, I.K.; Gouaux, E.
Deposited on : 2002-07-09
Resolution : 1.46 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

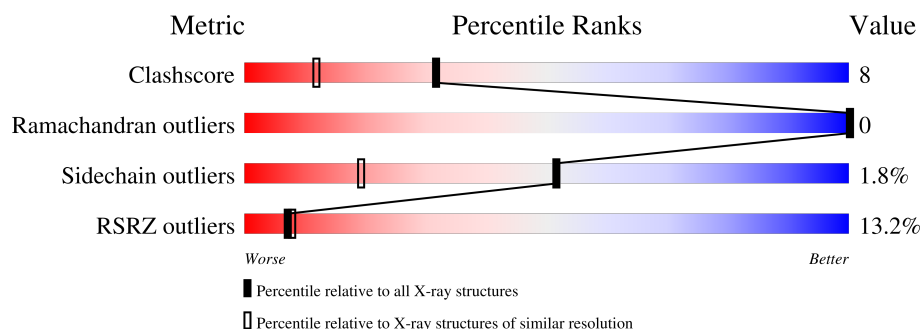
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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))
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	263	13% 81% 16% ..
1	B	263	9% 88% 10% ..
1	C	263	16% 78% 19% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7182 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	258	Total	C	N	O	S	0	4	0
			2049	1309	340	386	14			
1	B	258	Total	C	N	O	S	0	3	0
			2040	1301	339	386	14			
1	C	258	Total	C	N	O	S	0	5	0
			2057	1315	341	387	14			

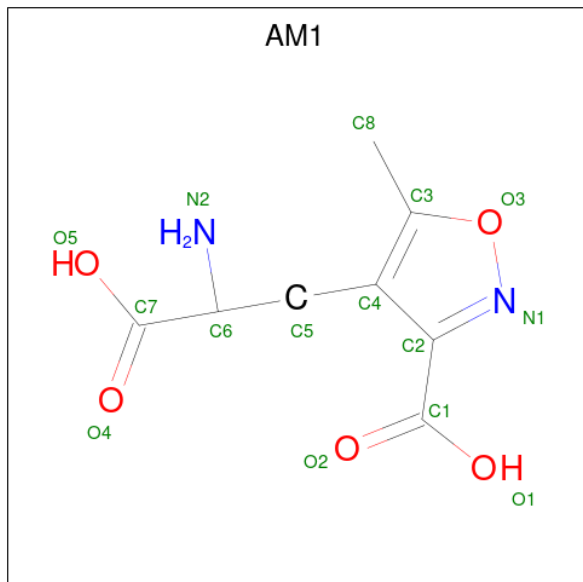
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P19491
A	2	ALA	-	cloning artifact	UNP P19491
A	118	GLY	-	linker	UNP P19491
A	119	THR	-	linker	UNP P19491
B	1	GLY	-	cloning artifact	UNP P19491
B	2	ALA	-	cloning artifact	UNP P19491
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
C	1	GLY	-	cloning artifact	UNP P19491
C	2	ALA	-	cloning artifact	UNP P19491
C	118	GLY	-	linker	UNP P19491
C	119	THR	-	linker	UNP P19491

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

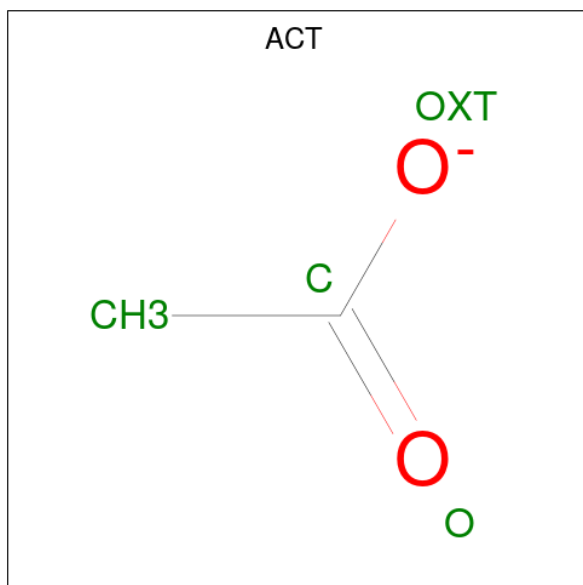
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	4	Total	Zn	0	0
			4	4		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (S)-2-AMINO-3-(3-CARBOXY-5-METHYLISOXAZOL-4-YL)PROPIONIC ACID (CCD ID: AM1) (formula: $C_8H_{10}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	2	5		
3	B	1	Total	C	N	O	0	0
			15	8	2	5		
3	C	1	Total	C	N	O	0	0
			15	8	2	5		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

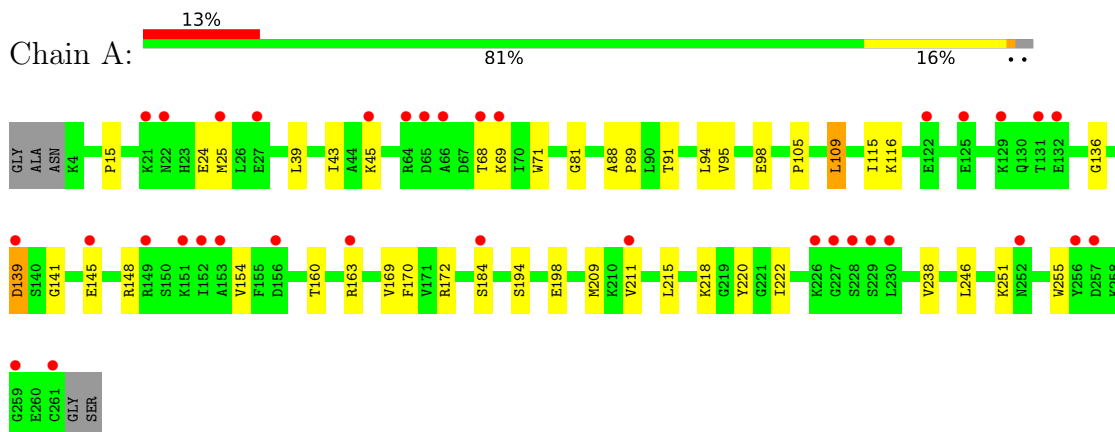
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	306	Total	O	0	0
			306	306		
5	B	387	Total	O	0	0
			387	387		
5	C	286	Total	O	0	0
			286	286		

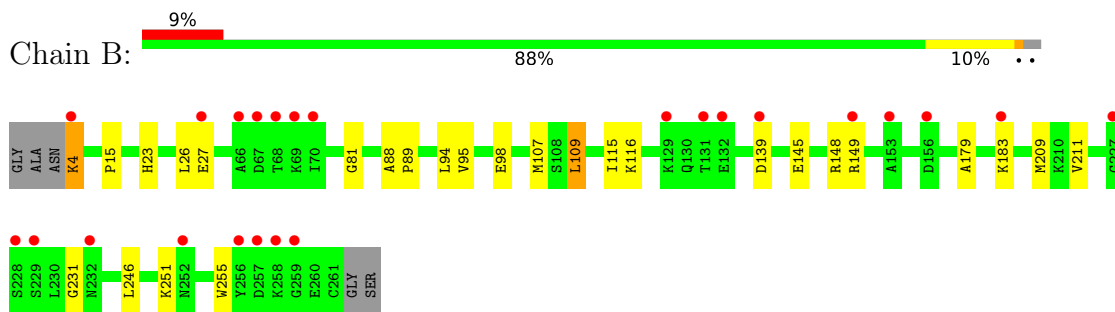
3 Residue-property plots [i](#)

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.

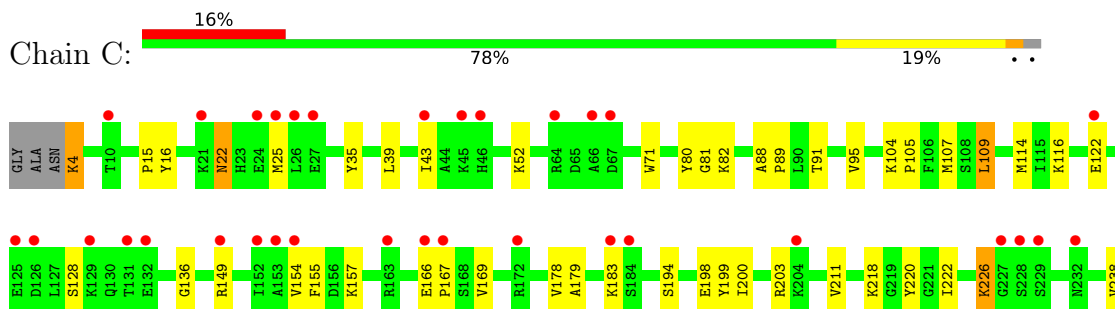
• Molecule 1: Glutamate receptor 2

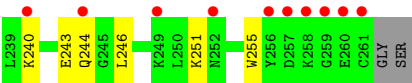


• Molecule 1: Glutamate receptor 2



• 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	114.05Å 163.16Å 46.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.75 – 1.46 16.75 – 1.46	Depositor EDS
% Data completeness (in resolution range)	97.3 (16.75-1.46) 97.4 (16.75-1.46)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.46Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.216 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7182	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.02% 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: AM1, ZN, ACT

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	0.31	0/2085	0.80	1/2805 (0.0%)
1	B	0.33	0/2076	0.81	2/2792 (0.1%)
1	C	0.31	0/2093	0.79	2/2816 (0.1%)
All	All	0.32	0/6254	0.80	5/8413 (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	C	116	LYS	N-CA-C	-6.52	99.89	110.20
1	A	116	LYS	N-CA-C	-6.39	100.10	110.20
1	B	116	LYS	N-CA-C	-6.21	100.38	110.20
1	B	231	GLY	N-CA-C	5.08	118.79	112.64
1	C	104	LYS	N-CA-C	-5.01	102.75	110.01

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	2049	0	2088	36	0
1	B	2040	0	2073	21	0
1	C	2057	0	2098	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	8	0	0
3	B	15	0	8	0	0
3	C	15	0	8	0	0
4	B	4	0	3	0	0
5	A	306	0	0	3	0
5	B	387	0	0	5	0
5	C	286	0	0	4	0
All	All	7182	0	6286	101	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 8.

All (101) 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:C:22:ASN:HB2	1:C:25:MET:HE2	1.51	0.90
1:B:179:ALA:O	1:B:183:LYS:HD3	1.73	0.89
1:C:179:ALA:O	1:C:183:LYS:HD3	1.76	0.84
1:B:107:MET:HE2	1:B:251:LYS:HD3	1.65	0.79
1:A:160:THR:HA	1:A:163:ARG:HH21	1.49	0.77
1:A:43[B]:ILE:HD13	1:A:222[B]:ILE:HD13	1.73	0.69
1:C:22:ASN:HD22	1:C:22:ASN:H	1.43	0.66
1:C:43[B]:ILE:HD13	1:C:222[B]:ILE:HD13	1.79	0.65
1:C:178:VAL:HG21	1:C:200[B]:ILE:HD13	1.79	0.64
1:C:39:LEU:HG	1:C:43[B]:ILE:HD11	1.78	0.64
1:C:71:TRP:HH2	1:C:95[B]:VAL:HG12	1.63	0.63
1:B:95:VAL:HG13	1:B:149:ARG:NH1	2.13	0.62
1:C:194:SER:O	1:C:198:GLU:HG3	2.00	0.62
1:C:82:LYS:N	1:C:82:LYS:HD2	2.16	0.61
1:C:243:GLU:HG3	5:C:1923:HOH:O	2.02	0.59
1:A:81:GLY:HA2	5:A:1781:HOH:O	2.02	0.59
1:C:35:TYR:CZ	1:C:107:MET:HE2	2.38	0.59
1:A:172:ARG:HH11	1:A:172:ARG:HG2	1.66	0.58
1:A:45:LYS:HE3	5:B:2098:HOH:O	2.03	0.58
1:C:91:THR:HG21	1:C:218:LYS:HE2	1.85	0.57
1:C:71:TRP:CH2	1:C:95[B]:VAL:HG12	2.38	0.57
1:A:194:SER:O	1:A:198:GLU:HG3	2.05	0.57
1:C:16:TYR:HE1	1:C:107:MET:HE1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ASN:HD22	1:C:22:ASN:N	2.01	0.57
1:C:81:GLY:HA2	5:C:1755:HOH:O	2.05	0.56
1:A:91:THR:HG21	1:A:218:LYS:HE2	1.87	0.56
1:B:81:GLY:HA2	5:B:1813:HOH:O	2.06	0.55
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.88	0.55
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.88	0.55
1:B:27:GLU:HG3	5:B:1934:HOH:O	2.05	0.55
1:A:222[B]:ILE:HD12	1:A:238:VAL:CG2	2.37	0.54
1:C:178:VAL:CG2	1:C:200[B]:ILE:HD13	2.36	0.54
1:C:109:LEU:N	1:C:109:LEU:HD13	2.23	0.53
1:C:4:LYS:NZ	1:C:4:LYS:HB2	2.24	0.53
1:A:24:GLU:O	1:A:25:MET:HE2	2.09	0.53
1:C:52:LYS:HE2	5:C:1919:HOH:O	2.08	0.52
1:A:246:LEU:C	1:A:246:LEU:HD13	2.36	0.51
1:C:22:ASN:H	1:C:22:ASN:ND2	2.07	0.50
1:B:107:MET:HE3	5:B:1738:HOH:O	2.10	0.50
1:A:43[B]:ILE:HD13	1:A:222[B]:ILE:CD1	2.41	0.50
1:C:246:LEU:C	1:C:246:LEU:HD13	2.37	0.49
1:C:122:GLU:HA	1:C:211:VAL:CG2	2.42	0.49
1:C:122:GLU:HA	1:C:211:VAL:HG21	1.95	0.48
1:C:226:LYS:HE3	5:C:1915:HOH:O	2.14	0.48
1:B:183:LYS:HE2	5:B:2020:HOH:O	2.13	0.48
1:A:24:GLU:C	1:A:25:MET:HE2	2.39	0.48
1:C:105:PRO:HA	1:C:220:TYR:O	2.14	0.48
1:A:109:LEU:HD13	1:A:109:LEU:N	2.28	0.47
1:B:88:ALA:HB1	1:B:89:PRO:HD2	1.95	0.47
1:C:39:LEU:HG	1:C:43[B]:ILE:CD1	2.45	0.47
1:C:251:LYS:O	1:C:255:TRP:HB2	2.15	0.47
1:A:115:ILE:CD1	1:A:211:VAL:HG11	2.44	0.47
1:A:209:MET:HE2	1:A:211:VAL:HG12	1.97	0.46
1:B:107:MET:CE	1:B:251:LYS:HD3	2.42	0.46
1:C:43[B]:ILE:HD13	1:C:222[B]:ILE:CD1	2.45	0.46
1:A:145:GLU:CD	1:A:148:ARG:HH21	2.24	0.46
1:C:199:TYR:O	1:C:203:ARG:HG2	2.15	0.46
1:B:4:LYS:HB2	1:B:4:LYS:NZ	2.30	0.46
1:B:209:MET:HE2	1:B:211:VAL:HG12	1.96	0.46
1:A:94:LEU:O	1:A:98:GLU:HG3	2.17	0.46
1:A:139:ASP:OD1	1:A:170:PHE:HB3	2.16	0.46
1:A:154:VAL:HG23	5:A:1938:HOH:O	2.15	0.45
1:A:71:TRP:HH2	1:A:95[B]:VAL:HG22	1.82	0.45
1:A:172:ARG:HG2	1:A:172:ARG:NH1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLY:HA3	1:C:169:VAL:O	2.17	0.45
1:B:251:LYS:HD2	1:B:255:TRP:CE3	2.52	0.45
1:A:109:LEU:HD22	1:A:218:LYS:HG2	2.00	0.44
1:C:80:TYR:HB3	1:C:82:LYS:HE2	1.98	0.44
1:A:68:THR:O	1:A:69:LYS:HB2	2.17	0.44
1:C:114:MET:HE1	1:C:200[B]:ILE:CD1	2.48	0.44
1:B:246:LEU:HD13	1:B:246:LEU:C	2.43	0.43
1:B:115:ILE:CD1	1:B:211:VAL:HG11	2.48	0.43
1:C:109:LEU:HD22	1:C:218:LYS:HG2	2.00	0.43
1:A:251:LYS:O	1:A:255:TRP:HB2	2.19	0.43
1:A:39:LEU:HG	1:A:43[B]:ILE:HD11	2.01	0.42
1:B:183:LYS:N	1:B:183:LYS:HD2	2.34	0.42
1:A:184:SER:HB3	5:A:1836:HOH:O	2.20	0.42
1:A:105:PRO:HA	1:A:220:TYR:O	2.19	0.42
1:B:94:LEU:O	1:B:98:GLU:HG3	2.18	0.42
1:B:145:GLU:OE1	1:B:148:ARG:NH1	2.52	0.42
1:C:39:LEU:O	1:C:43[B]:ILE:HG13	2.19	0.42
1:A:215[A]:LEU:HD12	1:A:215[A]:LEU:N	2.35	0.42
1:B:95:VAL:HG13	1:B:149:ARG:HH12	1.84	0.42
1:B:109:LEU:HD13	1:B:109:LEU:N	2.33	0.42
1:A:145:GLU:OE2	1:A:148:ARG:NH2	2.53	0.42
1:C:22:ASN:N	1:C:22:ASN:ND2	2.67	0.42
1:A:43[B]:ILE:CD1	1:A:222[B]:ILE:CD1	2.98	0.42
1:A:160:THR:HA	1:A:163:ARG:NH2	2.27	0.41
1:C:128:SER:O	1:C:157:LYS:HE3	2.20	0.41
1:A:136:GLY:HA3	1:A:169:VAL:O	2.21	0.41
1:A:71:TRP:CH2	1:A:95[B]:VAL:HG22	2.54	0.41
1:B:23:HIS:CD2	1:B:26:LEU:HD12	2.56	0.41
1:A:43[B]:ILE:HD11	1:A:222[B]:ILE:HD11	2.01	0.41
1:C:166:GLU:HA	1:C:167:PRO:C	2.46	0.41
1:C:114:MET:HE1	1:C:200[B]:ILE:HD12	2.01	0.41
1:C:154:VAL:HG13	1:C:155:PHE:N	2.36	0.41
1:C:222[B]:ILE:HD12	1:C:238:VAL:CG2	2.51	0.41
1:B:145:GLU:OE1	1:B:145:GLU:HA	2.21	0.40
1:C:149:ARG:HH11	1:C:149:ARG:HG2	1.85	0.40
1:A:141:GLY:O	1:A:145:GLU:HG2	2.22	0.40
1:C:240:LYS:HE2	1:C:244:GLN:OE1	2.22	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	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
1	B	259/263 (98%)	256 (99%)	3 (1%)	0	100	100
1	C	261/263 (99%)	259 (99%)	2 (1%)	0	100	100
All	All	780/789 (99%)	772 (99%)	8 (1%)	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	221/219 (101%)	218 (99%)	3 (1%)	59	28
1	B	220/219 (100%)	216 (98%)	4 (2%)	51	19
1	C	222/219 (101%)	217 (98%)	5 (2%)	44	13
All	All	663/657 (101%)	651 (98%)	12 (2%)	51	19

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PRO
1	A	109	LEU
1	A	139	ASP
1	B	4	LYS
1	B	15	PRO

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Mol	Chain	Res	Type
1	B	109	LEU
1	B	139	ASP
1	C	4	LYS
1	C	15	PRO
1	C	22	ASN
1	C	109	LEU
1	C	226	LYS

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	244	GLN
1	B	22	ASN
1	C	22	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	ACT	B	1703	2	3,3,3	0.60	0	3,3,3	0.43	0
3	AM1	A	1700	-	14,15,15	1.50	3 (21%)	13,21,21	1.11	1 (7%)
3	AM1	B	1701	-	14,15,15	1.55	3 (21%)	13,21,21	1.13	1 (7%)
3	AM1	C	1702	-	14,15,15	1.50	3 (21%)	13,21,21	1.16	1 (7%)

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	AM1	A	1700	-	-	0/12/12/12	0/1/1/1
3	AM1	B	1701	-	-	0/12/12/12	0/1/1/1
3	AM1	C	1702	-	-	0/12/12/12	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1701	AM1	O2-C1	2.85	1.29	1.22
3	A	1700	AM1	O2-C1	2.85	1.29	1.22
3	C	1702	AM1	O2-C1	2.74	1.29	1.22
3	B	1701	AM1	C4-C3	2.42	1.38	1.35
3	C	1702	AM1	C4-C3	2.42	1.38	1.35
3	A	1700	AM1	C4-C3	2.35	1.38	1.35
3	B	1701	AM1	O3-N1	-2.31	1.38	1.42
3	C	1702	AM1	O3-N1	-2.28	1.38	1.42
3	A	1700	AM1	O3-N1	-2.17	1.38	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1702	AM1	O5-C7-O4	2.80	130.42	124.08
3	B	1701	AM1	O5-C7-O4	2.77	130.35	124.08
3	A	1700	AM1	O5-C7-O4	2.73	130.27	124.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	258/263 (98%)	0.64	35 (13%) 7 7	6, 17, 31, 37	4 (1%)
1	B	258/263 (98%)	0.45	24 (9%) 14 14	5, 15, 29, 37	3 (1%)
1	C	258/263 (98%)	0.87	43 (16%) 4 4	3, 19, 33, 37	6 (2%)
All	All	774/789 (98%)	0.65	102 (13%) 7 8	3, 17, 31, 37	13 (1%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	GLY	5.1
1	C	10	THR	5.1
1	A	21	LYS	4.9
1	C	122	GLU	4.8
1	C	261	CYS	4.5
1	B	232	ASN	4.5
1	B	27	GLU	4.4
1	A	131	THR	4.1
1	C	131	THR	3.8
1	C	256	TYR	3.8
1	B	67	ASP	3.7
1	A	153	ALA	3.7
1	B	252	ASN	3.6
1	A	226	LYS	3.6
1	C	24	GLU	3.6
1	A	257	ASP	3.6
1	B	129	LYS	3.6
1	B	227	GLY	3.5
1	C	166	GLU	3.5
1	C	125	GLU	3.5
1	C	132	GLU	3.4
1	A	27	GLU	3.3
1	C	21	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	152	ILE	3.3
1	C	258	LYS	3.2
1	B	259	GLY	3.2
1	B	256	TYR	3.1
1	A	68	THR	3.0
1	A	229	SER	3.0
1	C	204	LYS	3.0
1	C	64	ARG	2.9
1	A	259	GLY	2.9
1	A	22	ASN	2.9
1	C	25	MET	2.9
1	C	183	LYS	2.9
1	C	228	SER	2.9
1	B	68	THR	2.8
1	A	256	TYR	2.8
1	A	261	CYS	2.8
1	B	4	LYS	2.8
1	B	149	ARG	2.8
1	C	153	ALA	2.7
1	B	229	SER	2.7
1	C	184	SER	2.7
1	C	46	HIS	2.7
1	A	184	SER	2.7
1	C	154	VAL	2.7
1	A	125	GLU	2.6
1	C	45	LYS	2.6
1	B	257	ASP	2.6
1	C	67	ASP	2.6
1	B	153	ALA	2.6
1	A	228	SER	2.6
1	B	183	LYS	2.6
1	A	252	ASN	2.6
1	B	258	LYS	2.5
1	A	211	VAL	2.5
1	C	252	ASN	2.5
1	A	156	ASP	2.5
1	C	126	ASP	2.5
1	A	45	LYS	2.5
1	A	163	ARG	2.5
1	A	149	ARG	2.5
1	C	249	LYS	2.4
1	A	230	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	66	ALA	2.4
1	A	129	LYS	2.3
1	C	129	LYS	2.3
1	B	228	SER	2.3
1	B	131	THR	2.3
1	C	227	GLY	2.3
1	A	65	ASP	2.3
1	C	257	ASP	2.3
1	C	149	ARG	2.3
1	C	163	ARG	2.3
1	B	69	LYS	2.3
1	B	132	GLU	2.3
1	C	240	LYS	2.3
1	B	70	ILE	2.3
1	B	66	ALA	2.2
1	C	232	ASN	2.2
1	A	139	ASP	2.2
1	A	145	GLU	2.2
1	C	172	ARG	2.2
1	C	260	GLU	2.2
1	A	151	LYS	2.2
1	C	167	PRO	2.2
1	A	69	LYS	2.2
1	A	122	GLU	2.1
1	C	229	SER	2.1
1	C	244	GLN	2.1
1	A	227	GLY	2.1
1	C	27	GLU	2.1
1	B	156	ASP	2.1
1	C	66	ALA	2.1
1	C	26	LEU	2.1
1	C	43[A]	ILE	2.1
1	B	139	ASP	2.1
1	C	152[A]	ILE	2.0
1	A	25	MET	2.0
1	A	64	ARG	2.0
1	A	132	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
4	ACT	B	1703	4/4	0.86	0.13	30,30,31,31	0
3	AM1	A	1700	15/15	0.93	0.11	10,15,21,23	0
2	ZN	C	1708	1/1	0.94	0.11	37,37,37,37	0
3	AM1	C	1702	15/15	0.95	0.08	9,15,22,24	0
3	AM1	B	1701	15/15	0.95	0.09	8,13,19,21	0
2	ZN	A	1704	1/1	0.96	0.06	23,23,23,23	0
2	ZN	A	1710	1/1	0.97	0.14	27,27,27,27	0
2	ZN	B	1709	1/1	0.98	0.20	30,30,30,30	0
2	ZN	A	1705	1/1	0.98	0.03	15,15,15,15	0
2	ZN	B	1707	1/1	0.98	0.03	16,16,16,16	0
2	ZN	B	1711	1/1	0.99	0.12	23,23,23,23	0
2	ZN	B	1706	1/1	0.99	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.