



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:36 PM UTC

PDB ID : 4RO2 / pdb_00004ro2
Title : Crystal Structure of CNG mimicking NaK-ETPP mutant cocrystallized with Methylammonium
Authors : De March, M.; Napolitano, L.M.R.; Onesti, S.
Deposited on : 2014-10-27
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:

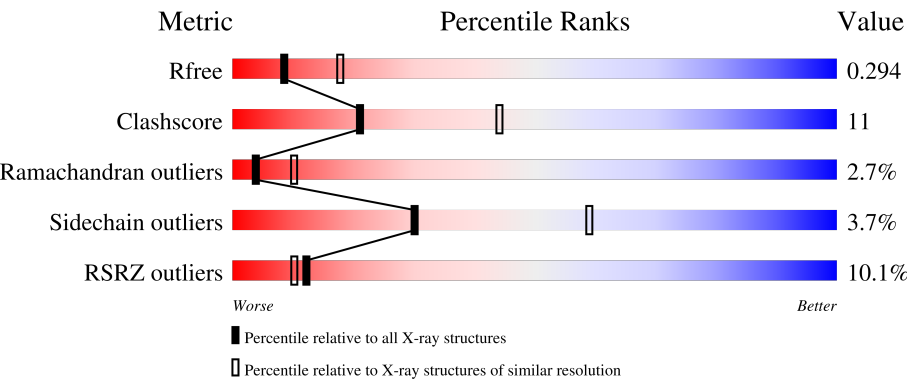
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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	96	3% 76% 8% 8% . .
1	B	96	3% 78% 11% 5% 5%
1	C	96	15% 69% 12% . 16%
1	D	96	16% 73% 10% . 15%

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	3P8	A	201	-	-	X	X
2	3P8	C	201	-	-	X	X
3	GLY	A	205	-	X	-	-
3	GLY	B	207	-	X	-	-
3	GLY	C	203	-	X	-	-
3	GLY	C	206	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2747 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 Potassium channel protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	0	0	0
			697	470	103	124			
1	B	91	Total	C	N	O	0	0	0
			683	465	101	117			
1	C	81	Total	C	N	O	0	0	0
			570	380	85	105			
1	D	82	Total	C	N	O	0	0	0
			570	378	86	106			

There are 44 discrepancies between the modelled and reference sequences:

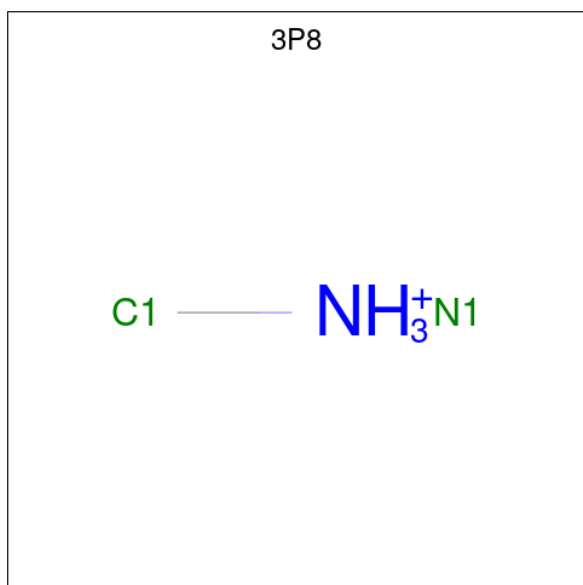
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP Q81HW2
A	19	ALA	-	expression tag	UNP Q81HW2
A	66	GLU	ASP	engineered mutation	UNP Q81HW2
A	67	THR	GLY	engineered mutation	UNP Q81HW2
A	68	PRO	ASN	engineered mutation	UNP Q81HW2
A	69	PRO	PHE	engineered mutation	UNP Q81HW2
A	?	-	SER	deletion	UNP Q81HW2
A	110	LEU	-	expression tag	UNP Q81HW2
A	111	VAL	-	expression tag	UNP Q81HW2
A	112	PRO	-	expression tag	UNP Q81HW2
A	113	ARG	-	expression tag	UNP Q81HW2
B	18	MET	-	expression tag	UNP Q81HW2
B	19	ALA	-	expression tag	UNP Q81HW2
B	66	GLU	ASP	engineered mutation	UNP Q81HW2
B	67	THR	GLY	engineered mutation	UNP Q81HW2
B	68	PRO	ASN	engineered mutation	UNP Q81HW2
B	69	PRO	PHE	engineered mutation	UNP Q81HW2
B	?	-	SER	deletion	UNP Q81HW2
B	110	LEU	-	expression tag	UNP Q81HW2
B	111	VAL	-	expression tag	UNP Q81HW2
B	112	PRO	-	expression tag	UNP Q81HW2

Continued on next page...

Continued from previous page...

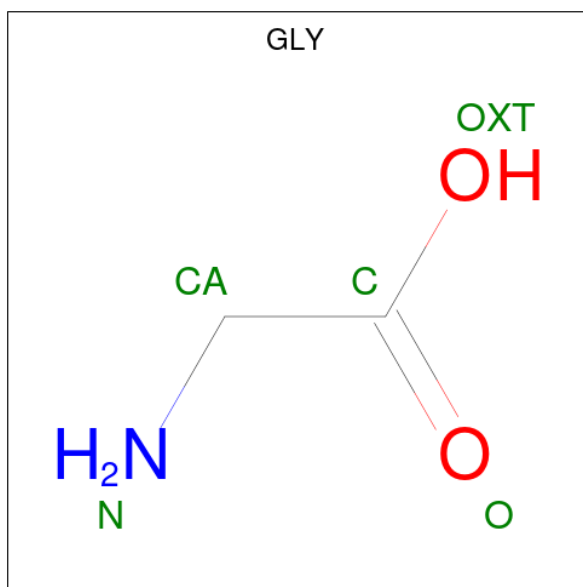
Chain	Residue	Modelled	Actual	Comment	Reference
B	113	ARG	-	expression tag	UNP Q81HW2
C	18	MET	-	expression tag	UNP Q81HW2
C	19	ALA	-	expression tag	UNP Q81HW2
C	66	GLU	ASP	engineered mutation	UNP Q81HW2
C	67	THR	GLY	engineered mutation	UNP Q81HW2
C	68	PRO	ASN	engineered mutation	UNP Q81HW2
C	69	PRO	PHE	engineered mutation	UNP Q81HW2
C	?	-	SER	deletion	UNP Q81HW2
C	110	LEU	-	expression tag	UNP Q81HW2
C	111	VAL	-	expression tag	UNP Q81HW2
C	112	PRO	-	expression tag	UNP Q81HW2
C	113	ARG	-	expression tag	UNP Q81HW2
D	18	MET	-	expression tag	UNP Q81HW2
D	19	ALA	-	expression tag	UNP Q81HW2
D	66	GLU	ASP	engineered mutation	UNP Q81HW2
D	67	THR	GLY	engineered mutation	UNP Q81HW2
D	68	PRO	ASN	engineered mutation	UNP Q81HW2
D	69	PRO	PHE	engineered mutation	UNP Q81HW2
D	?	-	SER	deletion	UNP Q81HW2
D	110	LEU	-	expression tag	UNP Q81HW2
D	111	VAL	-	expression tag	UNP Q81HW2
D	112	PRO	-	expression tag	UNP Q81HW2
D	113	ARG	-	expression tag	UNP Q81HW2

- Molecule 2 is methylammonium ion (CCD ID: 3P8) (formula: CH₅N).



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

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



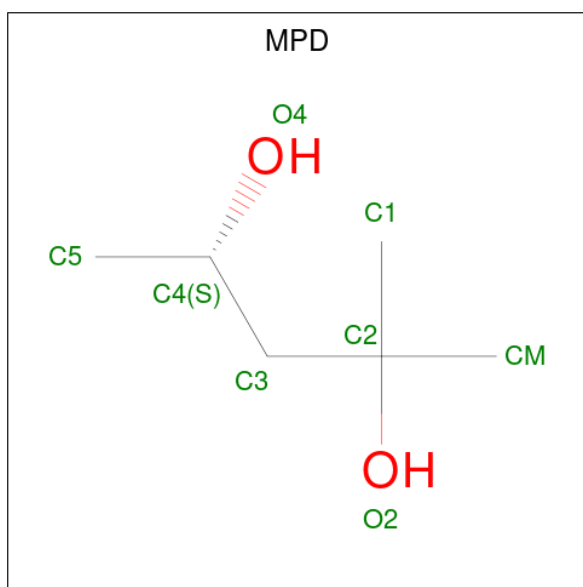
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	B	1	Total C N O 5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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

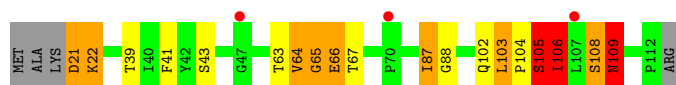
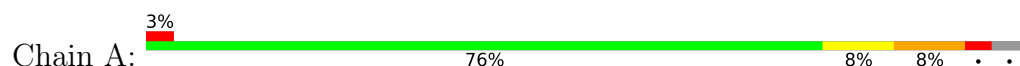
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	8	Total	O	0	0
			8	8		
5	C	17	Total	O	0	0
			17	17		
5	D	14	Total	O	0	0
			14	14		

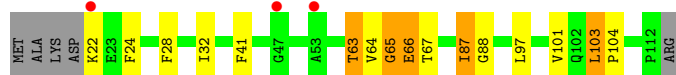
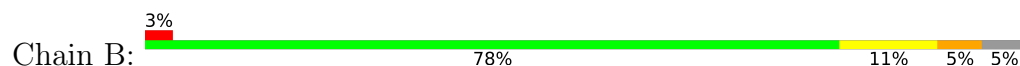
3 Residue-property plots [i](#)

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.

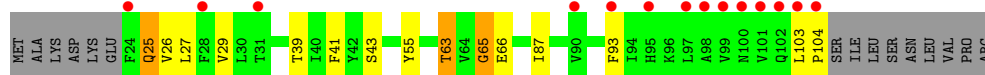
- Molecule 1: Potassium channel protein



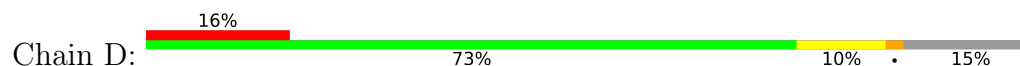
- Molecule 1: Potassium channel protein



- Molecule 1: Potassium channel protein



- Molecule 1: Potassium channel protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.70Å 91.05Å 67.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.52 – 2.70 45.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.52-2.70) 93.7 (45.52-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0	Depositor
R, R_{free}	0.248 , 0.283 0.262 , 0.294	Depositor DCC
R_{free} test set	545 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.178 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2747	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: 3P8, MPD

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	0.73	0/715	1.16	4/981 (0.4%)
1	B	0.75	0/701	1.03	2/960 (0.2%)
1	C	0.76	0/583	1.05	1/803 (0.1%)
1	D	0.75	0/584	1.06	3/804 (0.4%)
All	All	0.75	0/2583	1.08	10/3548 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	SER	N-CA-C	12.49	125.43	110.44
1	A	106	ILE	N-CA-C	6.61	123.09	109.34
1	A	65	GLY	N-CA-C	-6.34	98.15	113.18
1	A	105	SER	CA-C-O	-6.14	113.97	121.89
1	C	25	GLN	N-CA-C	-5.39	103.51	110.19
1	D	72	THR	CB-CA-C	-5.38	100.42	109.50
1	B	67	THR	CA-C-N	-5.28	114.94	120.38
1	B	67	THR	C-N-CA	-5.28	114.94	120.38
1	D	67	THR	CA-C-N	-5.05	115.18	120.38
1	D	67	THR	C-N-CA	-5.05	115.18	120.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	SER	Peptide
1	A	108	SER	Peptide
1	A	21	ASP	Peptide
1	A	64	VAL	Peptide

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	697	0	692	17	0
1	B	683	0	678	16	0
1	C	570	0	528	14	0
1	D	570	0	494	14	0
2	A	2	0	0	2	0
2	C	2	0	0	2	0
3	A	40	0	16	1	0
3	B	45	0	18	0	0
3	C	30	0	12	0	0
3	D	25	0	10	3	0
4	B	16	0	28	0	0
4	C	8	0	14	0	0
4	D	8	0	14	0	0
5	A	12	0	0	2	0
5	B	8	0	0	0	0
5	C	17	0	0	3	0
5	D	14	0	0	0	0
All	All	2747	0	2504	57	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 11.

All (57) 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:102:GLN:O	1:A:106:ILE:CB	1.78	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:THR:O	1:D:63:THR:HG22	1.66	0.94
3:D:201:GLY:OXT	3:D:203:GLY:N	2.03	0.90
1:A:66:GLU:O	1:A:66:GLU:HG2	1.85	0.75
1:C:66:GLU:OE2	5:C:301:HOH:O	2.07	0.72
1:B:22:LYS:HA	1:B:24:PHE:H	1.53	0.72
1:C:55:TYR:OH	1:C:66:GLU:OE1	2.11	0.68
1:B:28:PHE:CE2	1:B:32:ILE:HD11	2.30	0.67
1:D:64:VAL:HG12	1:D:66:GLU:HG2	1.77	0.66
1:B:28:PHE:CZ	1:B:32:ILE:HD11	2.30	0.65
5:A:301:HOH:O	1:B:66:GLU:HG2	1.96	0.65
1:A:67:THR:CB	5:A:311:HOH:O	2.48	0.61
1:A:21:ASP:N	3:A:204:GLY:HA2	2.16	0.60
1:D:28:PHE:H	3:D:205:GLY:HA2	1.66	0.59
1:B:64:VAL:HG12	1:B:66:GLU:HG3	1.84	0.59
1:B:103:LEU:HB3	1:B:104:PRO:HD3	1.84	0.58
1:C:87:ILE:HG21	1:D:94:ILE:HD13	1.85	0.58
1:C:93:PHE:CB	5:C:311:HOH:O	2.50	0.58
1:C:25:GLN:C	1:C:27:LEU:H	2.12	0.57
1:A:108:SER:O	1:A:109:ASN:HB2	2.04	0.57
1:A:103:LEU:HB3	1:A:104:PRO:HD3	1.88	0.55
1:D:63:THR:C	1:D:65:GLY:H	2.14	0.55
1:B:28:PHE:CE2	1:B:32:ILE:CD1	2.90	0.54
2:C:201:3P8:C1	1:D:63:THR:O	2.55	0.54
1:C:63:THR:C	1:C:65:GLY:H	2.15	0.53
1:A:39:THR:O	1:A:43:SER:OG	2.16	0.53
1:A:87:ILE:HG22	1:A:88:GLY:N	2.24	0.52
1:C:63:THR:O	2:C:201:3P8:C1	2.58	0.51
1:A:66:GLU:O	1:A:66:GLU:CG	2.51	0.51
1:B:87:ILE:HG22	1:B:88:GLY:N	2.27	0.50
1:A:103:LEU:O	1:A:106:ILE:CB	2.60	0.50
1:B:63:THR:C	1:B:65:GLY:H	2.22	0.48
1:A:65:GLY:O	1:B:66:GLU:HB3	2.14	0.48
2:A:201:3P8:C1	1:B:63:THR:O	2.62	0.47
1:D:72:THR:HB	1:D:75:GLY:H	1.80	0.47
1:B:41:PHE:CD1	1:B:41:PHE:C	2.93	0.47
1:A:103:LEU:C	1:A:103:LEU:HD23	2.39	0.46
1:C:39:THR:O	1:C:43:SER:HB3	2.16	0.46
1:B:103:LEU:C	1:B:103:LEU:HD23	2.41	0.46
1:D:62:THR:O	1:D:63:THR:CG2	2.52	0.46
1:A:41:PHE:C	1:A:41:PHE:CD1	2.93	0.46
1:A:105:SER:N	1:A:106:ILE:CB	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:O	2:A:201:3P8:C1	2.64	0.45
1:C:41:PHE:CD1	1:C:41:PHE:C	2.94	0.45
1:C:63:THR:HB	1:D:63:THR:HG23	1.99	0.45
5:C:303:HOH:O	1:D:63:THR:HG21	2.17	0.45
1:A:67:THR:O	1:B:66:GLU:HB2	2.18	0.44
1:D:63:THR:C	1:D:65:GLY:N	2.73	0.44
1:C:63:THR:C	1:C:65:GLY:N	2.75	0.44
1:D:27:LEU:N	3:D:205:GLY:HA2	2.33	0.43
1:A:21:ASP:O	1:A:22:LYS:CB	2.67	0.42
1:D:41:PHE:CD1	1:D:41:PHE:C	2.98	0.42
1:C:103:LEU:CB	1:C:104:PRO:HD3	2.49	0.42
1:C:87:ILE:HG23	1:D:94:ILE:HG21	2.02	0.42
1:C:25:GLN:C	1:C:27:LEU:N	2.78	0.41
1:B:97:LEU:HD12	1:B:101:VAL:HB	2.01	0.41
1:B:63:THR:C	1:B:65:GLY:N	2.78	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	90/96 (94%)	83 (92%)	3 (3%)	4 (4%)	2	4
1	B	89/96 (93%)	84 (94%)	4 (4%)	1 (1%)	11	29
1	C	79/96 (82%)	71 (90%)	5 (6%)	3 (4%)	2	5
1	D	80/96 (83%)	75 (94%)	4 (5%)	1 (1%)	9	25
All	All	338/384 (88%)	313 (93%)	16 (5%)	9 (3%)	4	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ILE
1	B	65	GLY
1	C	65	GLY
1	D	65	GLY
1	A	22	LYS
1	A	64	VAL
1	A	109	ASN
1	C	26	VAL
1	C	29	VAL

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	74/86 (86%)	70 (95%)	4 (5%)	20	45
1	B	69/86 (80%)	65 (94%)	4 (6%)	18	42
1	C	53/86 (62%)	52 (98%)	1 (2%)	50	77
1	D	47/86 (55%)	47 (100%)	0	100	100
All	All	243/344 (71%)	234 (96%)	9 (4%)	30	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	87	ILE
1	A	103	LEU
1	A	109	ASN
1	B	63	THR
1	B	66	GLU
1	B	87	ILE
1	B	103	LEU
1	C	63	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	100	ASN
1	A	102	GLN
1	A	109	ASN
1	B	102	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
3	GLY	C	207	-	4,4,4	1.26	0	3,4,4	0.94	0
2	3P8	A	201	-	1,1,1	0.77	0	-		
3	GLY	A	205	-	4,4,4	1.12	1 (25%)	3,4,4	1.83	1 (33%)
3	GLY	B	201	-	4,4,4	1.02	0	3,4,4	1.63	0
3	GLY	B	209	-	4,4,4	1.28	1 (25%)	3,4,4	1.32	0
3	GLY	C	204	-	4,4,4	1.08	1 (25%)	3,4,4	1.44	0
3	GLY	A	208	-	4,4,4	1.09	1 (25%)	3,4,4	1.48	0
3	GLY	B	206	-	4,4,4	1.21	1 (25%)	3,4,4	1.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	C	208	-	7,7,7	0.48	0	9,10,10	1.27	1 (11%)
4	MPD	B	211	-	7,7,7	0.35	0	9,10,10	0.48	0
3	GLY	B	207	-	4,4,4	1.11	1 (25%)	3,4,4	1.64	1 (33%)
3	GLY	A	207	-	4,4,4	1.09	0	3,4,4	1.64	1 (33%)
3	GLY	B	204	-	4,4,4	1.04	0	3,4,4	1.41	0
3	GLY	C	202	-	4,4,4	1.24	1 (25%)	3,4,4	1.24	0
3	GLY	C	206	-	4,4,4	1.07	0	3,4,4	1.91	2 (66%)
3	GLY	A	209	-	4,4,4	1.19	1 (25%)	3,4,4	1.45	0
3	GLY	D	205	-	4,4,4	1.20	0	3,4,4	0.99	0
4	MPD	D	206	-	7,7,7	0.34	0	9,10,10	0.23	0
2	3P8	C	201	-	1,1,1	0.29	0	-		
3	GLY	C	205	-	4,4,4	1.03	0	3,4,4	1.51	0
3	GLY	D	201	-	4,4,4	1.12	1 (25%)	3,4,4	2.83	2 (66%)
3	GLY	B	203	-	4,4,4	1.01	0	3,4,4	1.64	1 (33%)
3	GLY	B	202	-	4,4,4	1.19	1 (25%)	3,4,4	1.36	0
3	GLY	A	206	-	4,4,4	1.13	1 (25%)	3,4,4	1.46	0
3	GLY	A	203	-	4,4,4	1.07	1 (25%)	3,4,4	1.64	1 (33%)
3	GLY	D	202	-	4,4,4	1.00	0	3,4,4	1.64	1 (33%)
3	GLY	A	204	-	4,4,4	1.02	0	3,4,4	1.42	0
3	GLY	D	203	-	4,4,4	1.11	1 (25%)	3,4,4	0.92	0
4	MPD	B	210	-	7,7,7	0.39	0	9,10,10	0.47	0
3	GLY	B	205	-	4,4,4	1.10	1 (25%)	3,4,4	1.86	2 (66%)
3	GLY	C	203	-	4,4,4	1.20	1 (25%)	3,4,4	1.78	1 (33%)
3	GLY	A	202	-	4,4,4	1.04	0	3,4,4	1.59	0
3	GLY	B	208	-	4,4,4	0.96	0	3,4,4	1.79	2 (66%)
3	GLY	D	204	-	4,4,4	1.08	0	3,4,4	0.82	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	GLY	C	207	-	-	2/2/2/2	-
3	GLY	A	205	-	-	2/2/2/2	-
3	GLY	B	201	-	-	2/2/2/2	-
3	GLY	B	209	-	-	2/2/2/2	-
3	GLY	C	204	-	-	2/2/2/2	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	A	208	-	-	2/2/2/2	-
3	GLY	B	206	-	-	2/2/2/2	-
4	MPD	C	208	-	-	0/5/5/5	-
4	MPD	B	211	-	-	0/5/5/5	-
3	GLY	B	207	-	-	2/2/2/2	-
3	GLY	A	207	-	-	2/2/2/2	-
3	GLY	B	204	-	-	2/2/2/2	-
3	GLY	C	202	-	-	2/2/2/2	-
3	GLY	C	206	-	-	2/2/2/2	-
3	GLY	A	209	-	-	2/2/2/2	-
3	GLY	D	205	-	-	2/2/2/2	-
4	MPD	D	206	-	-	3/5/5/5	-
3	GLY	C	205	-	-	2/2/2/2	-
3	GLY	D	201	-	-	0/2/2/2	-
3	GLY	B	203	-	-	2/2/2/2	-
3	GLY	B	202	-	-	2/2/2/2	-
3	GLY	A	206	-	-	2/2/2/2	-
3	GLY	A	203	-	-	0/2/2/2	-
3	GLY	D	202	-	-	0/2/2/2	-
3	GLY	A	204	-	-	2/2/2/2	-
3	GLY	D	203	-	-	2/2/2/2	-
4	MPD	B	210	-	-	3/5/5/5	-
3	GLY	B	205	-	-	0/2/2/2	-
3	GLY	C	203	-	-	2/2/2/2	-
3	GLY	A	202	-	-	2/2/2/2	-
3	GLY	B	208	-	-	0/2/2/2	-
3	GLY	D	204	-	-	0/2/2/2	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	209	GLY	OXT-C	-2.39	1.22	1.30
3	C	202	GLY	OXT-C	-2.31	1.23	1.30
3	A	209	GLY	OXT-C	-2.27	1.23	1.30
3	B	206	GLY	OXT-C	-2.26	1.23	1.30
3	C	203	GLY	OXT-C	-2.23	1.23	1.30
3	B	202	GLY	OXT-C	-2.18	1.23	1.30
3	D	201	GLY	OXT-C	-2.14	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	207	GLY	OXT-C	-2.14	1.23	1.30
3	A	205	GLY	OXT-C	-2.12	1.23	1.30
3	A	206	GLY	OXT-C	-2.11	1.23	1.30
3	A	203	GLY	OXT-C	-2.06	1.24	1.30
3	A	208	GLY	OXT-C	-2.04	1.24	1.30
3	C	204	GLY	OXT-C	-2.03	1.24	1.30
3	D	203	GLY	OXT-C	-2.01	1.24	1.30
3	B	205	GLY	OXT-C	-2.00	1.24	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	GLY	OXT-C-O	-3.81	113.55	123.33
3	D	201	GLY	OXT-C-CA	3.07	125.58	113.38
3	C	203	GLY	OXT-C-O	-2.52	116.86	123.33
3	C	206	GLY	OXT-C-O	-2.49	116.94	123.33
3	A	205	GLY	OXT-C-O	-2.48	116.95	123.33
3	B	205	GLY	OXT-C-O	-2.39	117.18	123.33
3	A	207	GLY	OXT-C-O	-2.23	117.61	123.33
3	A	203	GLY	OXT-C-O	-2.22	117.61	123.33
3	B	208	GLY	OXT-C-O	-2.18	117.74	123.33
3	B	208	GLY	OXT-C-CA	2.16	121.98	113.38
4	C	208	MPD	CM-C2-C3	-2.16	100.88	110.20
3	B	203	GLY	OXT-C-CA	2.16	121.95	113.38
3	C	206	GLY	OXT-C-CA	2.16	121.95	113.38
3	B	205	GLY	OXT-C-CA	2.12	121.82	113.38
3	B	207	GLY	OXT-C-O	-2.05	118.05	123.33
3	D	202	GLY	OXT-C-CA	2.02	121.41	113.38

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	204	GLY	O-C-CA-N
3	A	207	GLY	OXT-C-CA-N
3	A	208	GLY	O-C-CA-N
3	A	208	GLY	OXT-C-CA-N
3	A	209	GLY	O-C-CA-N
3	A	209	GLY	OXT-C-CA-N
3	B	201	GLY	O-C-CA-N
3	B	201	GLY	OXT-C-CA-N
3	B	202	GLY	OXT-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	203	GLY	O-C-CA-N
3	B	203	GLY	OXT-C-CA-N
3	B	204	GLY	OXT-C-CA-N
3	B	206	GLY	O-C-CA-N
3	B	207	GLY	O-C-CA-N
3	B	207	GLY	OXT-C-CA-N
3	B	209	GLY	O-C-CA-N
3	B	209	GLY	OXT-C-CA-N
3	C	202	GLY	O-C-CA-N
3	C	202	GLY	OXT-C-CA-N
3	C	203	GLY	O-C-CA-N
3	C	203	GLY	OXT-C-CA-N
3	C	204	GLY	O-C-CA-N
3	C	205	GLY	O-C-CA-N
3	C	205	GLY	OXT-C-CA-N
3	C	207	GLY	O-C-CA-N
3	C	207	GLY	OXT-C-CA-N
3	D	203	GLY	O-C-CA-N
3	D	203	GLY	OXT-C-CA-N
3	D	205	GLY	O-C-CA-N
3	D	205	GLY	OXT-C-CA-N
4	B	210	MPD	C2-C3-C4-O4
3	A	206	GLY	O-C-CA-N
3	A	207	GLY	O-C-CA-N
3	B	202	GLY	O-C-CA-N
3	B	204	GLY	O-C-CA-N
3	C	206	GLY	O-C-CA-N
3	A	204	GLY	OXT-C-CA-N
3	A	205	GLY	OXT-C-CA-N
3	A	206	GLY	OXT-C-CA-N
3	B	206	GLY	OXT-C-CA-N
3	C	204	GLY	OXT-C-CA-N
3	A	205	GLY	O-C-CA-N
3	C	206	GLY	OXT-C-CA-N
4	D	206	MPD	CM-C2-C3-C4
4	B	210	MPD	C2-C3-C4-C5
3	A	202	GLY	OXT-C-CA-N
4	B	210	MPD	O2-C2-C3-C4
4	D	206	MPD	C2-C3-C4-O4
4	D	206	MPD	C1-C2-C3-C4
3	A	202	GLY	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	3P8	2	0
3	D	205	GLY	2	0
2	C	201	3P8	2	0
3	D	201	GLY	1	0
3	A	204	GLY	1	0
3	D	203	GLY	1	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	92/96 (95%)	0.60	3 (3%) 49 45	24, 44, 60, 68	0
1	B	91/96 (94%)	0.54	3 (3%) 49 45	24, 40, 57, 72	0
1	C	81/96 (84%)	1.01	14 (17%) 4 3	22, 42, 82, 97	7 (8%)
1	D	82/96 (85%)	1.14	15 (18%) 3 3	25, 41, 77, 90	5 (6%)
All	All	346/384 (90%)	0.81	35 (10%) 12 10	22, 42, 76, 97	12 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	PRO	7.3
1	D	97	LEU	6.5
1	D	98	ALA	5.9
1	D	100	ASN	5.4
1	C	99	VAL	5.1
1	C	100	ASN	5.0
1	D	95	HIS	4.7
1	D	99	VAL	4.5
1	D	101	VAL	4.5
1	C	98	ALA	4.2
1	C	103	LEU	4.2
1	A	47	GLY	4.2
1	B	22	LYS	4.0
1	C	102	GLN	3.7
1	B	47	GLY	3.4
1	C	101	VAL	3.1
1	D	105	SER	3.0
1	D	102	GLN	2.8
1	C	24	PHE	2.8
1	D	106	ILE	2.8
1	A	107	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	103	LEU	2.7
1	B	53	ALA	2.5
1	C	97	LEU	2.4
1	D	90	VAL	2.4
1	D	27	LEU	2.3
1	C	90	VAL	2.3
1	C	28	PHE	2.3
1	D	104	PRO	2.2
1	D	87	ILE	2.2
1	D	28	PHE	2.2
1	A	70	PRO	2.1
1	C	31	THR	2.1
1	C	95	HIS	2.1
1	C	93	PHE	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
4	MPD	B	211	8/8	0.38	0.23	65,72,76,76	0
3	GLY	D	202	5/5	0.52	0.24	55,57,66,67	0
3	GLY	B	206	5/5	0.52	0.17	69,71,77,78	0
3	GLY	A	209	5/5	0.58	0.18	69,69,72,74	0
3	GLY	A	207	5/5	0.61	0.17	65,67,69,71	0
3	GLY	A	204	5/5	0.62	0.20	70,71,77,78	0
3	GLY	B	205	5/5	0.63	0.18	54,55,59,62	0
4	MPD	D	206	8/8	0.63	0.17	61,63,64,68	0
3	GLY	D	205	5/5	0.65	0.15	29,30,32,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3P8	C	201	2/2	0.66	0.73	12,12,12,12	2
3	GLY	C	207	5/5	0.68	0.11	42,43,45,46	0
4	MPD	C	208	8/8	0.69	0.15	31,32,34,35	0
3	GLY	A	208	5/5	0.72	0.14	72,75,77,78	0
2	3P8	A	201	2/2	0.72	0.74	12,12,12,12	2
3	GLY	B	208	5/5	0.76	0.17	59,61,66,70	0
3	GLY	C	206	5/5	0.76	0.13	70,71,76,78	0
3	GLY	B	203	5/5	0.77	0.14	54,59,61,65	0
3	GLY	B	201	5/5	0.77	0.17	58,60,64,65	0
3	GLY	C	204	5/5	0.77	0.15	57,57,62,66	0
3	GLY	D	204	5/5	0.77	0.18	51,52,54,58	0
3	GLY	C	203	5/5	0.78	0.13	56,60,65,67	0
3	GLY	A	203	5/5	0.78	0.16	58,59,62,68	0
3	GLY	A	202	5/5	0.79	0.13	59,64,64,66	0
3	GLY	A	205	5/5	0.79	0.14	60,64,67,68	0
4	MPD	B	210	8/8	0.80	0.21	71,75,77,78	0
3	GLY	B	207	5/5	0.81	0.16	71,75,77,79	0
3	GLY	C	202	5/5	0.83	0.12	58,60,63,68	0
3	GLY	D	201	5/5	0.86	0.12	44,45,46,47	0
3	GLY	B	202	5/5	0.86	0.11	58,58,60,62	0
3	GLY	A	206	5/5	0.87	0.09	49,51,52,54	0
3	GLY	B	204	5/5	0.89	0.10	57,62,63,65	0
3	GLY	C	205	5/5	0.90	0.12	49,54,62,64	0
3	GLY	D	203	5/5	0.90	0.13	50,56,57,58	0
3	GLY	B	209	5/5	0.91	0.14	58,59,59,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.