



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 10:09 PM EST

PDB ID : 4FZ0  
Title : Crystal structure of acid-sensing ion channel in complex with psalmotoxin 1 at low pH  
Authors : Bacongus, I.; Gouaux, E.  
Deposited on : 2012-07-05  
Resolution : 2.80 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

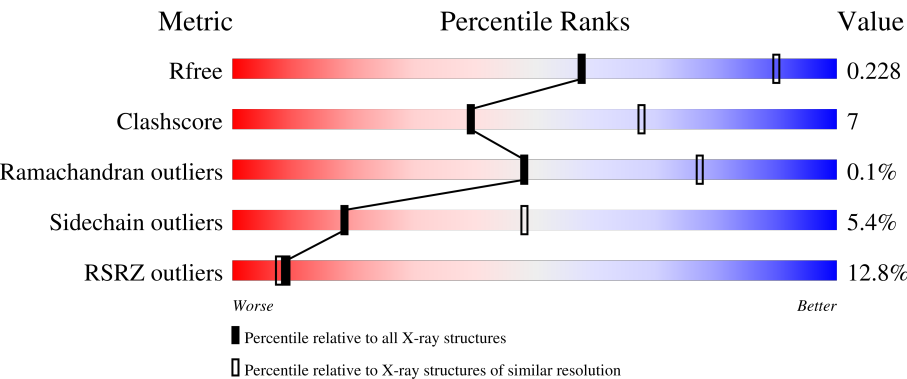
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	450	
1	B	450	
1	C	450	
2	M	40	
2	N	40	

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Mol	Chain	Length	Quality of chain
2	O	40	<div><div></div><div>5%</div><div>78%</div><div>15%</div><div>• 5%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10557 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 Acid-sensing ion channel 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3118	1983	515	596	24			
1	B	406	Total	C	N	O	S	0	0	0
			3138	2001	516	598	23			
1	C	410	Total	C	N	O	S	0	0	0
			3193	2041	522	605	25			

- Molecule 2 is a protein called Pi-theraphotoxin-Pc1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	37	Total	C	N	O	S	0	0	0
			293	182	55	50	6			
2	N	36	Total	C	N	O	S	0	0	0
			284	176	54	48	6			
2	O	38	Total	C	N	O	S	0	0	0
			302	187	56	53	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

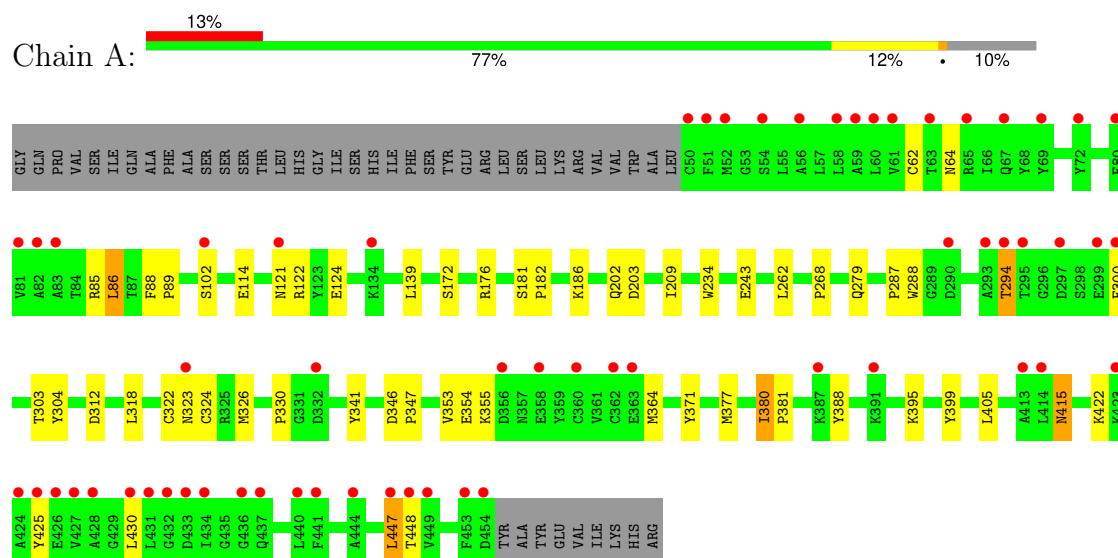
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	46	Total	O	0	0
			46	46		
6	C	48	Total	O	0	0
			48	48		
6	M	6	Total	O	0	0
			6	6		
6	N	2	Total	O	0	0
			2	2		
6	O	5	Total	O	0	0
			5	5		

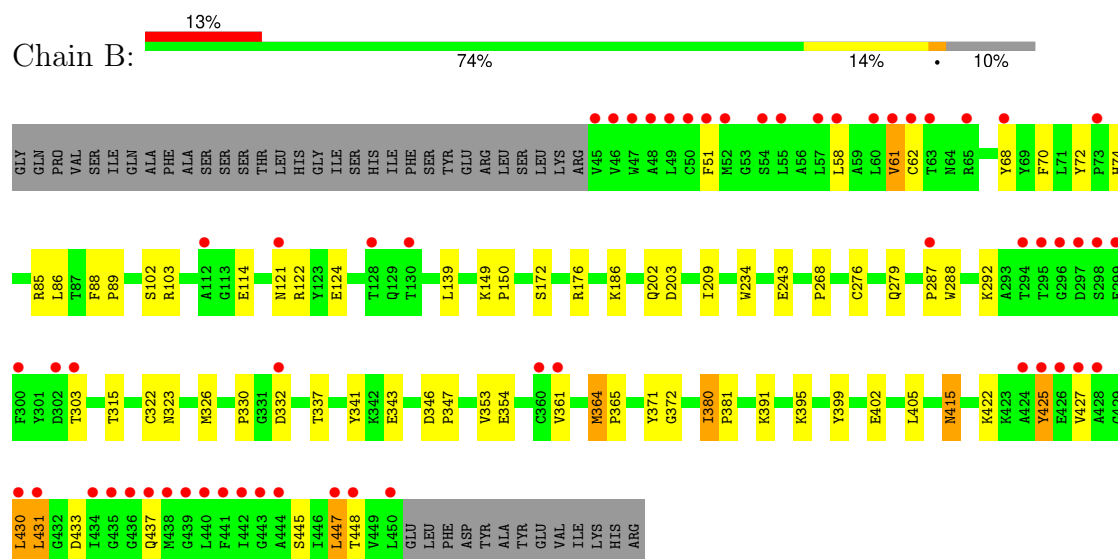
### 3 Residue-property plots [i](#)

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: Acid-sensing ion channel 1

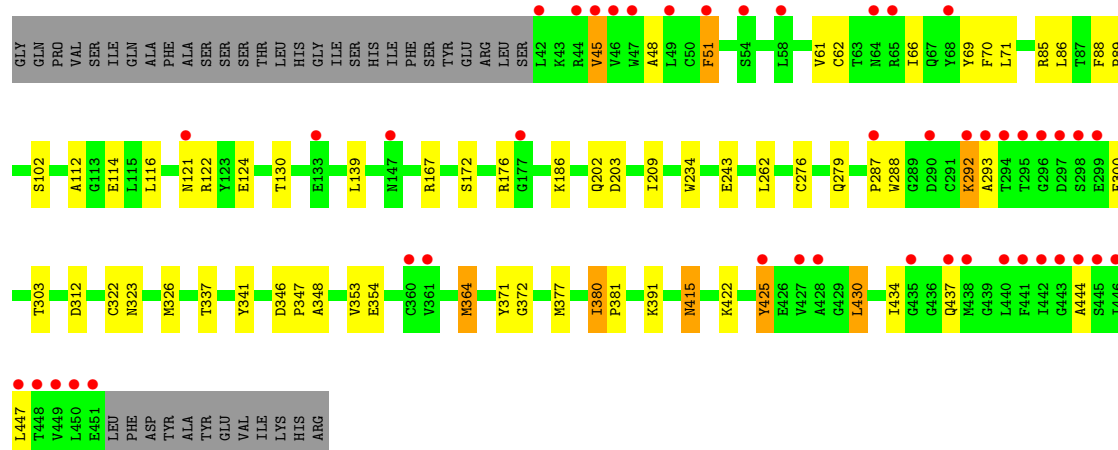


#### • Molecule 1: Acid-sensing ion channel 1



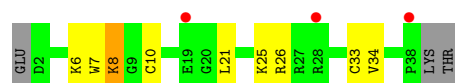
#### • Molecule 1: Acid-sensing ion channel 1

Chain C: 



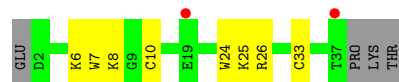
• Molecule 2: Pi-theraphotoxin-Pc1a

Chain M: 




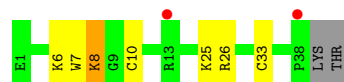
• Molecule 2: Pi-theraphotoxin-Pc1a

Chain N: 



• Molecule 2: Pi-theraphotoxin-Pc1a

Chain O: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.29Å 108.71Å 126.36Å 90.00° 119.78° 90.00°	Depositor
Resolution (Å)	38.37 – 2.80 38.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (38.37-2.80) 93.4 (38.37-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.202 , 0.231 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	3414 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, CL, 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	0.37	0/3190	0.54	0/4328
1	B	0.37	0/3212	0.55	0/4359
1	C	0.36	0/3267	0.54	0/4433
2	M	0.35	0/301	0.54	0/405
2	N	0.40	0/291	0.56	0/390
2	O	0.36	0/310	0.55	0/417
All	All	0.37	0/10571	0.55	0/14332

There are no bond length outliers.

There are no bond angle outliers.

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	3118	0	2878	34	0
1	B	3138	0	2910	51	0
1	C	3193	0	3009	41	0
2	M	293	0	275	7	0
2	N	284	0	263	6	0
2	O	302	0	284	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	1	0
3	C	1	0	0	0	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
4	C	28	0	26	0	0
5	C	12	0	16	0	0
6	A	37	0	0	1	0
6	B	46	0	0	2	0
6	C	48	0	0	2	0
6	M	6	0	0	0	0
6	N	2	0	0	0	0
6	O	5	0	0	0	0
All	All	10557	0	9700	133	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 7.

All (133) 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:68:TYR:HD2	1:B:425:TYR:CD2	2.05	0.75
2:M:10:CYS:HB3	2:M:33:CYS:SG	2.29	0.73
2:O:10:CYS:HB3	2:O:33:CYS:SG	2.30	0.71
1:C:62:CYS:SG	1:C:434:ILE:HD12	2.35	0.67
2:N:10:CYS:HB3	2:N:33:CYS:SG	2.33	0.67
1:B:68:TYR:CD2	1:B:425:TYR:CD2	2.84	0.65
1:B:427:VAL:O	1:B:430:LEU:HB3	1.99	0.62
6:C:638:HOH:O	2:M:8:LYS:HD3	1.98	0.62
1:A:355:LYS:HD2	2:N:24:TRP:NE1	2.15	0.62
1:C:322:CYS:O	1:C:323:ASN:HB2	2.00	0.62
1:B:51:PHE:CE1	1:B:445:SER:HA	2.36	0.61
1:B:353:VAL:HG12	3:B:501:CL:CL	2.39	0.60
1:C:300:PHE:HD2	1:C:312:ASP:OD1	1.85	0.60
1:B:322:CYS:O	1:B:323:ASN:HB2	2.01	0.59
1:C:45:VAL:HA	1:C:48:ALA:HB3	1.85	0.58
1:B:51:PHE:HE1	1:B:445:SER:HA	1.68	0.58
1:A:243:GLU:HG3	1:B:380:ILE:HG13	1.84	0.58
1:A:380:ILE:HG13	1:C:243:GLU:HG3	1.85	0.58
1:A:355:LYS:HD2	2:N:24:TRP:CE2	2.38	0.58
1:B:88:PHE:CG	1:B:89:PRO:HD2	2.41	0.56
1:A:380:ILE:HG12	1:A:381:PRO:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:HG3	1:C:380:ILE:HG13	1.89	0.55
1:C:66:ILE:HG12	1:C:430:LEU:HD11	1.87	0.55
1:A:122:ARG:HB3	1:A:124:GLU:HG3	1.88	0.54
1:A:322:CYS:O	1:A:323:ASN:HB2	2.08	0.54
1:C:139:LEU:HD13	1:C:234:TRP:CH2	2.43	0.54
1:B:427:VAL:C	1:B:430:LEU:HB3	2.28	0.53
1:A:86:LEU:HD13	1:A:415:ASN:HB2	1.89	0.53
1:B:139:LEU:HD13	1:B:234:TRP:CH2	2.44	0.53
1:C:61:VAL:HG21	1:C:437:GLN:NE2	2.23	0.53
1:C:122:ARG:HB3	1:C:124:GLU:HG3	1.91	0.53
1:A:139:LEU:HD13	1:A:234:TRP:CH2	2.44	0.52
1:B:326:MET:HG2	1:B:341:TYR:CZ	2.44	0.52
1:B:68:TYR:HD2	1:B:425:TYR:CE2	2.28	0.52
1:A:353:VAL:HG23	1:A:354:GLU:HG3	1.89	0.52
1:B:380:ILE:HG12	1:B:381:PRO:HA	1.91	0.52
1:A:287:PRO:HD2	1:A:288:TRP:CE3	2.45	0.51
1:B:122:ARG:HB3	1:B:124:GLU:HG3	1.90	0.51
1:A:300:PHE:HB3	1:A:330:PRO:HB2	1.92	0.51
1:B:86:LEU:HD13	1:B:415:ASN:HB2	1.91	0.51
1:C:353:VAL:HG23	1:C:354:GLU:HG3	1.91	0.51
1:C:380:ILE:HG12	1:C:381:PRO:HA	1.90	0.51
1:A:88:PHE:CG	1:A:89:PRO:HD2	2.45	0.51
1:A:447:LEU:HD23	1:A:448:THR:N	2.26	0.51
1:C:326:MET:HG2	1:C:341:TYR:CZ	2.46	0.50
1:C:88:PHE:CG	1:C:89:PRO:HD2	2.46	0.50
1:A:294:THR:HA	1:A:304:TYR:HB3	1.93	0.50
1:A:326:MET:HG2	1:A:341:TYR:CZ	2.47	0.50
1:A:355:LYS:HD2	2:N:24:TRP:CD1	2.46	0.50
1:B:427:VAL:HA	1:B:430:LEU:HB3	1.94	0.50
1:A:346:ASP:HB2	1:A:347:PRO:HD3	1.93	0.49
1:B:343:GLU:OE1	2:O:8:LYS:HE3	2.12	0.49
1:B:353:VAL:HG23	1:B:354:GLU:HG3	1.93	0.49
1:B:427:VAL:O	1:B:431:LEU:N	2.45	0.49
1:C:346:ASP:HB2	1:C:347:PRO:HD3	1.94	0.49
2:N:25:LYS:HD2	2:N:26:ARG:H	1.78	0.48
1:C:287:PRO:HD2	1:C:288:TRP:CE3	2.49	0.47
1:B:287:PRO:HD2	1:B:288:TRP:CE3	2.50	0.47
1:B:70:PHE:HD1	1:B:72:TYR:HH	1.62	0.47
1:B:346:ASP:HB2	1:B:347:PRO:HD3	1.97	0.47
2:N:6:LYS:HD2	2:N:7:TRP:CE2	2.50	0.47
1:A:287:PRO:HD2	1:A:288:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:TYR:CE2	1:C:430:LEU:HB2	2.51	0.46
2:O:25:LYS:HD2	2:O:26:ARG:H	1.81	0.45
1:B:326:MET:HG2	1:B:341:TYR:CE2	2.52	0.45
1:A:395:LYS:HD2	1:A:399:TYR:CE2	2.52	0.45
1:B:61:VAL:HG12	1:B:62:CYS:N	2.31	0.45
1:B:68:TYR:CE2	1:B:425:TYR:CG	3.04	0.45
1:A:89:PRO:HB3	1:A:371:TYR:CZ	2.52	0.45
1:B:74:HIS:CD2	6:B:645:HOH:O	2.70	0.45
1:B:422:LYS:HE3	1:B:422:LYS:HB3	1.84	0.45
1:C:86:LEU:HD13	1:C:415:ASN:HB2	1.98	0.45
1:B:391:LYS:HE2	1:B:391:LYS:HB3	1.86	0.45
1:A:326:MET:HG2	1:A:341:TYR:CE2	2.52	0.45
1:C:391:LYS:HE2	1:C:391:LYS:HB3	1.86	0.45
1:B:89:PRO:HB3	1:B:371:TYR:CZ	2.53	0.44
1:B:447:LEU:HD13	1:B:447:LEU:HA	1.86	0.44
1:C:276:CYS:HA	1:C:372:GLY:O	2.17	0.44
2:M:25:LYS:HD2	2:M:26:ARG:H	1.83	0.44
1:B:315:THR:OG1	1:B:330:PRO:HD2	2.18	0.44
1:B:276:CYS:HA	1:B:372:GLY:O	2.17	0.44
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.75	0.44
1:C:287:PRO:HD2	1:C:288:TRP:CZ3	2.53	0.43
2:M:6:LYS:HD2	2:M:7:TRP:CE2	2.53	0.43
1:B:74:HIS:HD2	6:B:645:HOH:O	2.00	0.43
1:B:202:GLN:O	1:B:203:ASP:HB2	2.18	0.43
1:B:332:ASP:CG	1:B:332:ASP:O	2.57	0.43
1:C:69:TYR:HD2	1:C:70:PHE:CD1	2.36	0.43
1:A:300:PHE:HD2	1:A:312:ASP:OD1	2.02	0.43
1:A:388:TYR:HA	1:C:130:THR:HG21	2.00	0.43
1:C:202:GLN:O	1:C:203:ASP:HB2	2.19	0.43
1:C:202:GLN:HE21	1:C:202:GLN:HB3	1.70	0.43
1:B:58:LEU:HD13	1:B:437:GLN:C	2.39	0.42
1:B:88:PHE:CD2	1:B:89:PRO:HD2	2.54	0.42
1:A:294:THR:HA	1:A:304:TYR:CB	2.49	0.42
1:A:318:LEU:HD12	1:A:318:LEU:HA	1.88	0.42
1:C:51:PHE:CD2	1:C:51:PHE:C	2.93	0.42
1:C:348:ALA:HA	2:M:7:TRP:CZ3	2.54	0.42
1:C:364:MET:HE3	1:C:364:MET:HB3	1.93	0.42
1:B:149:LYS:HA	1:B:150:PRO:HD3	1.92	0.42
1:A:377:MET:HE3	1:C:377:MET:HE3	2.02	0.42
1:B:287:PRO:HD2	1:B:288:TRP:CZ3	2.54	0.42
1:C:380:ILE:HA	1:C:381:PRO:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:LYS:HB3	1:C:422:LYS:HE3	1.85	0.42
2:O:6:LYS:HD2	2:O:7:TRP:CE2	2.55	0.42
1:B:427:VAL:CA	1:B:430:LEU:HB3	2.50	0.42
1:C:61:VAL:HG21	1:C:437:GLN:CD	2.40	0.42
2:M:21:LEU:HA	2:M:34:VAL:O	2.20	0.42
1:B:85:ARG:HB2	1:B:209:ILE:HD12	2.02	0.41
1:C:89:PRO:HB3	1:C:371:TYR:CZ	2.55	0.41
1:B:364:MET:HE3	1:B:364:MET:HB3	1.92	0.41
1:C:186:LYS:HD3	1:C:202:GLN:OE1	2.21	0.41
1:C:292:LYS:HG2	1:C:293:ALA:N	2.34	0.41
1:A:324:CYS:HB3	6:A:619:HOH:O	2.20	0.41
1:B:395:LYS:HD2	1:B:399:TYR:CE2	2.56	0.41
1:A:422:LYS:HE3	1:A:422:LYS:HB3	1.85	0.41
1:B:61:VAL:HG21	1:B:437:GLN:NE2	2.36	0.41
2:M:8:LYS:HA	2:M:8:LYS:HD2	1.89	0.41
1:A:186:LYS:HD3	1:A:202:GLN:OE1	2.21	0.41
1:C:167:ARG:HD2	6:C:621:HOH:O	2.21	0.41
1:A:202:GLN:O	1:A:203:ASP:HB2	2.21	0.41
1:A:268:PRO:HA	1:A:405:LEU:HB3	2.03	0.41
1:A:181:SER:HB2	1:A:182:PRO:HD2	2.03	0.40
1:B:268:PRO:HA	1:B:405:LEU:HB3	2.03	0.40
1:B:364:MET:HA	1:B:365:PRO:HD3	1.85	0.40
1:C:112:ALA:O	1:C:116:LEU:HG	2.20	0.40
1:A:85:ARG:HB2	1:A:209:ILE:HD12	2.03	0.40
1:B:186:LYS:HD3	1:B:202:GLN:OE1	2.21	0.40
1:C:85:ARG:HB2	1:C:209:ILE:HD12	2.03	0.40
1:C:444:ALA:HA	1:C:447:LEU:HD13	2.02	0.40
1:B:268:PRO:HB2	1:B:402:GLU:O	2.22	0.40
1:C:326:MET:HG2	1:C:341:TYR:CE2	2.56	0.40
1:B:103:ARG:HA	1:B:103:ARG:HD3	1.92	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	403/450 (90%)	394 (98%)	8 (2%)	1 (0%)	44	73
1	B	404/450 (90%)	398 (98%)	6 (2%)	0	100	100
1	C	408/450 (91%)	399 (98%)	9 (2%)	0	100	100
2	M	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
2	N	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
2	O	36/40 (90%)	33 (92%)	3 (8%)	0	100	100
All	All	1320/1470 (90%)	1289 (98%)	30 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	THR

### 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	315/392 (80%)	298 (95%)	17 (5%)	18	48
1	B	319/392 (81%)	299 (94%)	20 (6%)	15	42
1	C	332/392 (85%)	315 (95%)	17 (5%)	20	51
2	M	33/37 (89%)	32 (97%)	1 (3%)	36	70
2	N	31/37 (84%)	30 (97%)	1 (3%)	34	68
2	O	34/37 (92%)	33 (97%)	1 (3%)	37	71
All	All	1064/1287 (83%)	1007 (95%)	57 (5%)	18	48

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	CYS

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Mol	Chain	Res	Type
1	A	64	ASN
1	A	86	LEU
1	A	102	SER
1	A	114	GLU
1	A	121	ASN
1	A	172	SER
1	A	176	ARG
1	A	262	LEU
1	A	279	GLN
1	A	303	THR
1	A	364	MET
1	A	380	ILE
1	A	415	ASN
1	A	425	TYR
1	A	430	LEU
1	A	447	LEU
1	B	61	VAL
1	B	102	SER
1	B	114	GLU
1	B	121	ASN
1	B	172	SER
1	B	176	ARG
1	B	279	GLN
1	B	292	LYS
1	B	303	THR
1	B	337	THR
1	B	361	VAL
1	B	364	MET
1	B	380	ILE
1	B	415	ASN
1	B	425	TYR
1	B	430	LEU
1	B	431	LEU
1	B	433	ASP
1	B	447	LEU
1	B	448	THR
1	C	45	VAL
1	C	51	PHE
1	C	102	SER
1	C	114	GLU
1	C	121	ASN
1	C	172	SER

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Mol	Chain	Res	Type
1	C	176	ARG
1	C	262	LEU
1	C	279	GLN
1	C	292	LYS
1	C	303	THR
1	C	337	THR
1	C	364	MET
1	C	380	ILE
1	C	415	ASN
1	C	425	TYR
1	C	430	LEU
2	M	8	LYS
2	N	8	LYS
2	O	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN

### 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](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	NAG	A	502	1	14,14,15	0.64	0	17,19,21	1.49	2 (11%)
5	GOL	C	502	-	5,5,5	0.35	0	5,5,5	0.29	0
5	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.44	0
4	NAG	C	504	1	14,14,15	0.55	0	17,19,21	1.03	1 (5%)
4	NAG	C	505	1	14,14,15	0.55	0	17,19,21	0.75	0
4	NAG	B	502	1	14,14,15	0.47	0	17,19,21	0.92	1 (5%)
4	NAG	A	503	1	14,14,15	0.42	0	17,19,21	0.75	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
4	NAG	A	502	1	-	4/6/23/26	0/1/1/1
5	GOL	C	502	-	-	0/4/4/4	-
5	GOL	C	503	-	-	2/4/4/4	-
4	NAG	C	504	1	-	4/6/23/26	0/1/1/1
4	NAG	C	505	1	-	2/6/23/26	0/1/1/1
4	NAG	B	502	1	-	1/6/23/26	0/1/1/1
4	NAG	A	503	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	NAG	C1-O5-C5	4.94	118.81	112.19
4	C	504	NAG	C1-O5-C5	3.37	116.71	112.19
4	B	502	NAG	C2-N2-C7	-2.62	119.39	122.90
4	A	502	NAG	O5-C1-C2	2.42	115.04	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	NAG	C8-C7-N2-C2
4	A	502	NAG	O7-C7-N2-C2
4	A	503	NAG	C8-C7-N2-C2
4	A	503	NAG	O7-C7-N2-C2
4	C	504	NAG	O7-C7-N2-C2
4	A	503	NAG	O5-C5-C6-O6
4	C	504	NAG	C8-C7-N2-C2
4	C	505	NAG	O5-C5-C6-O6
4	C	505	NAG	C4-C5-C6-O6
4	C	504	NAG	O5-C5-C6-O6
4	A	503	NAG	C4-C5-C6-O6
4	A	502	NAG	C4-C5-C6-O6
4	A	502	NAG	O5-C5-C6-O6
5	C	503	GOL	O1-C1-C2-O2
4	B	502	NAG	O5-C5-C6-O6
5	C	503	GOL	O2-C2-C3-O3
4	C	504	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/450 (90%)	0.53	60 (14%) <b>7</b> <b>6</b>	35, 61, 159, 174	0
1	B	406/450 (90%)	0.53	57 (14%) <b>7</b> <b>7</b>	35, 61, 143, 157	0
1	C	410/450 (91%)	0.43	46 (11%) <b>11</b> <b>9</b>	36, 60, 130, 159	0
2	M	37/40 (92%)	0.39	3 (8%) <b>19</b> <b>15</b>	51, 66, 104, 112	0
2	N	36/40 (90%)	0.51	2 (5%) <b>31</b> <b>24</b>	51, 68, 101, 106	0
2	O	38/40 (95%)	0.45	2 (5%) <b>33</b> <b>26</b>	52, 71, 106, 114	0
All	All	1332/1470 (90%)	0.49	170 (12%) <b>9</b> <b>8</b>	35, 62, 145, 174	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	VAL	10.4
1	C	451	GLU	6.7
1	A	425	TYR	6.6
1	A	426	GLU	6.3
1	B	436	GLY	5.9
1	B	297	ASP	5.8
1	C	295	THR	5.8
2	N	37	THR	5.8
1	A	432	GLY	5.7
1	B	437	GLN	5.7
1	A	428	ALA	5.6
1	C	448	THR	5.6
1	B	425	TYR	5.4
1	B	62	CYS	5.3
1	C	297	ASP	5.2
1	B	450	LEU	5.1
1	C	447	LEU	5.0
1	A	437	GLN	4.9
1	B	439	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	299	GLU	4.9
1	B	427	VAL	4.8
1	C	443	GLY	4.8
1	A	295	THR	4.7
1	C	449	VAL	4.7
1	C	299	GLU	4.6
1	A	54	SER	4.6
1	B	440	LEU	4.4
1	B	294	THR	4.4
1	B	50	CYS	4.3
1	A	440	LEU	4.3
1	A	431	LEU	4.3
1	B	60	LEU	4.3
1	B	444	ALA	4.2
1	C	296	GLY	4.2
1	C	49	LEU	4.2
1	C	442	ILE	4.2
1	C	444	ALA	4.2
1	A	65	ARG	4.1
1	A	360	CYS	4.1
1	B	47	TRP	4.0
1	C	450	LEU	4.0
1	C	294	THR	4.0
1	A	50	CYS	4.0
1	B	46	VAL	4.0
2	O	38	PRO	3.9
1	C	360	CYS	3.9
1	C	425	TYR	3.9
1	B	300	PHE	3.7
1	B	45	VAL	3.7
1	A	430	LEU	3.6
1	B	61	VAL	3.6
1	B	435	GLY	3.5
1	A	81	VAL	3.5
1	C	147	ASN	3.5
1	A	58	LEU	3.5
1	C	51	PHE	3.5
1	B	443	GLY	3.5
1	A	63	THR	3.5
1	C	438	MET	3.4
1	B	68	TYR	3.4
1	C	427	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	51	PHE	3.4
1	B	296	GLY	3.3
1	A	51	PHE	3.3
1	A	448	THR	3.3
1	B	434	ILE	3.2
1	B	441	PHE	3.2
2	M	38	PRO	3.2
1	B	428	ALA	3.2
1	B	298	SER	3.2
1	C	58	LEU	3.2
1	A	299	GLU	3.2
1	C	68	TYR	3.1
1	B	302	ASP	3.1
1	C	440	LEU	3.1
1	B	57	LEU	3.0
2	M	28	ARG	3.0
1	C	445	SER	3.0
1	A	454	ASP	3.0
1	A	294	THR	3.0
2	M	19	GLU	3.0
1	B	332	ASP	2.9
1	B	360	CYS	2.9
1	B	426	GLU	2.9
1	C	446	ILE	2.9
1	B	424	ALA	2.9
1	C	45	VAL	2.9
1	B	65	ARG	2.9
1	B	54	SER	2.9
1	B	448	THR	2.9
1	C	47	TRP	2.9
1	A	293	ALA	2.9
1	B	295	THR	2.8
1	C	133	GLU	2.8
1	A	414	LEU	2.8
1	A	436	GLY	2.8
1	C	177	GLY	2.8
1	A	72	TYR	2.7
1	A	413	ALA	2.7
1	C	46	VAL	2.7
1	A	391	LYS	2.7
1	A	297	ASP	2.7
1	A	434	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	453	PHE	2.7
1	B	128	THR	2.7
1	A	362	CYS	2.7
1	A	423	LYS	2.7
1	C	54	SER	2.7
1	A	424	ALA	2.6
1	A	69	TYR	2.6
1	B	130	THR	2.6
1	B	442	ILE	2.6
1	C	65	ARG	2.6
1	A	59	ALA	2.6
1	C	44	ARG	2.6
1	A	61	VAL	2.6
1	A	300	PHE	2.6
1	A	102	SER	2.6
1	A	332	ASP	2.5
1	A	447	LEU	2.5
1	A	449	VAL	2.5
1	C	290	ASP	2.4
1	A	83	ALA	2.4
1	C	292	LYS	2.4
1	A	82	ALA	2.4
1	B	430	LEU	2.4
2	N	19	GLU	2.4
1	A	444	ALA	2.4
1	A	441	PHE	2.3
1	A	323	ASN	2.3
1	B	303	THR	2.3
1	B	52	MET	2.3
1	C	287	PRO	2.3
1	C	361	VAL	2.3
1	B	121	ASN	2.3
1	B	438	MET	2.3
1	C	298	SER	2.3
1	A	52	MET	2.3
1	B	447	LEU	2.3
1	C	64	ASN	2.3
1	C	121	ASN	2.2
1	A	80	GLU	2.2
1	C	293	ALA	2.2
1	B	431	LEU	2.2
1	A	121	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	287	PRO	2.2
1	C	435	GLY	2.2
1	A	67	GLN	2.2
1	A	358	GLU	2.2
1	A	356	ASP	2.2
1	B	63	THR	2.2
1	A	60	LEU	2.2
1	A	363	GLU	2.2
1	A	387	LYS	2.2
1	B	48	ALA	2.1
1	B	55	LEU	2.1
1	C	42	LEU	2.1
1	B	73	PRO	2.1
1	A	433	ASP	2.1
1	A	56	ALA	2.1
1	B	58	LEU	2.1
1	B	49	LEU	2.1
1	B	112	ALA	2.1
1	C	428	ALA	2.1
1	C	441	PHE	2.1
1	A	290	ASP	2.1
1	B	361	VAL	2.1
1	C	437	GLN	2.0
2	O	13	ARG	2.0
1	A	134	LYS	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	NAG	A	503	14/15	0.69	0.14	100,120,130,133	0
4	NAG	C	505	14/15	0.73	0.12	89,107,115,118	0
4	NAG	A	502	14/15	0.76	0.18	95,116,134,134	0
4	NAG	C	504	14/15	0.82	0.14	91,105,115,119	0
4	NAG	B	502	14/15	0.82	0.14	73,94,110,113	0
5	GOL	C	502	6/6	0.84	0.17	72,81,85,92	0
3	CL	A	501	1/1	0.93	0.18	81,81,81,81	0
5	GOL	C	503	6/6	0.93	0.15	53,66,71,76	0
3	CL	B	501	1/1	0.95	0.15	71,71,71,71	0
3	CL	C	501	1/1	0.97	0.14	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.