



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:49 PM BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

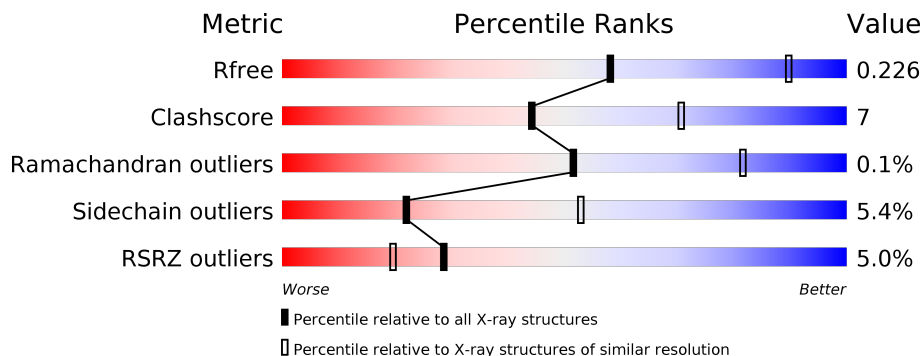
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	450	 2% 77% 12% • 10%
1	B	450	 8% 74% 14% • 10%
1	C	450	 4% 76% 13% • 9%
2	M	40	 70% 20% • 8%
2	N	40	 70% 20% 10%
2	O	40	 5% 78% 15% • 5%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	405	Total 3118	C 1983	N 515	O 596	S 24	0	0	0
1	B	406	Total 3138	C 2001	N 516	O 598	S 23	0	0	0
1	C	410	Total 3193	C 2041	N 522	O 605	S 25	0	0	0

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

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

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

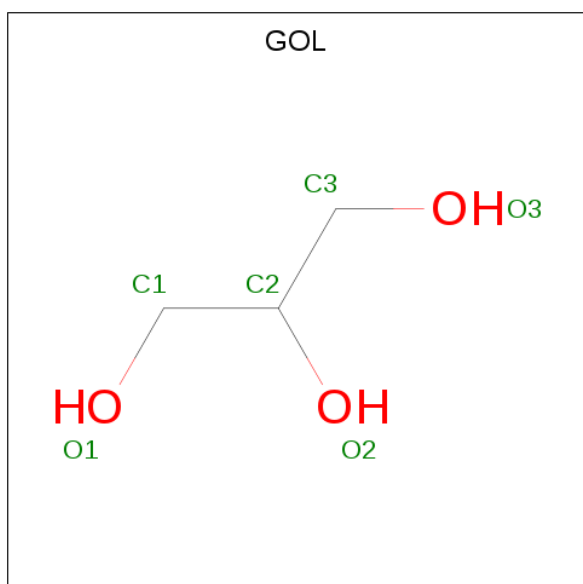
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- 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		

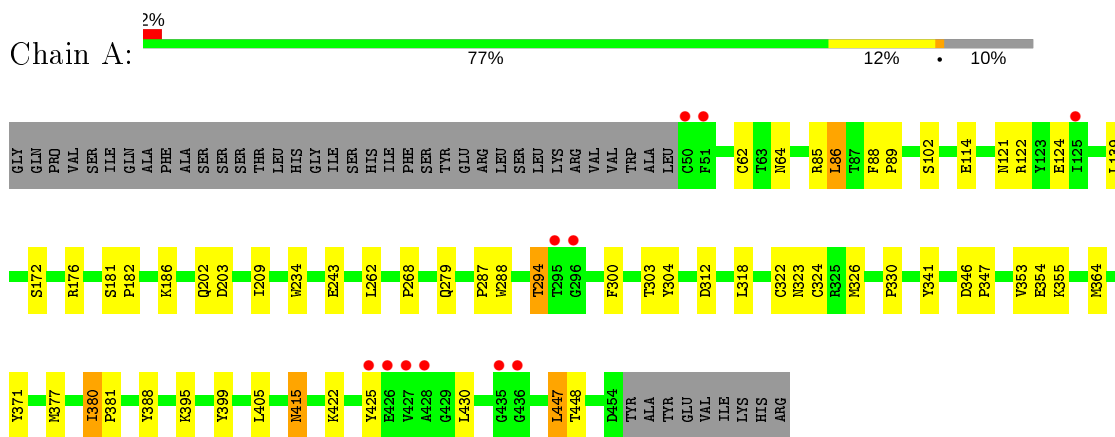
- Molecule 6 is water.

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		

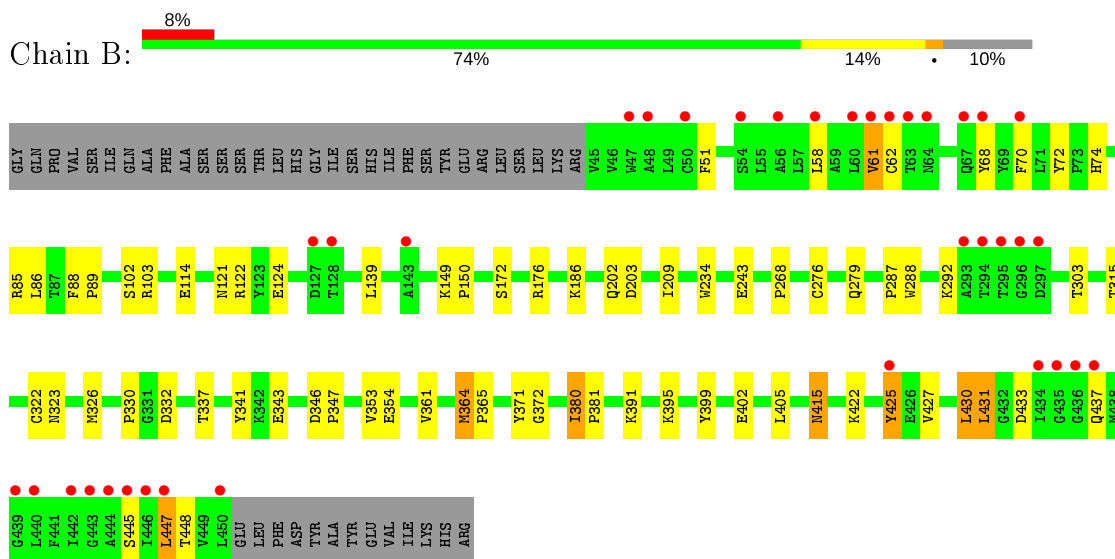
3 Residue-property plots [i](#)

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.

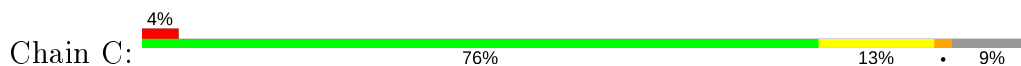
- Molecule 1: Acid-sensing ion channel 1

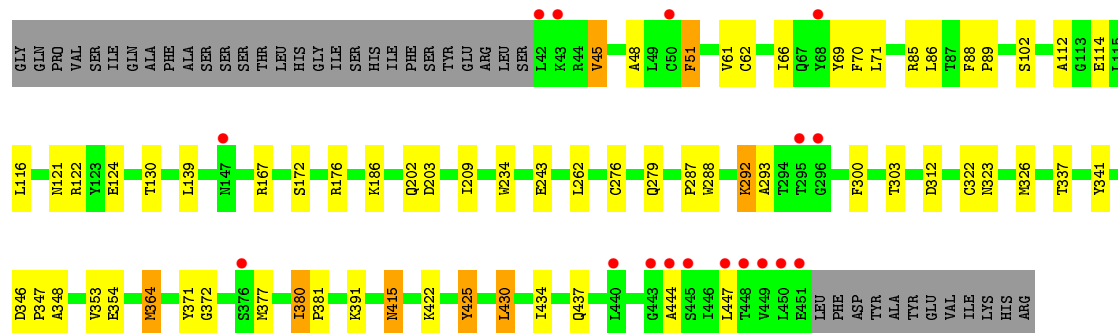


- Molecule 1: Acid-sensing ion channel 1



- Molecule 1: Acid-sensing ion channel 1





- Molecule 2: Pi-theraphotoxin-Pc1a

Chain M: 70% 20% 8%



- Molecule 2: Pi-theraphotoxin-Pc1a

Chain N: 70% 20% 10%



- Molecule 2: Pi-theraphotoxin-Pc1a

Chain O: 5% 78% 15% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.29Å 108.71Å 126.36Å 90.00° 119.78° 90.00°	Depositor
Resolution (Å)	38.37 – 2.80 48.21 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.2 (38.37-2.80) 92.7 (48.21-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.202 , 0.231 0.198 , 0.226	Depositor DCC
R_{free} test set	3436 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtrriage
Anisotropy	0.416	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10557	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage'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.*

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: GOL, NAG, CL

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:447:LEU:HD23	1:A:448:THR:N	2.26	0.51
1:A:88:PHE:CG	1:A:89:PRO:HD2	2.45	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:B:427:VAL:HA	1:B:430:LEU:HB3	1.94	0.50
1:A:355:LYS:HD2	2:N:24:TRP:CD1	2.46	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:422:LYS:HB3	1:B:422:LYS:HE3	1.84	0.45
1:B:74:HIS:CD2	6:B:645:HOH:O	2.70	0.45
1:C:86:LEU:HD13	1:C:415:ASN:HB2	1.98	0.45
1:B:391:LYS:HB3	1:B:391:LYS:HE2	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:HA	1:C:71:LEU:HD23	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:202:GLN:O	1:B:203:ASP:HB2	2.18	0.43
1:B:74:HIS:HD2	6:B:645:HOH:O	2.00	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:HB3	1:C:202:GLN:HE21	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:348:ALA:HA	2:M:7:TRP:CZ3	2.54	0.42
1:C:364:MET:HB3	1:C:364:MET:HE3	1.93	0.42
1:C:51:PHE:CD2	1:C:51:PHE:C	2.93	0.42
1:B:149:LYS:HA	1:B:150:PRO:HD3	1.92	0.42
1:B:287:PRO:HD2	1:B:288:TRP:CZ3	2.54	0.42
1:A:377:MET:HE3	1:C:377:MET:HE3	2.02	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:HE3	1:C:422:LYS:HB3	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:HB3	1:A:422:LYS:HE3	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:364:MET:HA	1:B:365:PRO:HD3	1.85	0.40
1:B:268:PRO:HA	1:B:405:LEU:HB3	2.03	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:444:ALA:HA	1:C:447:LEU:HD13	2.02	0.40
1:C:85:ARG:HB2	1:C:209:ILE:HD12	2.03	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:HD3	1:B:103:ARG:HA	1.92	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	403/450 (90%)	394 (98%)	8 (2%)	1 (0%)	47	78
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%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/392 (80%)	298 (95%)	17 (5%)	22	53
1	B	319/392 (81%)	299 (94%)	20 (6%)	18	46
1	C	332/392 (85%)	315 (95%)	17 (5%)	24	55
2	M	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	N	31/37 (84%)	30 (97%)	1 (3%)	39	73
2	O	34/37 (92%)	33 (97%)	1 (3%)	42	76
All	All	1064/1287 (83%)	1007 (95%)	57 (5%)	22	53

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

Some 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 monosaccharides 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	B	502	1	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
4	NAG	C	504	1	14,14,15	0.56	0	17,19,21	1.04	1 (5%)
4	NAG	A	503	1	14,14,15	0.43	0	17,19,21	0.79	0
5	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.40	0
4	NAG	A	502	1	14,14,15	0.62	0	17,19,21	1.47	2 (11%)
5	GOL	C	502	-	5,5,5	0.34	0	5,5,5	0.27	0
4	NAG	C	505	1	14,14,15	0.55	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	B	502	1	-	1/6/23/26	0/1/1/1
4	NAG	C	504	1	-	4/6/23/26	0/1/1/1
4	NAG	A	503	1	-	4/6/23/26	0/1/1/1
5	GOL	C	503	-	-	4/4/4/4	-
4	NAG	A	502	1	-	4/6/23/26	0/1/1/1
5	GOL	C	502	-	-	0/4/4/4	-
4	NAG	C	505	1	-	2/6/23/26	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	4.88	118.81	112.19
4	C	504	NAG	C1-O5-C5	3.33	116.71	112.19
4	B	502	NAG	C2-N2-C7	-2.47	119.39	122.90
4	A	502	NAG	O5-C1-C2	2.37	115.04	111.29

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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 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	405/450 (90%)	-0.14	11 (2%) 54 44	35, 61, 159, 174	0
1	B	406/450 (90%)	0.14	36 (8%) 9 5	35, 61, 143, 157	0
1	C	410/450 (91%)	-0.06	17 (4%) 37 27	36, 60, 130, 159	0
2	M	37/40 (92%)	-0.25	0 100 100	51, 66, 104, 112	0
2	N	36/40 (90%)	-0.11	0 100 100	51, 68, 101, 106	0
2	O	38/40 (95%)	0.12	2 (5%) 26 17	52, 71, 106, 114	0
All	All	1332/1470 (90%)	-0.03	66 (4%) 28 19	35, 62, 145, 174	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	447	LEU	6.7
1	B	439	GLY	5.8
1	B	437	GLN	5.7
1	C	451	GLU	5.5
2	O	38	PRO	5.2
1	B	48	ALA	5.2
1	C	295	THR	5.0
1	B	443	GLY	4.8
1	B	440	LEU	4.6
1	A	426	GLU	4.4
1	B	293	ALA	4.3
1	B	68	TYR	4.2
1	A	425	TYR	4.2
1	B	294	THR	4.1
1	B	444	ALA	4.0
1	B	435	GLY	4.0
1	C	449	VAL	4.0
1	C	444	ALA	3.9
1	B	62	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	448	THR	3.8
1	A	296	GLY	3.8
1	A	427	VAL	3.8
1	B	436	GLY	3.7
1	B	295	THR	3.7
1	B	61	VAL	3.7
1	B	447	LEU	3.6
1	B	47	TRP	3.4
1	B	446	ILE	3.3
1	A	295	THR	3.2
1	B	50	CYS	3.2
1	B	425	TYR	3.1
1	C	450	LEU	3.1
1	C	42	LEU	3.1
1	A	51	PHE	3.1
1	B	442	ILE	3.1
1	C	50	CYS	3.0
1	B	296	GLY	3.0
1	C	147	ASN	3.0
1	A	435	GLY	2.9
1	B	450	LEU	2.9
1	C	445	SER	2.8
1	C	440	LEU	2.8
1	B	128	THR	2.8
1	C	443	GLY	2.7
1	A	50	CYS	2.7
1	B	60	LEU	2.6
1	C	376	SER	2.5
1	B	67	GLN	2.5
1	C	296	GLY	2.4
1	B	127	ASP	2.4
1	A	125	ILE	2.4
1	B	434	ILE	2.4
1	B	445	SER	2.4
1	B	54	SER	2.4
2	O	20	GLY	2.3
1	B	56	ALA	2.3
1	B	58	LEU	2.3
1	B	63	THR	2.2
1	A	428	ALA	2.2
1	A	436	GLY	2.1
1	B	143	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	297	ASP	2.1
1	B	64	ASN	2.1
1	C	43	LYS	2.1
1	B	70	PHE	2.1
1	C	68	TYR	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 monosaccharides 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
4	NAG	A	502	14/15	0.85	0.26	95,116,134,134	0
5	GOL	C	502	6/6	0.89	0.16	72,81,85,92	0
4	NAG	B	502	14/15	0.90	0.29	73,94,110,113	0
4	NAG	C	504	14/15	0.90	0.20	91,105,115,119	0
4	NAG	A	503	14/15	0.91	0.20	100,120,130,133	0
3	CL	A	501	1/1	0.91	0.17	81,81,81,81	0
5	GOL	C	503	6/6	0.93	0.16	53,66,71,76	0
4	NAG	C	505	14/15	0.93	0.28	89,107,115,118	0
3	CL	C	501	1/1	0.93	0.16	77,77,77,77	0
3	CL	B	501	1/1	0.94	0.14	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.