



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 03:34 AM GMT

PDB ID : 3S3X  
Title : Structure of chicken acid-sensing ion channel 1 AT 3.0 Å resolution in complex with psalmotoxin  
Authors : Dawson, R.J.P.; Benz, J.; Stohler, P.; Tetaz, T.; Joseph, C.; Huber, S.; Schmid, G.; Huegin, D.; Pflimlin, P.; Trube, G.; Rudolph, M.G.; Hennig, M.; Ruf, A.  
Deposited on : 2011-05-18  
Resolution : 2.99 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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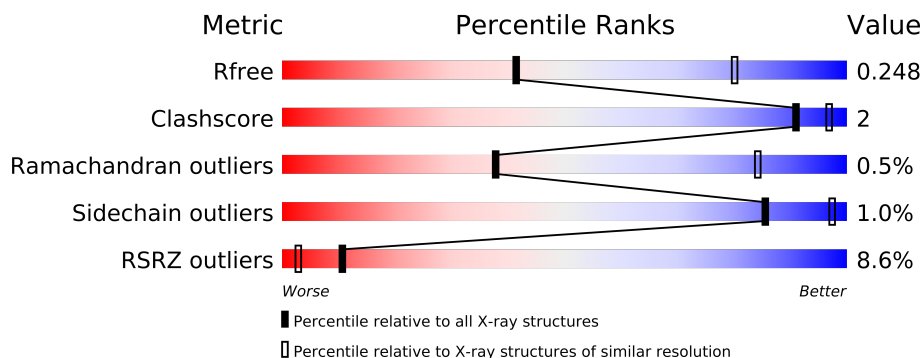
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.99 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	459	
1	B	459	
1	C	459	
2	D	37	
2	E	37	
2	F	37	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	600	-	X
3	NAG	B	600	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	C	600	-	X
4	K	A	1	-	X
5	CL	A	464	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10519 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Amiloride-sensitive cation channel 2, neuronal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3209	2054	521	607	27			
1	B	391	Total	C	N	O	S	0	0	0
			3139	2008	510	594	27			
1	C	396	Total	C	N	O	S	0	0	0
			3168	2026	515	600	27			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	EXPRESSION TAG	UNP Q1XA76
A	6	SER	-	EXPRESSION TAG	UNP Q1XA76
A	7	TYR	-	EXPRESSION TAG	UNP Q1XA76
A	8	TYR	-	EXPRESSION TAG	UNP Q1XA76
A	9	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	10	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	11	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	12	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	13	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	14	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	15	GLY	-	EXPRESSION TAG	UNP Q1XA76
A	16	ALA	-	EXPRESSION TAG	UNP Q1XA76
A	17	SER	-	EXPRESSION TAG	UNP Q1XA76
A	18	LEU	-	EXPRESSION TAG	UNP Q1XA76
A	19	VAL	-	EXPRESSION TAG	UNP Q1XA76
A	20	PRO	-	EXPRESSION TAG	UNP Q1XA76
A	21	ARG	-	EXPRESSION TAG	UNP Q1XA76
A	22	GLY	-	EXPRESSION TAG	UNP Q1XA76
A	23	SER	-	EXPRESSION TAG	UNP Q1XA76
A	24	HIS	-	EXPRESSION TAG	UNP Q1XA76
A	25	MET	-	EXPRESSION TAG	UNP Q1XA76
B	5	MET	-	EXPRESSION TAG	UNP Q1XA76
B	6	SER	-	EXPRESSION TAG	UNP Q1XA76

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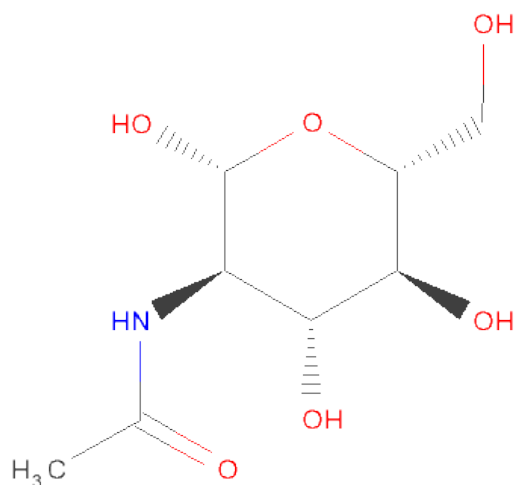
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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	TYR	-	EXPRESSION TAG	UNP Q1XA76
B	8	TYR	-	EXPRESSION TAG	UNP Q1XA76
B	9	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	10	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	11	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	12	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	13	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	14	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	15	GLY	-	EXPRESSION TAG	UNP Q1XA76
B	16	ALA	-	EXPRESSION TAG	UNP Q1XA76
B	17	SER	-	EXPRESSION TAG	UNP Q1XA76
B	18	LEU	-	EXPRESSION TAG	UNP Q1XA76
B	19	VAL	-	EXPRESSION TAG	UNP Q1XA76
B	20	PRO	-	EXPRESSION TAG	UNP Q1XA76
B	21	ARG	-	EXPRESSION TAG	UNP Q1XA76
B	22	GLY	-	EXPRESSION TAG	UNP Q1XA76
B	23	SER	-	EXPRESSION TAG	UNP Q1XA76
B	24	HIS	-	EXPRESSION TAG	UNP Q1XA76
B	25	MET	-	EXPRESSION TAG	UNP Q1XA76
C	5	MET	-	EXPRESSION TAG	UNP Q1XA76
C	6	SER	-	EXPRESSION TAG	UNP Q1XA76
C	7	TYR	-	EXPRESSION TAG	UNP Q1XA76
C	8	TYR	-	EXPRESSION TAG	UNP Q1XA76
C	9	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	10	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	11	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	12	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	13	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	14	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	15	GLY	-	EXPRESSION TAG	UNP Q1XA76
C	16	ALA	-	EXPRESSION TAG	UNP Q1XA76
C	17	SER	-	EXPRESSION TAG	UNP Q1XA76
C	18	LEU	-	EXPRESSION TAG	UNP Q1XA76
C	19	VAL	-	EXPRESSION TAG	UNP Q1XA76
C	20	PRO	-	EXPRESSION TAG	UNP Q1XA76
C	21	ARG	-	EXPRESSION TAG	UNP Q1XA76
C	22	GLY	-	EXPRESSION TAG	UNP Q1XA76
C	23	SER	-	EXPRESSION TAG	UNP Q1XA76
C	24	HIS	-	EXPRESSION TAG	UNP Q1XA76
C	25	MET	-	EXPRESSION TAG	UNP Q1XA76

- Molecule 2 is a protein called Psalmotoxin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	37	Total	C	N	O	S	0	0	0
			299	185	58	50	6			
2	E	37	Total	C	N	O	S	0	0	0
			299	185	58	50	6			
2	F	37	Total	C	N	O	S	0	0	0
			299	185	58	50	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

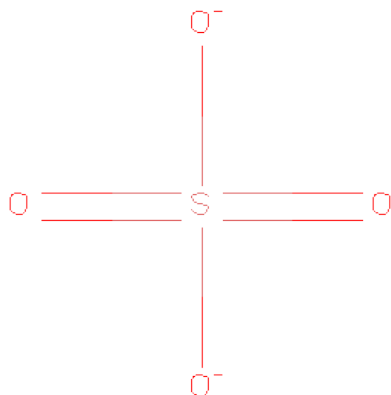
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

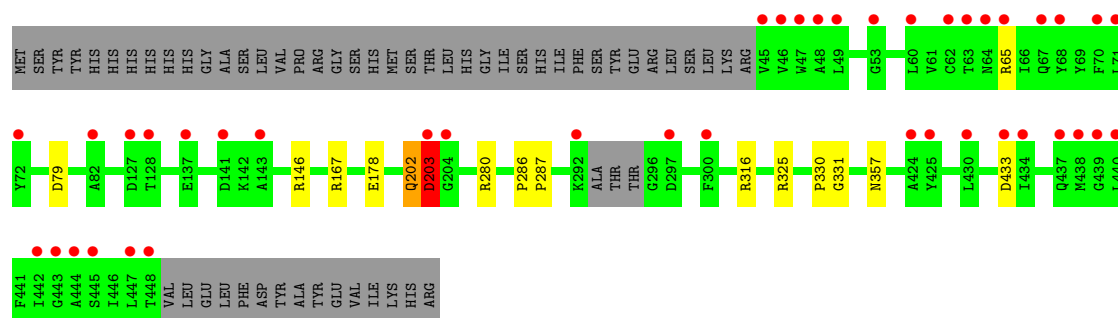
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total O 4 4	0	0
7	B	3	Total O 3 3	0	0
7	C	6	Total O 6 6	0	0
7	E	1	Total O 1 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

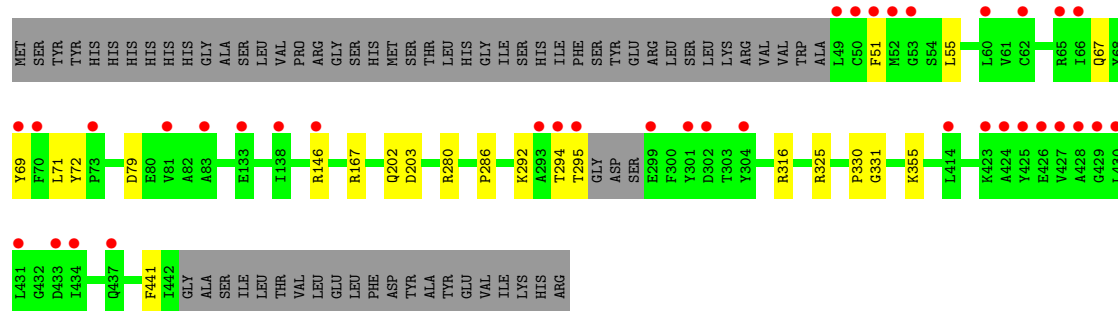
- Molecule 1: Amiloride-sensitive cation channel 2, neuronal

Chain A: 



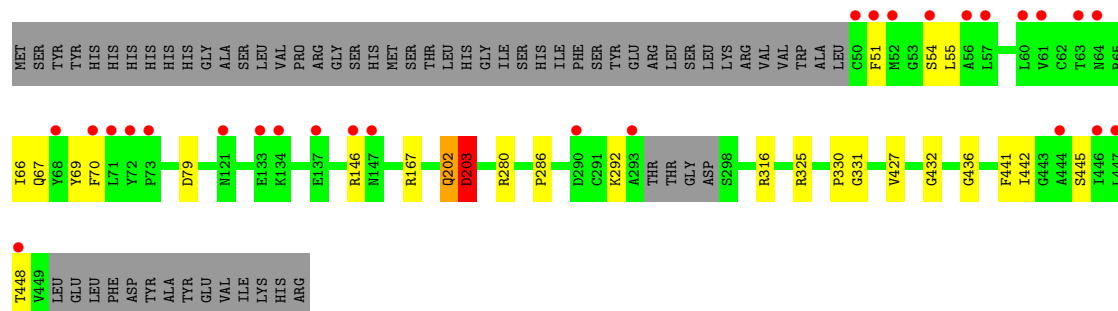
- Molecule 1: Amiloride-sensitive cation channel 2, neuronal

Chain B: 



- Molecule 1: Amiloride-sensitive cation channel 2, neuronal

Chain C: 





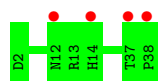
- Molecule 2: Psalmotoxin-1

Chain D: 



- Molecule 2: Psalmotoxin-1

Chain E: 



- Molecule 2: Psalmotoxin-1

Chain F: 

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.40Å 109.44Å 127.27Å 90.00° 119.81° 90.00°	Depositor
Resolution (Å)	29.91 – 2.99 29.92 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.91-2.99) 93.0 (29.92-2.99)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.218 , 0.249 0.218 , 0.248	Depositor DCC
$R_{free}$ test set	2658 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.6	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 55795 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CL, SO4, NAG

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	0.29	2/3284 (0.1%)	0.50	8/4445 (0.2%)
1	B	0.25	0/3212	0.51	8/4346 (0.2%)
1	C	0.26	0/3241	0.82	12/4385 (0.3%)
2	D	0.19	0/307	0.40	0/412
2	E	0.20	0/307	0.39	0/412
2	F	0.20	0/307	0.39	0/412
All	All	0.26	2/10658 (0.0%)	0.61	28/14412 (0.2%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	ASN	CG-ND2	-7.41	1.14	1.32
1	A	357	ASN	CG-OD1	-6.98	1.08	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ARG	NE-CZ-NH2	19.65	130.12	120.30
1	C	280	ARG	NE-CZ-NH1	-17.81	111.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ARG	NE-CZ-NH1	-15.54	112.53	120.30
1	C	146	ARG	NE-CZ-NH2	-15.49	112.55	120.30
1	C	167	ARG	NE-CZ-NH1	-15.18	112.71	120.30
1	C	146	ARG	NE-CZ-NH1	14.98	127.79	120.30
1	C	316	ARG	NE-CZ-NH2	14.95	127.78	120.30
1	C	167	ARG	NE-CZ-NH2	14.64	127.62	120.30
1	B	316	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	316	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	146	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	A	146	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	167	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	167	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	316	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	316	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	B	146	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	146	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	146	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	C	316	ARG	CD-NE-CZ	7.32	133.85	123.60
1	C	167	ARG	CD-NE-CZ	7.28	133.79	123.60
1	A	167	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	B	167	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	280	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	280	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	280	ARG	CD-NE-CZ	5.90	131.85	123.60
1	B	280	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	280	ARG	NE-CZ-NH1	5.64	123.12	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	PRO	Peptide
1	B	286	PRO	Peptide
1	C	286	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	0	4	0
1	B	3139	0	0	8	0
1	C	3168	0	0	10	0
2	D	299	0	0	0	0
2	E	299	0	0	0	0
2	F	299	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
7	C	6	0	0	0	0
7	E	1	0	0	0	0
All	All	10519	0	0	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:442:ILE:O	1:C:445:SER:OG	2.10	0.69
1:C:445:SER:O	1:C:448:THR:OG1	2.14	0.66
1:A:65:ARG:NH2	1:A:433:ASP:CB	2.59	0.65
1:A:202:GLN:O	1:A:203:ASP:CB	2.49	0.60
1:C:67:GLN:O	1:C:70:PHE:N	2.36	0.58
1:B:51:PHE:O	1:B:55:LEU:CG	2.53	0.56
1:B:325:ARG:NH1	1:B:331:GLY:O	2.39	0.56
1:C:202:GLN:O	1:C:203:ASP:CB	2.53	0.56
1:B:69:TYR:C	1:B:71:LEU:N	2.58	0.56
1:A:325:ARG:NH1	1:A:331:GLY:O	2.39	0.54
1:C:325:ARG:NH1	1:C:331:GLY:O	2.40	0.54
1:B:55:LEU:CB	1:B:441:PHE:CE1	2.94	0.50
1:C:55:LEU:N	1:C:441:PHE:CE1	2.82	0.47
1:C:432:GLY:O	1:C:436:GLY:N	2.47	0.46
1:B:202:GLN:O	1:B:203:ASP:CB	2.63	0.46
1:C:51:PHE:O	1:C:54:SER:OG	2.33	0.46
1:B:69:TYR:O	1:B:72:TYR:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:67:GLN:O	1:B:71:LEU:CG	2.68	0.42
1:A:178:GLU:OE1	1:B:355:LYS:NZ	2.53	0.41
1:C:69:TYR:OH	1:C:427:VAL:CG2	2.69	0.41
1:C:66:ILE:CG2	1:C:67:GLN:N	2.84	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	397/459 (86%)	375 (94%)	19 (5%)	3 (1%)	27	76
1	B	387/459 (84%)	365 (94%)	21 (5%)	1 (0%)	50	90
1	C	392/459 (85%)	369 (94%)	21 (5%)	2 (0%)	38	84
2	D	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
2	E	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
2	F	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	1281/1488 (86%)	1211 (94%)	64 (5%)	6 (0%)	38	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASP
1	C	203	ASP
1	A	287	PRO
1	A	330	PRO
1	B	330	PRO
1	C	330	PRO

### 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	349/401 (87%)	346 (99%)	3 (1%)	87	98
1	B	342/401 (85%)	338 (99%)	4 (1%)	82	97
1	C	345/401 (86%)	341 (99%)	4 (1%)	82	97
2	D	34/34 (100%)	34 (100%)	0	100	100
2	E	34/34 (100%)	34 (100%)	0	100	100
2	F	34/34 (100%)	34 (100%)	0	100	100
All	All	1138/1305 (87%)	1127 (99%)	11 (1%)	85	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	202	GLN
1	A	203	ASP
1	B	79	ASP
1	B	292	LYS
1	B	294	THR
1	B	295	THR
1	C	79	ASP
1	C	202	GLN
1	C	203	ASP
1	C	292	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
6	SO4	A	465	-	4,4,4	0.76	0	6,6,6	0.73	0
3	NAG	A	600	1	12,14,15	0.66	0	15,19,21	0.78	0
3	NAG	A	700	1	12,14,15	0.70	1 (8%)	15,19,21	1.02	1 (6%)
3	NAG	B	600	1	12,14,15	0.67	0	15,19,21	0.80	0
3	NAG	B	700	1	12,14,15	0.71	1 (8%)	15,19,21	1.02	1 (6%)
3	NAG	C	600	1	12,14,15	0.63	0	15,19,21	0.95	1 (6%)
3	NAG	C	700	1	12,14,15	0.69	1 (8%)	15,19,21	1.03	1 (6%)

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
6	SO4	A	465	-	-	0/0/0/0	0/0/0/0
3	NAG	A	600	1	-	0/6/23/26	0/1/1/1
3	NAG	A	700	1	-	0/6/23/26	0/1/1/1
3	NAG	B	600	1	-	0/6/23/26	0/1/1/1
3	NAG	B	700	1	-	0/6/23/26	0/1/1/1
3	NAG	C	600	1	-	0/6/23/26	0/1/1/1
3	NAG	C	700	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAG	O5-C5	-2.12	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	NAG	O5-C5	-2.12	1.41	1.45
3	C	700	NAG	O5-C5	-2.07	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	NAG	O5-C5-C6	2.88	110.00	106.98
3	C	700	NAG	O5-C5-C6	2.85	109.97	106.98
3	B	700	NAG	O5-C5-C6	2.79	109.91	106.98
3	C	600	NAG	O5-C5-C6	2.63	109.74	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	401/459 (87%)	0.34	42 (10%) 7 2	51, 86, 198, 251	0
1	B	391/459 (85%)	0.35	37 (9%) 8 2	47, 88, 203, 236	0
1	C	396/459 (86%)	0.14	27 (6%) 17 4	49, 82, 182, 236	0
2	D	37/37 (100%)	0.32	1 (2%) 52 10	71, 100, 147, 180	0
2	E	37/37 (100%)	0.35	4 (10%) 6 2	81, 109, 149, 177	0
2	F	37/37 (100%)	0.19	0 100 100	74, 102, 145, 176	0
All	All	1299/1488 (87%)	0.28	111 (8%) 11 3	47, 88, 194, 251	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	11.7
1	B	50	CYS	9.4
1	A	434	ILE	9.1
1	B	426	GLU	7.9
1	B	51	PHE	7.5
2	D	38	PRO	7.4
1	A	438	MET	7.2
1	C	57	LEU	6.3
1	A	63	THR	6.2
1	A	48	ALA	6.2
1	C	50	CYS	5.9
1	C	60	LEU	5.8
1	A	45	VAL	5.6
1	C	293	ALA	5.6
1	A	440	LEU	5.5
1	A	67	GLN	5.5
1	A	128	THR	5.3
1	C	447	LEU	5.3
1	B	431	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	68	TYR	5.0
1	B	428	ALA	4.9
1	B	425	TYR	4.8
1	B	66	ILE	4.8
1	A	443	GLY	4.8
1	B	427	VAL	4.4
1	C	72	TYR	4.4
1	A	127	ASP	4.3
1	A	64	ASN	4.3
1	A	447	LEU	4.3
1	B	70	PHE	4.3
1	A	46	VAL	4.3
1	A	439	GLY	4.2
1	B	65	ARG	4.2
1	C	54	SER	4.0
2	E	38	PRO	3.9
1	B	299	GLU	3.8
1	A	203	ASP	3.8
1	A	433	ASP	3.8
1	B	83	ALA	3.8
1	B	52	MET	3.8
1	B	294	THR	3.6
1	A	49	LEU	3.6
1	C	448	THR	3.6
1	B	424	ALA	3.6
1	B	295	THR	3.5
1	A	297	ASP	3.5
1	C	56	ALA	3.4
1	B	53	GLY	3.4
1	A	430	LEU	3.4
1	A	60	LEU	3.4
1	B	423	LYS	3.3
1	B	429	GLY	3.3
1	C	121	ASN	3.3
1	B	433	ASP	3.3
1	C	71	LEU	3.3
1	C	61	VAL	3.2
1	B	293	ALA	3.2
1	C	70	PHE	3.1
1	B	60	LEU	3.1
1	A	437	GLN	3.0
1	C	51	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	47	TRP	2.9
1	B	62	CYS	2.9
1	C	52	MET	2.9
1	A	143	ALA	2.9
1	B	146	ARG	2.8
1	A	425	TYR	2.8
1	A	71	LEU	2.8
1	A	70	PHE	2.8
1	B	414	LEU	2.8
1	C	446	ILE	2.7
1	C	444	ALA	2.7
2	E	37	THR	2.6
1	A	292	LYS	2.6
1	A	300	PHE	2.6
1	C	68	TYR	2.6
1	C	134	LYS	2.6
1	B	138	ILE	2.6
1	A	82	ALA	2.5
1	B	301	TYR	2.5
1	A	442	ILE	2.5
2	E	14	HIS	2.5
1	A	137	GLU	2.5
1	C	146	ARG	2.4
1	A	448	THR	2.4
1	B	302	ASP	2.4
1	B	69	TYR	2.4
1	C	73	PRO	2.4
1	C	137	GLU	2.3
1	A	65	ARG	2.3
1	B	430	LEU	2.3
1	B	437	GLN	2.2
1	A	445	SER	2.2
1	A	204	GLY	2.2
1	A	141	ASP	2.2
1	A	444	ALA	2.2
1	A	53	GLY	2.2
1	C	147	ASN	2.1
1	B	81	VAL	2.1
1	C	290	ASP	2.1
1	A	72	TYR	2.1
1	C	64	ASN	2.1
1	B	73	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	63	THR	2.1
2	E	12	ASN	2.1
1	C	133	GLU	2.1
1	A	424	ALA	2.0
1	B	304	TYR	2.0
1	A	62	CYS	2.0
1	B	133	GLU	2.0
1	B	434	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	K	A	1	1/1	0.83	101.49	146,146,146,146	0
3	NAG	B	600	14/15	0.43	10.28	79,147,166,168	0
3	NAG	C	600	14/15	0.34	3.55	89,150,167,170	0
5	CL	A	464	1/1	0.28	3.17	94,94,94,94	0
3	NAG	A	600	14/15	0.37	2.73	86,145,166,168	0
4	K	A	2	1/1	0.26	1.86	96,96,96,96	0
6	SO4	A	465	5/5	0.25	0.95	126,187,225,234	0
3	NAG	C	700	14/15	0.51	-	132,163,181,184	0
3	NAG	A	700	14/15	0.39	-	131,162,184,186	0
3	NAG	B	700	14/15	0.40	-	134,162,183,184	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.