wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 04:10 PM EDT

PDB ID	:	3S3X
Title	:	Structure of chicken acid-sensing ion channel 1 AT 3.0 A 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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

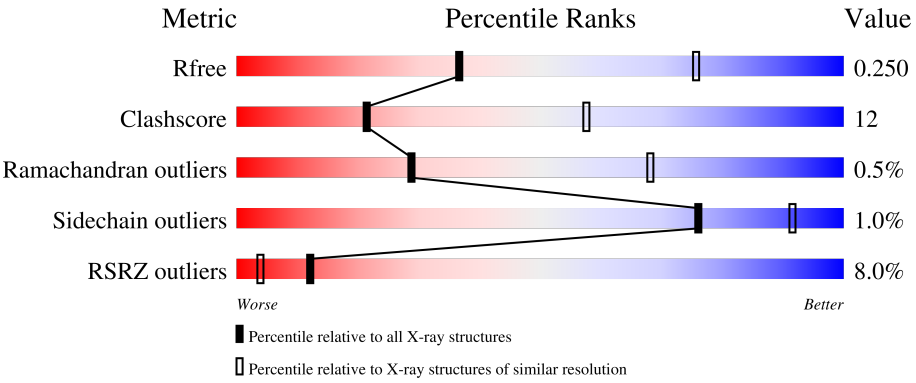
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.99 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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 <=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	459	8% 64% 23% • 13%
1	B	459	8% 61% 24% 15%
1	C	459	5% 61% 25% • 14%
2	D	37	3% 49% 51%
2	E	37	8% 59% 41%

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Mol	Chain	Length	Quality of chain
2	F	37	49% 51%

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
3	NAG	A	700	-	-	-	X
3	NAG	B	700	-	-	-	X
3	NAG	C	700	-	-	-	X
4	K	A	1	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10519 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 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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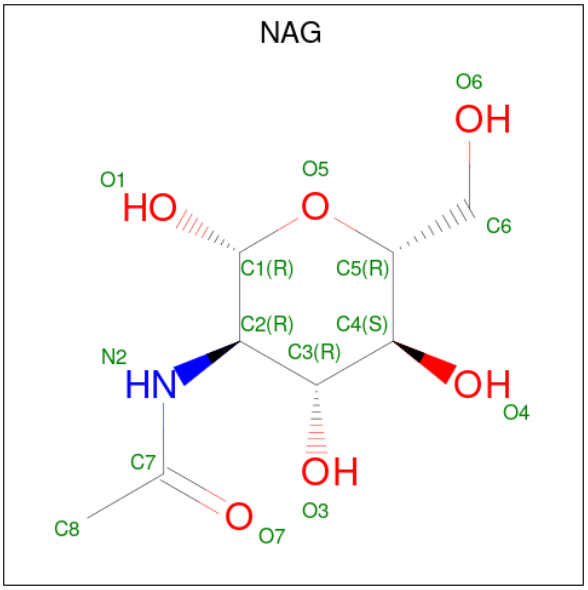
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	TYR	-	expression tag	UNP Q1XA76
B	8	TYR	-	expression tag	UNP Q1XA76
B	9	HIS	-	expression tag	UNP Q1XA76
B	10	HIS	-	expression tag	UNP Q1XA76
B	11	HIS	-	expression tag	UNP Q1XA76
B	12	HIS	-	expression tag	UNP Q1XA76
B	13	HIS	-	expression tag	UNP Q1XA76
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 2-acetamido-2-deoxy-beta-D-glucopyranose (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		

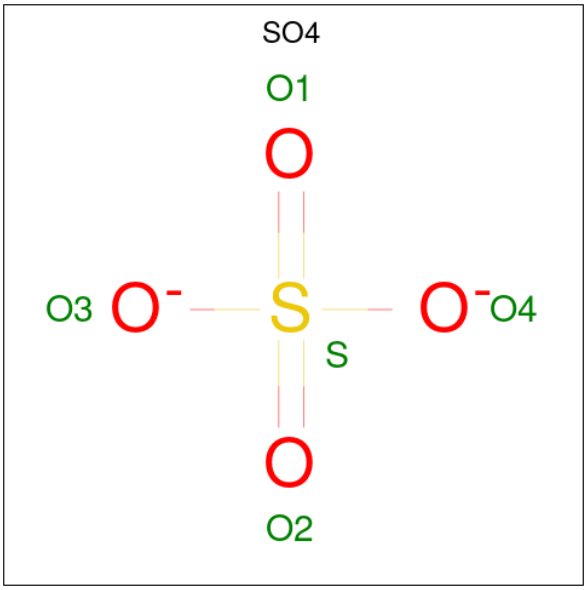
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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_4S).



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

- Molecule 7 is water.

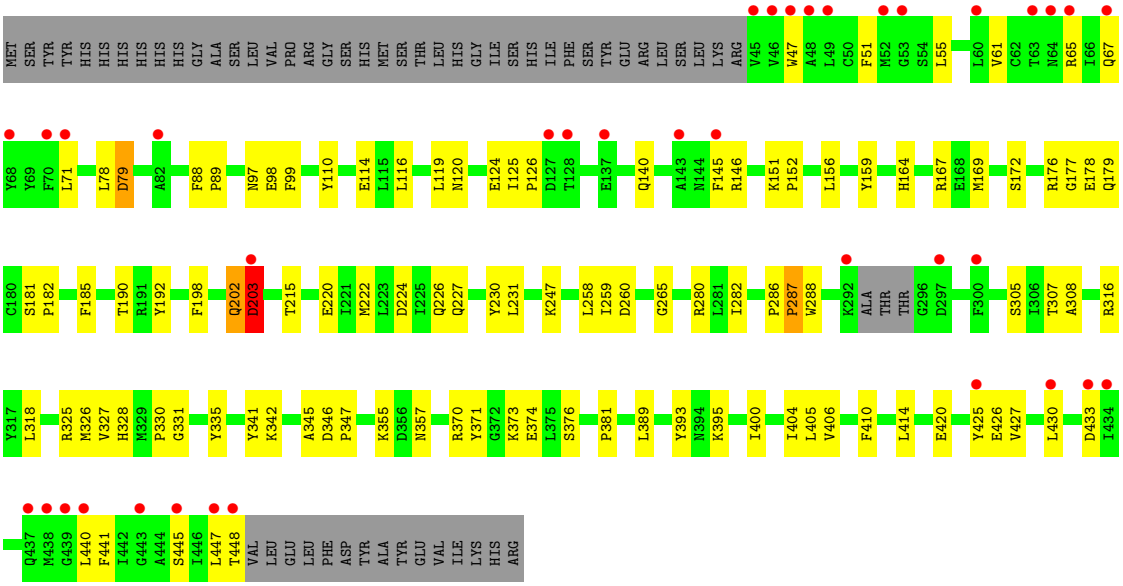
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total O 4 4	0	0
7	B	3	Total O 3 3	0	0
7	C	6	Total O 6 6	0	0
7	E	1	Total O 1 1	0	0

3 Residue-property plots (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.

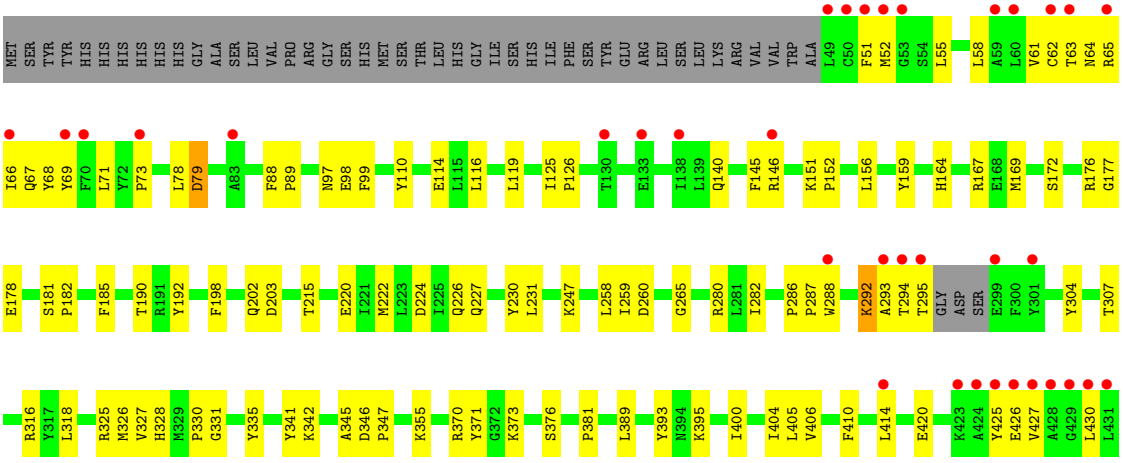
• Molecule 1: Amiloride-sensitive cation channel 2, neuronal

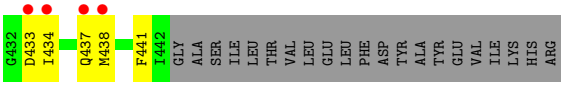
Chain A:



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

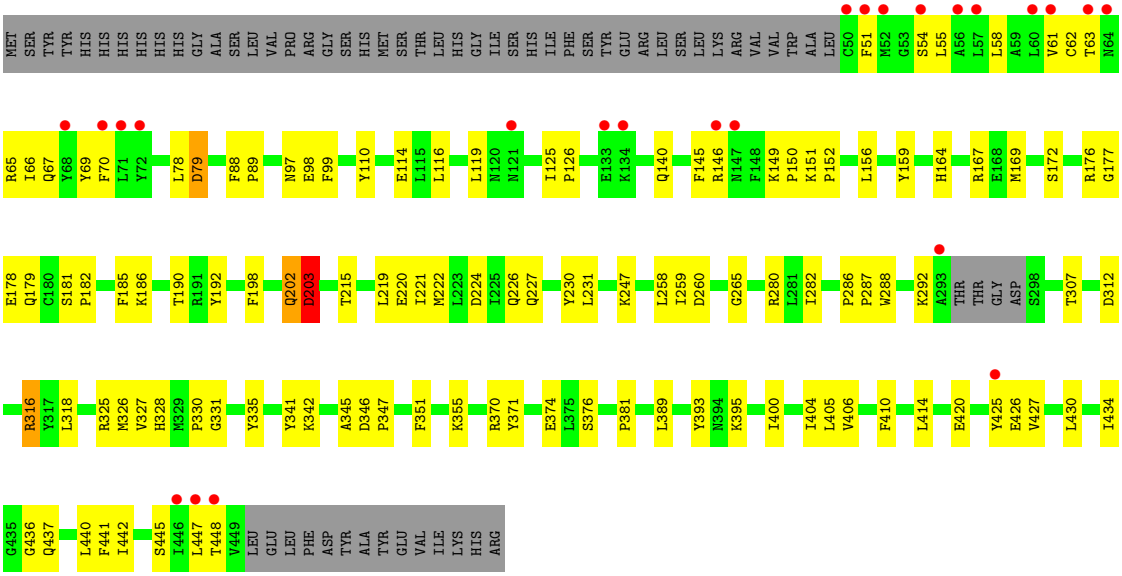
Chain B:





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

Chain C:

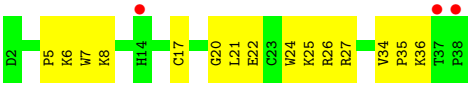


• Molecule 2: Psalmotoxin-1

Chain D:

• Molecule 2: Psalmotoxin-1

Chain E:



• Molecule 2: Psalmotoxin-1

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.26 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.218 , 0.249 0.219 , 0.250	Depositor DCC
R_{free} test set	2829 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10519	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, CL, NAG, K

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

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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

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 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	3209	0	3102	74	0
1	B	3139	0	3034	76	0
1	C	3168	0	3065	88	0
2	D	299	0	286	14	0
2	E	299	0	286	11	0
2	F	299	0	286	15	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	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	10137	248	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 12.

The worst 5 of 248 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:440:LEU:HA	1:C:447:LEU:HD11	1.34	1.10
1:B:51:PHE:O	1:B:55:LEU:HG	1.56	1.05
1:B:66:ILE:HB	1:B:434:ILE:HD11	1.49	0.91
1:B:55:LEU:HB3	1:B:441:PHE:CE1	2.06	0.91
1:C:202:GLN:O	1:C:203:ASP:HB2	1.72	0.88

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	397/459 (86%)	375 (94%)	19 (5%)	3 (1%)	19 57
1	B	387/459 (84%)	365 (94%)	21 (5%)	1 (0%)	41 76
1	C	392/459 (85%)	369 (94%)	21 (5%)	2 (0%)	29 68
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%)	29 68

5 of 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

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	349/401 (87%)	346 (99%)	3 (1%)	78 92
1	B	342/401 (85%)	338 (99%)	4 (1%)	71 90
1	C	345/401 (86%)	341 (99%)	4 (1%)	71 90
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%)	76 91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	ASP
1	C	202	GLN
1	C	292	LYS
1	C	203	ASP
1	B	292	LYS

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	328	HIS
1	A	357	ASN
1	B	328	HIS
1	C	202	GLN
1	C	328	HIS

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	$\#\|Z\| > 2$
3	NAG	B	700	1	14,14,15	0.55	0	17,19,21	0.67	0
3	NAG	C	600	1	14,14,15	0.49	0	17,19,21	0.81	0
3	NAG	A	700	1	14,14,15	0.55	0	17,19,21	0.69	0
6	SO4	A	465	-	4,4,4	0.51	0	6,6,6	0.62	0
3	NAG	A	600	1	14,14,15	0.51	0	17,19,21	0.72	0
3	NAG	B	600	1	14,14,15	0.52	0	17,19,21	0.72	0
3	NAG	C	700	1	14,14,15	0.54	0	17,19,21	0.69	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	NAG	B	700	1	-	2/6/23/26	0/1/1/1
3	NAG	C	600	1	-	1/6/23/26	0/1/1/1
3	NAG	A	700	1	-	2/6/23/26	0/1/1/1
3	NAG	A	600	1	-	2/6/23/26	0/1/1/1
3	NAG	B	600	1	-	2/6/23/26	0/1/1/1
3	NAG	C	700	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	NAG	O5-C5-C6-O6
3	A	700	NAG	O5-C5-C6-O6
3	C	700	NAG	O5-C5-C6-O6
3	A	700	NAG	C4-C5-C6-O6
3	B	700	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^{th} 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	401/459 (87%)	0.33	37 (9%) 9 3	51, 86, 198, 251	0
1	B	391/459 (85%)	0.33	39 (9%) 7 2	47, 88, 203, 236	0
1	C	396/459 (86%)	0.09	24 (6%) 21 7	49, 82, 182, 236	0
2	D	37/37 (100%)	0.17	1 (2%) 54 26	71, 100, 147, 180	0
2	E	37/37 (100%)	0.44	3 (8%) 12 3	81, 109, 149, 177	0
2	F	37/37 (100%)	0.20	0 100 100	74, 102, 145, 176	0
All	All	1299/1488 (87%)	0.26	104 (8%) 12 4	47, 88, 194, 251	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	9.5
1	A	434	ILE	8.1
1	B	426	GLU	7.7
1	B	50	CYS	7.7
1	A	48	ALA	6.5

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^{th} 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	K	A	1	1/1	0.54	0.88	146,146,146,146	0
3	NAG	B	700	14/15	0.69	0.43	134,162,183,184	0
3	NAG	A	700	14/15	0.72	0.40	131,162,184,186	0
4	K	A	2	1/1	0.74	0.30	96,96,96,96	0
3	NAG	C	700	14/15	0.78	0.48	132,163,181,184	0
6	SO4	A	465	5/5	0.78	0.26	126,187,225,234	0
3	NAG	B	600	14/15	0.79	0.34	79,147,166,168	0
3	NAG	C	600	14/15	0.80	0.31	89,150,167,170	0
3	NAG	A	600	14/15	0.84	0.29	86,145,166,168	0
5	CL	A	464	1/1	0.87	0.28	94,94,94,94	0

6.5 Other polymers

There are no such residues in this entry.