



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:33 PM UTC

PDB ID : 3S3X / pdb_00003s3x
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

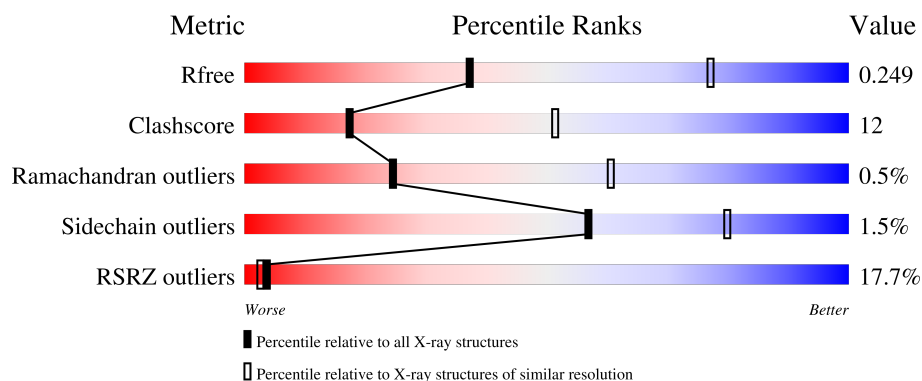
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	459	17% 64% 22% 13%
1	B	459	15% 61% 23% 15%
1	C	459	14% 60% 25% 14%
2	D	37	14% 49% 49% .
2	E	37	8% 59% 38% .

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Mol	Chain	Length	Quality of chain
2	F	37	24% 49% 49%

2 Entry composition

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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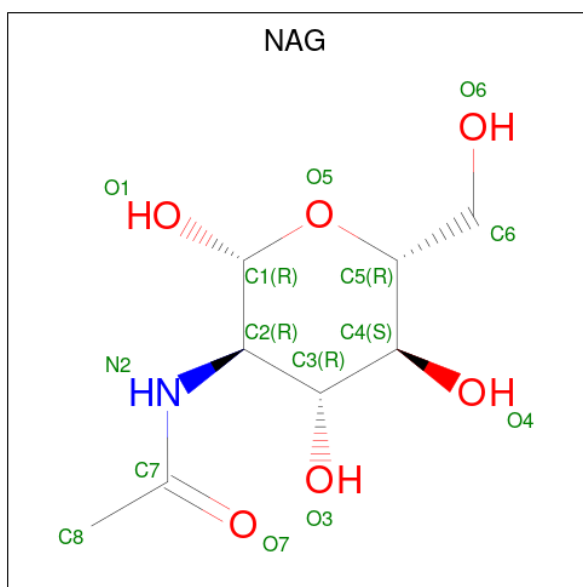
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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	TYR	-	expression tag	UNP Q1XA76
B	8	TYR	-	expression tag	UNP Q1XA76
B	9	HIS	-	expression tag	UNP Q1XA76
B	10	HIS	-	expression tag	UNP Q1XA76
B	11	HIS	-	expression tag	UNP Q1XA76
B	12	HIS	-	expression 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 (CCD ID: 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		

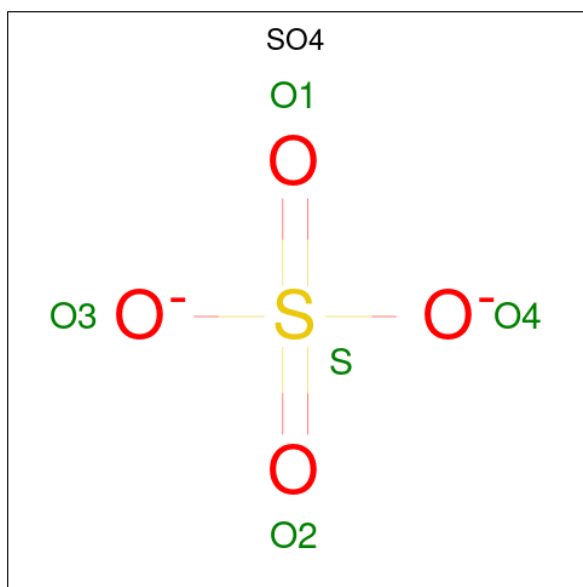
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

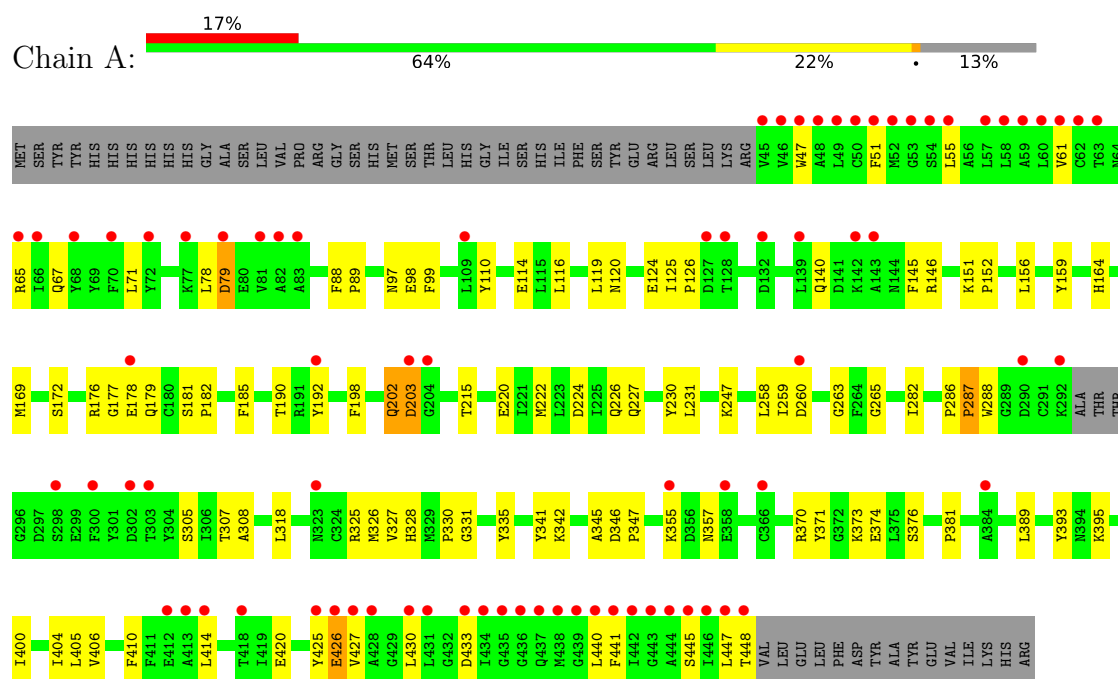
- Molecule 7 is water.

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

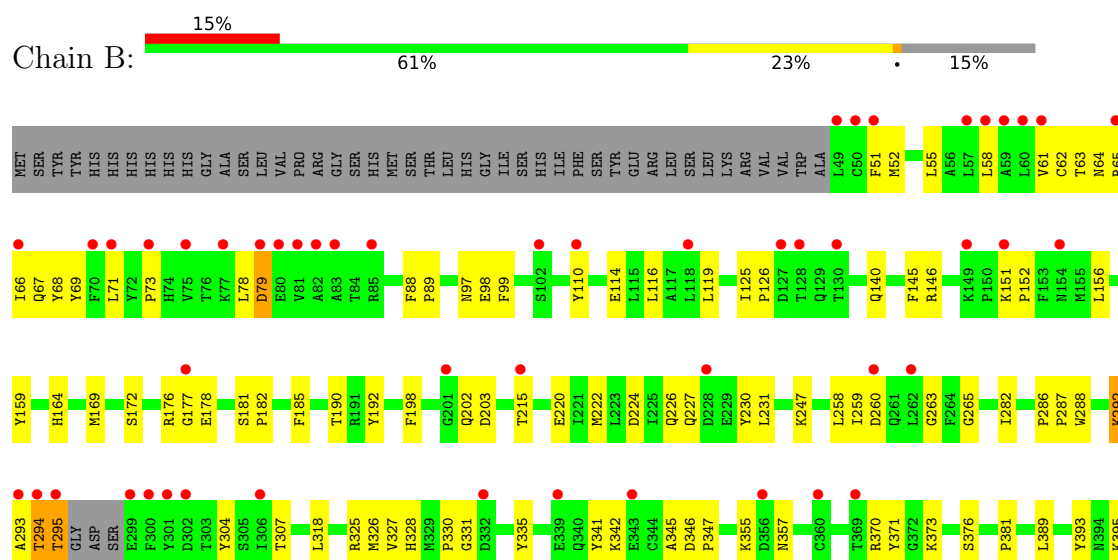
3 Residue-property plots

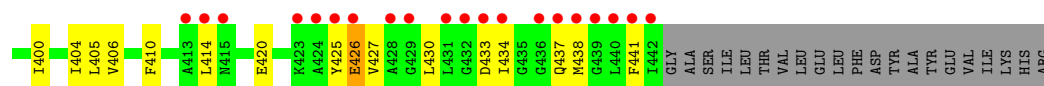
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

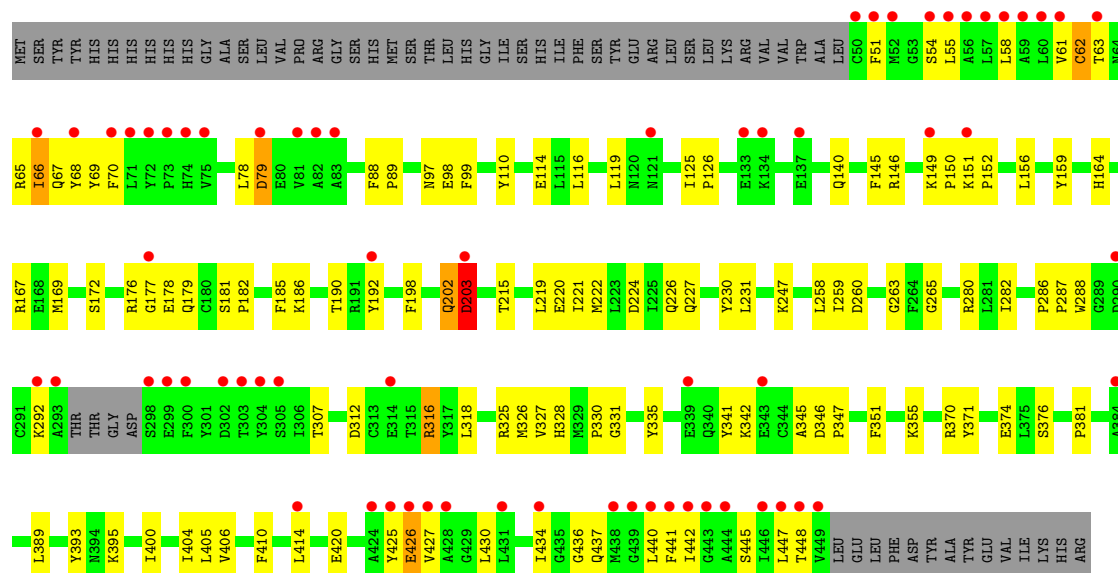


- Molecule 1: Amiloride-sensitive cation channel 2, neuronal

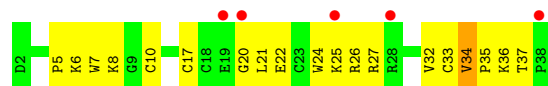




- Molecule 1: Amiloride-sensitive cation channel 2, neuronal



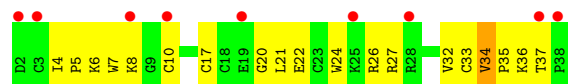
- Molecule 2: Psalmotoxin-1



- Molecule 2: Psalmotoxin-1



- Molecule 2: Psalmotoxin-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.40 Å 109.44 Å 127.27 Å 90.00° 119.81° 90.00°	Depositor
Resolution (Å)	29.91 – 2.99 29.91 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.91-2.99) 92.9 (29.91-2.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.00 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.218 , 0.249 0.220 , 0.249	Depositor DCC
R_{free} test set	2829 reflections (5.04%)	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)	0.28 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	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.*

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: NAG, K, SO4, 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	0.33	2/3284 (0.1%)	0.67	2/4445 (0.0%)
1	B	0.29	1/3212 (0.0%)	0.68	2/4346 (0.0%)
1	C	0.30	0/3241	0.79	13/4385 (0.3%)
2	D	0.26	0/307	0.69	0/412
2	E	0.26	0/307	0.69	0/412
2	F	0.26	0/307	0.69	0/412
All	All	0.30	3/10658 (0.0%)	0.71	17/14412 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	ASN	CG-ND2	-9.01	1.14	1.33
1	A	357	ASN	CG-OD1	-7.87	1.08	1.23
1	B	357	ASN	CG-ND2	-5.30	1.22	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ARG	NE-CZ-NH2	12.14	130.12	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ARG	NE-CZ-NH1	-10.10	111.40	121.50
1	C	316	ARG	NE-CZ-NH2	9.53	127.78	119.20
1	C	167	ARG	NE-CZ-NH2	9.35	127.62	119.20
1	C	316	ARG	NE-CZ-NH1	-8.97	112.53	121.50
1	C	167	ARG	NE-CZ-NH1	-8.79	112.71	121.50
1	C	146	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	C	146	ARG	CD-NE-CZ	6.90	134.06	124.40
1	C	316	ARG	CD-NE-CZ	6.75	133.85	124.40
1	C	167	ARG	CD-NE-CZ	6.71	133.79	124.40
1	C	146	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	C	62	CYS	N-CA-C	5.56	117.15	111.14
1	B	146	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	280	ARG	CD-NE-CZ	5.32	131.85	124.40
1	A	146	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	146	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	146	ARG	NE-CZ-NH1	-5.09	116.41	121.50

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	77	0
1	B	3139	0	3034	80	0
1	C	3168	0	3065	90	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	257	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.

All (257) 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
1:B:67:GLN:O	1:B:71:LEU:HG	1.73	0.87
1:C:341:TYR:HA	1:C:345:ALA:HB3	1.57	0.85
1:A:341:TYR:HA	1:A:345:ALA:HB3	1.57	0.85
1:B:341:TYR:HA	1:B:345:ALA:HB3	1.58	0.84
1:C:69:TYR:OH	1:C:427:VAL:HG22	1.81	0.81
1:A:65:ARG:NH2	1:A:433:ASP:HB3	1.97	0.80
1:A:202:GLN:O	1:A:203:ASP:HB2	1.81	0.80
1:A:177:GLY:H	2:E:27:ARG:HH21	1.28	0.80
1:B:114:GLU:HG2	1:B:342:LYS:HE3	1.64	0.79
1:C:114:GLU:HG2	1:C:342:LYS:HE3	1.64	0.79
1:A:61:VAL:HG11	1:C:436:GLY:HA2	1.66	0.77
1:A:114:GLU:HG2	1:A:342:LYS:HE3	1.65	0.77
1:C:177:GLY:H	2:D:27:ARG:HH21	1.34	0.75
1:B:177:GLY:H	2:F:27:ARG:HH21	1.34	0.75
1:B:292:LYS:HD2	1:B:293:ALA:O	1.87	0.74
1:B:318:LEU:HD11	1:B:345:ALA:HA	1.70	0.73
1:A:440:LEU:HD11	1:C:440:LEU:HD12	1.70	0.72
1:C:318:LEU:HD11	1:C:345:ALA:HA	1.70	0.72
1:B:414:LEU:HD12	1:C:370:ARG:HD2	1.70	0.71
1:A:318:LEU:HD11	1:A:345:ALA:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:O	1:C:65:ARG:HG2	1.89	0.71
1:B:400:ILE:HA	1:B:404:ILE:HD13	1.74	0.70
1:A:282:ILE:HB	1:A:420:GLU:HG3	1.74	0.69
1:A:400:ILE:HA	1:A:404:ILE:HD13	1.74	0.69
1:C:282:ILE:HB	1:C:420:GLU:HG3	1.73	0.69
1:B:282:ILE:HB	1:B:420:GLU:HG3	1.73	0.69
1:C:400:ILE:HA	1:C:404:ILE:HD13	1.75	0.69
1:B:65:ARG:HD3	1:B:425:TYR:OH	1.90	0.69
1:C:186:LYS:HG2	1:C:202:GLN:NE2	2.08	0.68
1:B:202:GLN:O	1:B:203:ASP:HB2	1.93	0.68
1:B:292:LYS:HE3	1:B:304:TYR:CE1	2.29	0.68
1:A:326:MET:HE3	1:A:341:TYR:HE2	1.59	0.67
1:C:62:CYS:SG	1:C:434:ILE:HG23	2.34	0.67
1:C:442:ILE:O	1:C:445:SER:OG	2.10	0.66
1:C:326:MET:HE3	1:C:341:TYR:HE2	1.60	0.66
1:B:326:MET:HE3	1:B:341:TYR:HE2	1.59	0.66
1:A:65:ARG:NH2	1:A:433:ASP:CB	2.59	0.65
1:C:63:THR:O	1:C:66:ILE:HG22	1.97	0.65
1:A:287:PRO:HD2	1:A:288:TRP:CE3	2.33	0.64
1:B:69:TYR:C	1:B:71:LEU:H	2.05	0.63
1:A:67:GLN:O	1:A:71:LEU:HG	1.99	0.63
1:C:312:ASP:OD2	1:C:316:ARG:HD3	1.99	0.63
1:B:52:MET:SD	1:B:55:LEU:HD12	2.39	0.63
2:F:20:GLY:HA2	2:F:36:LYS:HE2	1.82	0.62
2:E:20:GLY:HA2	2:E:36:LYS:HE2	1.81	0.62
2:D:20:GLY:HA2	2:D:36:LYS:HE2	1.81	0.61
1:A:202:GLN:O	1:A:203:ASP:CB	2.49	0.60
1:A:414:LEU:HD12	1:B:370:ARG:HD2	1.83	0.60
2:D:6:LYS:HE2	2:D:7:TRP:CZ2	2.37	0.60
1:B:62:CYS:SG	1:B:434:ILE:HG23	2.41	0.60
1:B:426:GLU:HG3	1:B:427:VAL:H	1.66	0.60
1:A:89:PRO:HB3	1:A:371:TYR:CZ	2.37	0.60
1:B:89:PRO:HB3	1:B:371:TYR:CZ	2.36	0.60
1:C:89:PRO:HB3	1:C:371:TYR:CZ	2.36	0.60
2:F:6:LYS:HE2	2:F:7:TRP:CZ2	2.37	0.59
1:B:69:TYR:C	1:B:71:LEU:N	2.58	0.59
2:E:6:LYS:HE2	2:E:7:TRP:CZ2	2.36	0.59
1:A:440:LEU:CA	1:C:447:LEU:HD11	2.23	0.58
1:C:346:ASP:HB2	1:C:347:PRO:HD3	1.85	0.58
1:C:69:TYR:HE1	1:C:426:GLU:C	2.11	0.58
1:B:66:ILE:HB	1:B:434:ILE:CD1	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HH21	1:A:433:ASP:HB3	1.69	0.58
1:A:370:ARG:HD2	1:C:414:LEU:HD12	1.85	0.57
1:B:55:LEU:HD22	1:B:441:PHE:CD1	2.39	0.57
1:B:119:LEU:HA	1:B:126:PRO:HD3	1.87	0.57
1:A:346:ASP:HB2	1:A:347:PRO:HD3	1.86	0.57
1:A:440:LEU:O	1:C:447:LEU:HD21	2.05	0.57
1:B:346:ASP:HB2	1:B:347:PRO:HD3	1.86	0.57
1:A:119:LEU:HA	1:A:126:PRO:HD3	1.87	0.56
1:C:69:TYR:CG	1:C:430:LEU:HD22	2.40	0.56
1:B:62:CYS:HA	1:B:437:GLN:OE1	2.05	0.56
1:B:325:ARG:NH1	1:B:331:GLY:O	2.39	0.56
1:C:119:LEU:HA	1:C:126:PRO:HD3	1.86	0.56
1:A:227:GLN:HA	1:A:230:TYR:CD1	2.41	0.56
1:B:227:GLN:HA	1:B:230:TYR:CD1	2.40	0.56
1:A:65:ARG:HH21	1:A:433:ASP:CB	2.17	0.55
1:C:51:PHE:HE1	1:C:445:SER:HB3	1.71	0.55
1:C:51:PHE:CE1	1:C:445:SER:HB3	2.41	0.55
1:C:227:GLN:HA	1:C:230:TYR:CD1	2.41	0.55
2:E:22:GLU:HG3	2:E:36:LYS:HB3	1.88	0.55
1:A:177:GLY:H	2:E:27:ARG:NH2	2.01	0.55
1:B:326:MET:HE3	1:B:341:TYR:CE2	2.41	0.55
1:C:69:TYR:CD2	1:C:430:LEU:HD22	2.42	0.55
2:D:22:GLU:HG3	2:D:36:LYS:HB3	1.88	0.54
2:F:22:GLU:HG3	2:F:36:LYS:HB3	1.88	0.54
1:A:325:ARG:NH1	1:A:331:GLY:O	2.39	0.54
1:C:287:PRO:HD2	1:C:288:TRP:CE3	2.43	0.54
1:C:58:LEU:HD13	1:C:437:GLN:HG3	1.89	0.54
1:B:287:PRO:HD2	1:B:288:TRP:CE3	2.43	0.54
1:C:325:ARG:NH1	1:C:331:GLY:O	2.40	0.54
1:A:426:GLU:HG3	1:A:427:VAL:H	1.73	0.53
1:B:65:ARG:HD2	1:B:433:ASP:HB3	1.90	0.53
1:C:355:LYS:HE3	2:F:37:THR:OG1	2.07	0.53
1:A:181:SER:HB2	1:A:182:PRO:HD2	1.91	0.53
1:C:445:SER:O	1:C:448:THR:OG1	2.14	0.53
1:B:68:TYR:CE2	1:B:73:PRO:HG3	2.44	0.52
1:A:156:LEU:HD22	1:A:335:TYR:CE2	2.45	0.52
1:C:258:LEU:HB2	1:C:307:THR:HG23	1.92	0.52
1:C:156:LEU:HD22	1:C:335:TYR:CE2	2.45	0.52
1:B:68:TYR:HA	1:B:71:LEU:HD12	1.91	0.52
1:A:326:MET:HE3	1:A:341:TYR:CE2	2.41	0.52
1:B:61:VAL:HA	1:B:64:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD22	1:B:335:TYR:CE2	2.45	0.51
1:C:181:SER:HB2	1:C:182:PRO:HD2	1.91	0.51
1:B:181:SER:HB2	1:B:182:PRO:HD2	1.91	0.51
1:B:99:PHE:HB2	1:B:231:LEU:HD11	1.92	0.51
1:B:68:TYR:O	1:B:71:LEU:HB2	2.10	0.51
1:C:326:MET:HE3	1:C:341:TYR:CE2	2.42	0.51
1:A:99:PHE:HB2	1:A:231:LEU:HD11	1.92	0.51
1:A:425:TYR:HE2	1:A:430:LEU:HD13	1.76	0.51
1:B:258:LEU:HB2	1:B:307:THR:HG23	1.93	0.51
1:C:99:PHE:HB2	1:C:231:LEU:HD11	1.92	0.50
1:C:381:PRO:HB3	1:C:389:LEU:HD12	1.93	0.50
1:A:258:LEU:HB2	1:A:307:THR:HG23	1.92	0.50
2:D:34:VAL:HG13	2:D:35:PRO:HD2	1.93	0.50
1:A:381:PRO:HB3	1:A:389:LEU:HD12	1.93	0.50
1:B:381:PRO:HB3	1:B:389:LEU:HD12	1.93	0.50
1:C:156:LEU:HD13	1:C:327:VAL:HG13	1.94	0.50
1:C:192:TYR:HE2	1:C:260:ASP:HA	1.77	0.50
1:C:55:LEU:N	1:C:441:PHE:HE1	2.10	0.50
1:C:318:LEU:HD21	1:C:326:MET:HG3	1.93	0.49
1:A:98:GLU:HG2	1:A:192:TYR:O	2.13	0.49
1:A:156:LEU:HD13	1:A:327:VAL:HG13	1.95	0.49
1:A:318:LEU:HD21	1:A:326:MET:HG3	1.94	0.49
1:C:405:LEU:C	1:C:405:LEU:HD23	2.38	0.49
1:B:318:LEU:HD21	1:B:326:MET:HG3	1.94	0.49
1:B:98:GLU:HG2	1:B:192:TYR:O	2.13	0.49
1:B:190:THR:HA	1:B:328:HIS:HB2	1.95	0.49
1:A:355:LYS:HE3	2:D:37:THR:OG1	2.13	0.49
1:A:405:LEU:C	1:A:405:LEU:HD23	2.38	0.49
1:B:192:TYR:HE2	1:B:260:ASP:HA	1.77	0.49
1:A:190:THR:HA	1:A:328:HIS:HB2	1.95	0.48
1:A:65:ARG:HH22	1:A:433:ASP:HB3	1.74	0.48
1:A:192:TYR:HE2	1:A:260:ASP:HA	1.78	0.48
1:C:98:GLU:HG2	1:C:192:TYR:O	2.13	0.48
1:C:177:GLY:H	2:D:27:ARG:NH2	2.09	0.48
2:F:34:VAL:HG13	2:F:35:PRO:HD2	1.94	0.48
1:B:63:THR:O	1:B:67:GLN:HG3	2.14	0.48
2:D:5:PRO:HD2	2:D:8:LYS:HG3	1.94	0.48
2:F:5:PRO:HD2	2:F:8:LYS:HG3	1.95	0.48
1:C:190:THR:HA	1:C:328:HIS:HB2	1.95	0.48
2:D:17:CYS:HB3	2:D:21:LEU:HB2	1.96	0.48
1:B:156:LEU:HD13	1:B:327:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LYS:HE3	1:B:304:TYR:CD1	2.49	0.47
1:B:405:LEU:C	1:B:405:LEU:HD23	2.39	0.47
2:E:17:CYS:HB3	2:E:21:LEU:HB2	1.96	0.47
1:C:66:ILE:HG12	1:C:70:PHE:CZ	2.49	0.47
1:C:55:LEU:N	1:C:441:PHE:CE1	2.82	0.47
1:C:125:ILE:HD12	1:C:140:GLN:HG2	1.97	0.47
2:E:5:PRO:HD2	2:E:8:LYS:HG3	1.95	0.47
1:B:247:LYS:O	1:B:259:ILE:HD11	2.15	0.47
1:B:438:MET:O	1:B:441:PHE:HB3	2.14	0.47
2:F:24:TRP:CZ3	2:F:26:ARG:HG2	2.50	0.47
1:A:376:SER:HB2	1:B:265:GLY:H	1.80	0.47
1:C:67:GLN:O	1:C:70:PHE:N	2.36	0.47
1:C:110:TYR:HB2	1:C:145:PHE:CE1	2.50	0.47
1:A:151:LYS:HB3	1:A:152:PRO:HD2	1.97	0.47
1:B:125:ILE:HD12	1:B:140:GLN:HG2	1.97	0.47
1:C:247:LYS:O	1:C:259:ILE:HD11	2.15	0.47
2:D:24:TRP:CZ3	2:D:26:ARG:HG2	2.49	0.47
1:A:159:TYR:HD1	1:A:327:VAL:HG21	1.80	0.47
1:A:176:ARG:C	1:A:178:GLU:H	2.22	0.47
2:F:4:ILE:HA	2:F:5:PRO:HD3	1.77	0.47
1:A:110:TYR:HB2	1:A:145:PHE:CE1	2.50	0.46
1:A:265:GLY:H	1:C:376:SER:HB2	1.80	0.46
1:B:151:LYS:HB3	1:B:152:PRO:HD2	1.98	0.46
2:E:24:TRP:CZ3	2:E:26:ARG:HG2	2.49	0.46
1:C:151:LYS:HB3	1:C:152:PRO:HD2	1.97	0.46
2:E:34:VAL:HG13	2:E:35:PRO:HD2	1.96	0.46
1:A:374:GLU:OE1	1:B:373:LYS:HE2	2.15	0.46
2:F:17:CYS:HB3	2:F:21:LEU:HB2	1.96	0.46
1:C:202:GLN:O	1:C:203:ASP:CB	2.53	0.46
1:B:110:TYR:HB2	1:B:145:PHE:CE1	2.50	0.46
1:B:176:ARG:C	1:B:178:GLU:H	2.23	0.46
1:A:125:ILE:HD12	1:A:140:GLN:HG2	1.97	0.46
1:A:97:ASN:HB2	1:A:230:TYR:CE2	2.51	0.46
1:C:159:TYR:HD1	1:C:327:VAL:HG21	1.81	0.46
1:C:220:GLU:OE2	2:D:27:ARG:HD3	2.16	0.46
1:B:58:LEU:O	1:B:62:CYS:HB2	2.15	0.45
1:B:97:ASN:HB2	1:B:230:TYR:CE2	2.51	0.45
1:C:176:ARG:C	1:C:178:GLU:H	2.23	0.45
1:C:351:PHE:CZ	2:F:35:PRO:HG2	2.51	0.45
1:A:247:LYS:O	1:A:259:ILE:HD11	2.16	0.45
1:C:347:PRO:HB3	2:F:32:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TRP:HZ3	1:A:447:LEU:HD13	1.81	0.45
1:A:51:PHE:HE2	1:A:445:SER:HA	1.81	0.45
1:C:186:LYS:HG2	1:C:202:GLN:HE21	1.81	0.45
1:C:69:TYR:HD1	1:C:425:TYR:HD2	1.65	0.45
1:A:347:PRO:HB3	2:D:32:VAL:HG11	1.98	0.45
1:C:99:PHE:CE2	1:C:116:LEU:HD21	2.52	0.45
1:B:99:PHE:CE2	1:B:116:LEU:HD21	2.52	0.45
1:C:97:ASN:HB2	1:C:230:TYR:CE2	2.52	0.44
1:A:172:SER:HB3	1:A:222:MET:HB3	1.99	0.44
1:B:222:MET:HA	1:B:405:LEU:O	2.18	0.44
1:B:177:GLY:H	2:F:27:ARG:NH2	2.08	0.44
1:A:99:PHE:CE2	1:A:116:LEU:HD21	2.52	0.44
1:A:179:GLN:OE1	2:E:25:LYS:HD2	2.18	0.44
1:C:222:MET:HA	1:C:405:LEU:O	2.18	0.44
1:A:88:PHE:CG	1:A:89:PRO:HD2	2.53	0.44
1:B:55:LEU:HD22	1:B:441:PHE:CG	2.53	0.44
1:B:185:PHE:CE1	1:B:198:PHE:HB2	2.52	0.44
1:C:164:HIS:HB3	1:C:169:MET:SD	2.58	0.44
1:C:185:PHE:CE1	1:C:198:PHE:HB2	2.53	0.44
1:C:88:PHE:CG	1:C:89:PRO:HD2	2.54	0.43
1:C:426:GLU:HG3	1:C:427:VAL:H	1.83	0.43
1:B:88:PHE:CG	1:B:89:PRO:HD2	2.53	0.43
1:C:69:TYR:HB2	1:C:430:LEU:HD13	2.00	0.43
1:A:51:PHE:HB2	1:A:448:THR:HG21	2.01	0.43
1:A:55:LEU:HD13	1:A:441:PHE:CE2	2.53	0.43
1:A:393:TYR:O	1:A:395:LYS:HG2	2.19	0.43
1:B:159:TYR:HD1	1:B:327:VAL:HG21	1.82	0.43
1:A:164:HIS:HB3	1:A:169:MET:SD	2.59	0.43
1:A:222:MET:HA	1:A:405:LEU:O	2.19	0.43
1:C:393:TYR:O	1:C:395:LYS:HG2	2.19	0.43
1:A:185:PHE:CE1	1:A:198:PHE:HB2	2.53	0.43
1:B:172:SER:HB3	1:B:222:MET:HB3	2.01	0.43
1:B:376:SER:HB2	1:C:265:GLY:H	1.83	0.43
1:B:425:TYR:HE2	1:B:430:LEU:HA	1.84	0.43
1:B:393:TYR:O	1:B:395:LYS:HG2	2.19	0.43
1:C:172:SER:HB3	1:C:222:MET:HB3	2.00	0.43
1:C:51:PHE:O	1:C:54:SER:OG	2.33	0.42
1:B:164:HIS:HB3	1:B:169:MET:SD	2.59	0.42
1:C:58:LEU:CD1	1:C:437:GLN:HG3	2.49	0.42
1:C:224:ASP:O	1:C:226:GLN:HG3	2.19	0.42
1:C:179:GLN:OE1	2:D:25:LYS:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLN:O	1:C:68:TYR:C	2.63	0.41
1:A:215:THR:HG22	1:A:410:PHE:CE1	2.55	0.41
1:B:224:ASP:O	1:B:226:GLN:HG3	2.20	0.41
2:D:10:CYS:HB3	2:D:33:CYS:SG	2.60	0.41
1:A:178:GLU:OE1	1:B:355:LYS:NZ	2.53	0.41
1:A:373:LYS:HE2	1:C:374:GLU:OE1	2.21	0.41
1:B:78:LEU:HD12	1:B:79:ASP:H	1.85	0.41
1:A:405:LEU:HD23	1:A:406:VAL:N	2.36	0.41
1:A:224:ASP:O	1:A:226:GLN:HG3	2.20	0.41
1:C:78:LEU:HD12	1:C:79:ASP:H	1.85	0.41
1:C:247:LYS:HE2	1:C:263:GLY:C	2.46	0.41
1:B:405:LEU:HD23	1:B:406:VAL:N	2.36	0.41
1:A:78:LEU:HD12	1:A:79:ASP:H	1.85	0.41
1:B:215:THR:HG22	1:B:410:PHE:CE1	2.56	0.41
1:C:215:THR:HG22	1:C:410:PHE:CE1	2.56	0.41
1:C:69:TYR:HD1	1:C:425:TYR:CD2	2.39	0.41
1:C:405:LEU:HD23	1:C:406:VAL:N	2.36	0.41
1:B:247:LYS:HE2	1:B:263:GLY:C	2.46	0.41
1:A:220:GLU:OE2	2:E:27:ARG:HD3	2.21	0.40
1:B:220:GLU:OE2	2:F:27:ARG:HD3	2.21	0.40
1:B:294:THR:O	1:B:295:THR:C	2.64	0.40
1:C:219:LEU:HD21	1:C:221:ILE:HD11	2.03	0.40
1:A:120:ASN:HD21	1:A:124:GLU:HB2	1.87	0.40
1:A:305:SER:HB2	1:A:308:ALA:H	1.86	0.40
2:F:10:CYS:HB3	2:F:33:CYS:SG	2.62	0.40
1:A:247:LYS:HE2	1:A:263:GLY:C	2.46	0.40
1:C:149:LYS:HA	1:C:150:PRO:HD3	1.89	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	397/459 (86%)	375 (94%)	19 (5%)	3 (1%)	16	50
1	B	387/459 (84%)	365 (94%)	21 (5%)	1 (0%)	36	70
1	C	392/459 (85%)	369 (94%)	21 (5%)	2 (0%)	24	60
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%)	24	60

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%)	70	85
1	B	342/401 (85%)	337 (98%)	5 (2%)	57	80
1	C	345/401 (86%)	339 (98%)	6 (2%)	53	78
2	D	34/34 (100%)	33 (97%)	1 (3%)	37	70
2	E	34/34 (100%)	33 (97%)	1 (3%)	37	70
2	F	34/34 (100%)	33 (97%)	1 (3%)	37	70
All	All	1138/1305 (87%)	1121 (98%)	17 (2%)	57	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	202	GLN
1	A	426	GLU
1	B	79	ASP
1	B	292	LYS
1	B	294	THR
1	B	295	THR
1	B	426	GLU
1	C	66	ILE
1	C	79	ASP
1	C	202	GLN
1	C	203	ASP
1	C	292	LYS
1	C	426	GLU
2	D	34	VAL
2	E	34	VAL
2	F	34	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	C	202	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	600	1	14,14,15	0.50	0	17,19,21	0.70	0
3	NAG	A	600	1	14,14,15	0.50	0	17,19,21	0.70	0
3	NAG	A	700	1	14,14,15	0.54	0	17,19,21	0.62	0
6	SO4	A	465	-	4,4,4	0.59	0	6,6,6	0.62	0
3	NAG	B	700	1	14,14,15	0.54	0	17,19,21	0.60	0
3	NAG	C	600	1	14,14,15	0.47	0	17,19,21	0.76	0
3	NAG	C	700	1	14,14,15	0.53	0	17,19,21	0.62	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	600	1	-	2/6/23/26	0/1/1/1
3	NAG	A	600	1	-	2/6/23/26	0/1/1/1
3	NAG	A	700	1	-	2/6/23/26	0/1/1/1
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	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.

All (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

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Mol	Chain	Res	Type	Atoms
3	C	700	NAG	C4-C5-C6-O6
3	A	600	NAG	C4-C5-C6-O6
3	B	600	NAG	C4-C5-C6-O6
3	C	600	NAG	C4-C5-C6-O6
3	A	600	NAG	O5-C5-C6-O6
3	B	600	NAG	O5-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, 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	401/459 (87%)	1.22	77 (19%) 3 2	51, 86, 198, 251	0
1	B	391/459 (85%)	1.17	70 (17%) 3 2	47, 88, 203, 236	0
1	C	396/459 (86%)	1.14	66 (16%) 4 3	49, 82, 182, 236	0
2	D	37/37 (100%)	1.17	5 (13%) 7 4	71, 100, 147, 180	0
2	E	37/37 (100%)	0.98	3 (8%) 18 9	81, 109, 149, 177	0
2	F	37/37 (100%)	1.31	9 (24%) 2 1	74, 102, 145, 176	0
All	All	1299/1488 (87%)	1.17	230 (17%) 4 2	47, 88, 194, 251	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	ILE	8.0
1	A	440	LEU	7.7
1	B	442	ILE	6.6
1	C	449	VAL	6.4
1	B	81	VAL	6.3
1	C	447	LEU	6.1
1	A	128	THR	5.7
1	B	440	LEU	5.5
1	B	80	GLU	5.5
1	B	426	GLU	5.4
1	A	439	GLY	5.4
2	F	38	PRO	5.4
1	A	438	MET	5.4
1	C	442	ILE	5.2
1	C	293	ALA	5.2
2	D	38	PRO	5.2
1	C	121	ASN	5.0
1	A	60	LEU	5.0
1	B	51	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	437	GLN	4.9
1	B	295	THR	4.9
1	C	446	ILE	4.8
1	A	57	LEU	4.8
1	C	57	LEU	4.7
1	C	58	LEU	4.7
1	B	58	LEU	4.6
1	B	49	LEU	4.5
1	A	61	VAL	4.4
1	A	203	ASP	4.4
1	B	293	ALA	4.3
1	C	298	SER	4.3
1	B	425	TYR	4.3
1	A	441	PHE	4.3
1	A	49	LEU	4.3
2	E	38	PRO	4.2
1	B	61	VAL	4.2
1	C	299	GLU	4.1
1	B	228	ASP	4.1
1	C	71	LEU	4.1
1	A	81	VAL	4.1
1	A	292	LYS	4.1
1	A	68	TYR	4.0
1	B	414	LEU	4.0
1	B	66	ILE	4.0
1	A	443	GLY	4.0
1	B	82	ALA	3.9
1	A	447	LEU	3.9
1	A	45	VAL	3.9
1	B	60	LEU	3.8
1	C	55	LEU	3.8
1	A	48	ALA	3.8
1	B	83	ALA	3.8
1	A	46	VAL	3.8
1	C	438	MET	3.8
1	B	57	LEU	3.7
1	C	60	LEU	3.7
1	A	53	GLY	3.7
1	A	433	ASP	3.7
1	A	55	LEU	3.6
1	C	72	TYR	3.6
1	C	149	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	446	ILE	3.5
1	B	433	ASP	3.5
1	C	81	VAL	3.5
1	B	424	ALA	3.5
1	A	51	PHE	3.5
1	A	302	ASP	3.5
1	A	435	GLY	3.5
1	C	52	MET	3.5
1	A	430	LEU	3.5
1	C	448	THR	3.5
1	B	413	ALA	3.4
1	C	425	TYR	3.4
1	C	439	GLY	3.4
1	C	50	CYS	3.3
1	B	339	GLU	3.3
1	B	50	CYS	3.3
1	A	436	GLY	3.3
1	A	65	ARG	3.3
1	B	299	GLU	3.3
1	C	54	SER	3.3
1	C	73	PRO	3.2
1	B	438	MET	3.2
1	A	384	ALA	3.2
1	B	428	ALA	3.2
1	B	441	PHE	3.2
1	C	292	LYS	3.1
1	A	427	VAL	3.1
1	C	431	LEU	3.1
2	E	28	ARG	3.1
1	A	63	THR	3.1
1	C	290	ASP	3.1
1	A	444	ALA	3.0
1	A	204	GLY	3.0
1	A	47	TRP	3.0
1	B	70	PHE	3.0
1	B	436	GLY	3.0
2	D	19	GLU	3.0
1	B	294	THR	3.0
1	C	444	ALA	3.0
1	B	151	LYS	2.9
2	F	3	CYS	2.9
1	A	413	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	441	PHE	2.9
1	A	442	ILE	2.9
1	A	82	ALA	2.9
1	A	62	CYS	2.9
1	C	79	ASP	2.9
1	A	58	LEU	2.9
1	A	425	TYR	2.8
1	B	154	ASN	2.8
1	B	79	ASP	2.8
1	A	127	ASP	2.8
1	A	290	ASP	2.7
1	B	75	VAL	2.7
1	A	414	LEU	2.7
1	B	59	ALA	2.7
1	C	300	PHE	2.7
1	B	423	LYS	2.7
1	B	177	GLY	2.7
1	C	203	ASP	2.7
1	A	54	SER	2.7
1	A	298	SER	2.7
1	C	61	VAL	2.7
1	B	431	LEU	2.7
1	A	83	ALA	2.7
1	A	300	PHE	2.7
1	C	82	ALA	2.7
1	B	149	LYS	2.6
1	A	70	PHE	2.6
1	A	72	TYR	2.6
1	C	68	TYR	2.6
1	A	428	ALA	2.6
1	C	134	LYS	2.6
1	B	369	THR	2.6
1	B	437	GLN	2.6
1	A	52	MET	2.6
1	C	70	PHE	2.6
1	B	65	ARG	2.5
1	A	178	GLU	2.5
1	C	63	THR	2.5
2	F	2	ASP	2.5
1	C	192	TYR	2.5
2	F	28	ARG	2.5
1	B	332	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	414	LEU	2.5
1	C	83	ALA	2.5
1	A	50	CYS	2.5
2	F	8	LYS	2.5
1	A	79	ASP	2.5
1	B	71	LEU	2.5
1	C	434	ILE	2.5
1	B	300	PHE	2.5
1	C	133	GLU	2.4
1	C	428	ALA	2.4
1	A	431	LEU	2.4
1	A	77	LYS	2.4
1	A	445	SER	2.4
1	C	56	ALA	2.4
1	A	323	ASN	2.4
1	A	142	LYS	2.4
1	B	432	GLY	2.4
1	C	177	GLY	2.4
1	C	343	GLU	2.4
2	F	25	LYS	2.3
1	B	201	GLY	2.3
1	A	426	GLU	2.3
1	A	139	LEU	2.3
1	B	110	TYR	2.3
2	F	37	THR	2.3
1	A	355	LYS	2.3
1	B	77	LYS	2.3
2	D	25	LYS	2.3
1	B	415	ASN	2.3
1	C	51	PHE	2.3
1	A	412	GLU	2.3
1	A	418	THR	2.3
1	A	143	ALA	2.3
1	C	427	VAL	2.3
1	A	59	ALA	2.2
1	B	343	GLU	2.2
1	C	59	ALA	2.2
1	B	128	THR	2.2
2	E	9	GLY	2.2
1	A	66	ILE	2.2
1	C	302	ASP	2.2
1	C	75	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	130	THR	2.2
1	B	360	CYS	2.2
1	C	443	GLY	2.2
1	B	262	LEU	2.2
1	C	440	LEU	2.2
1	C	339	GLU	2.2
1	C	426	GLU	2.2
1	A	260	ASP	2.2
1	B	73	PRO	2.2
1	B	356	ASP	2.2
1	A	303	THR	2.2
1	A	448	THR	2.2
1	C	137	GLU	2.2
1	C	74	HIS	2.1
1	C	303	THR	2.1
1	C	305	SER	2.1
1	C	424	ALA	2.1
1	B	215	THR	2.1
1	B	85	ARG	2.1
1	C	66	ILE	2.1
1	C	314	GLU	2.1
1	B	260	ASP	2.1
2	D	20	GLY	2.1
1	A	358	GLU	2.1
1	B	306	ILE	2.1
1	B	434	ILE	2.1
1	B	302	ASP	2.1
1	C	304	TYR	2.1
1	C	151	LYS	2.0
2	F	10	CYS	2.0
1	A	109	LEU	2.0
1	B	429	GLY	2.0
1	B	439	GLY	2.0
1	C	384	ALA	2.0
1	B	301	TYR	2.0
1	B	102	SER	2.0
1	A	366	CYS	2.0
1	B	118	LEU	2.0
2	D	28	ARG	2.0
1	A	132	ASP	2.0
1	B	127	ASP	2.0
2	F	19	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	192	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	700	14/15	0.55	0.17	131,162,184,186	0
3	NAG	B	700	14/15	0.56	0.15	134,162,183,184	0
3	NAG	B	600	14/15	0.59	0.20	79,147,166,168	0
3	NAG	C	700	14/15	0.59	0.16	132,163,181,184	0
4	K	A	1	1/1	0.64	0.27	146,146,146,146	0
3	NAG	C	600	14/15	0.69	0.17	89,150,167,170	0
6	SO4	A	465	5/5	0.71	0.18	126,187,225,234	0
3	NAG	A	600	14/15	0.78	0.16	86,145,166,168	0
4	K	A	2	1/1	0.85	0.21	96,96,96,96	0
5	CL	A	464	1/1	0.90	0.27	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.