



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2020 – 12:12 PM JST

PDB ID : 6L6I
Title : hASIC1a co-crystallized with Mamb-1
Authors : Lei, F.; Jian, S.
Deposited on : 2019-10-29
Resolution : 3.24 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.

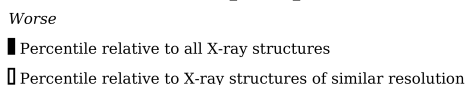
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

i

X-RAY DIFFRACTION

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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	454	
1	B	454	
1	C	454	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acid-sensing ion channel 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3440	2201	563	647	29			
1	B	443	Total	C	N	O	S	0	0	0
			3551	2275	582	665	29			
1	C	410	Total	C	N	O	S	0	0	0
			3279	2095	537	618	29			

There are 42 discrepancies between the modelled and reference sequences:

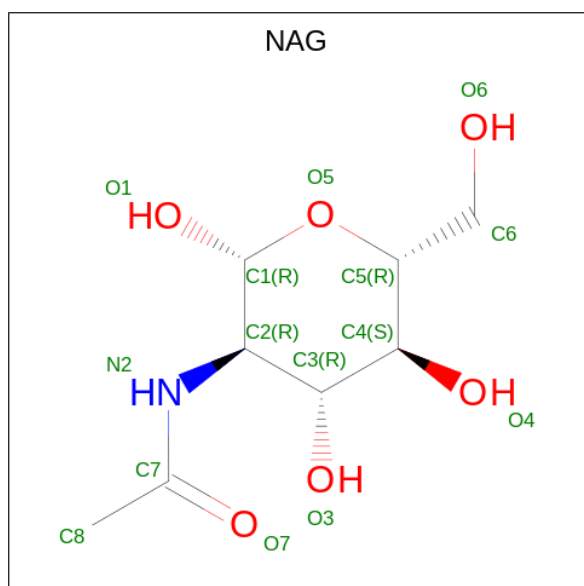
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP P78348
A	12	SER	-	expression tag	UNP P78348
A	13	GLY	-	expression tag	UNP P78348
A	14	GLY	-	expression tag	UNP P78348
A	15	SER	-	expression tag	UNP P78348
A	16	GLY	-	expression tag	UNP P78348
A	17	LEU	-	expression tag	UNP P78348
A	18	GLU	-	expression tag	UNP P78348
A	19	VAL	-	expression tag	UNP P78348
A	20	LEU	-	expression tag	UNP P78348
A	21	PHE	-	expression tag	UNP P78348
A	22	GLN	-	expression tag	UNP P78348
A	23	GLY	-	expression tag	UNP P78348
A	24	PRO	-	expression tag	UNP P78348
B	11	GLY	-	expression tag	UNP P78348
B	12	SER	-	expression tag	UNP P78348
B	13	GLY	-	expression tag	UNP P78348
B	14	GLY	-	expression tag	UNP P78348
B	15	SER	-	expression tag	UNP P78348
B	16	GLY	-	expression tag	UNP P78348
B	17	LEU	-	expression tag	UNP P78348
B	18	GLU	-	expression tag	UNP P78348
B	19	VAL	-	expression tag	UNP P78348

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	LEU	-	expression tag	UNP P78348
B	21	PHE	-	expression tag	UNP P78348
B	22	GLN	-	expression tag	UNP P78348
B	23	GLY	-	expression tag	UNP P78348
B	24	PRO	-	expression tag	UNP P78348
C	11	GLY	-	expression tag	UNP P78348
C	12	SER	-	expression tag	UNP P78348
C	13	GLY	-	expression tag	UNP P78348
C	14	GLY	-	expression tag	UNP P78348
C	15	SER	-	expression tag	UNP P78348
C	16	GLY	-	expression tag	UNP P78348
C	17	LEU	-	expression tag	UNP P78348
C	18	GLU	-	expression tag	UNP P78348
C	19	VAL	-	expression tag	UNP P78348
C	20	LEU	-	expression tag	UNP P78348
C	21	PHE	-	expression tag	UNP P78348
C	22	GLN	-	expression tag	UNP P78348
C	23	GLY	-	expression tag	UNP P78348
C	24	PRO	-	expression tag	UNP P78348

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

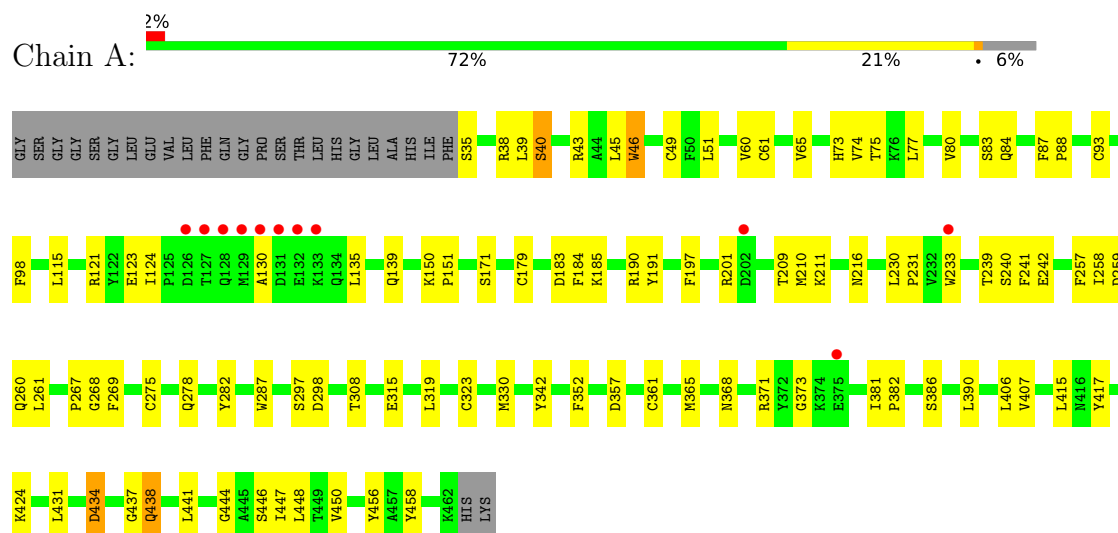
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	4	Total	O	0	0
			4	4		
3	C	2	Total	O	0	0
			2	2		

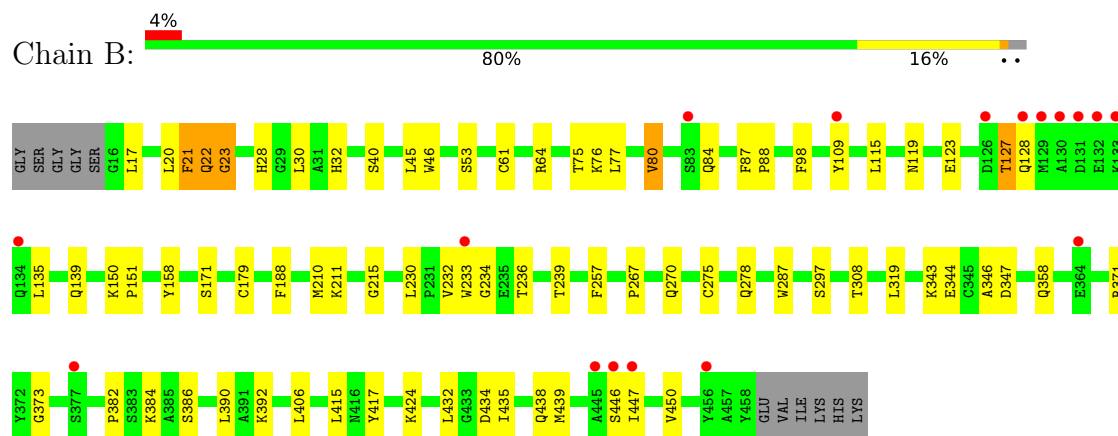
3 Residue-property plots [i](#)

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.

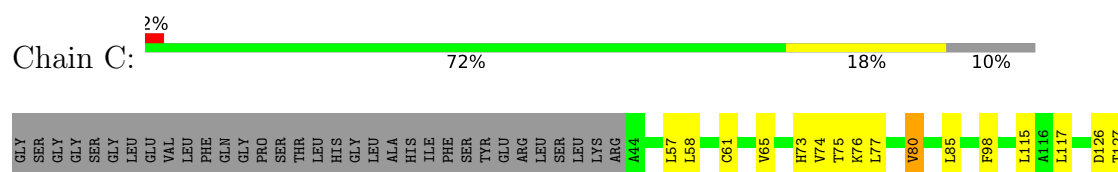
• Molecule 1: Acid-sensing ion channel 1

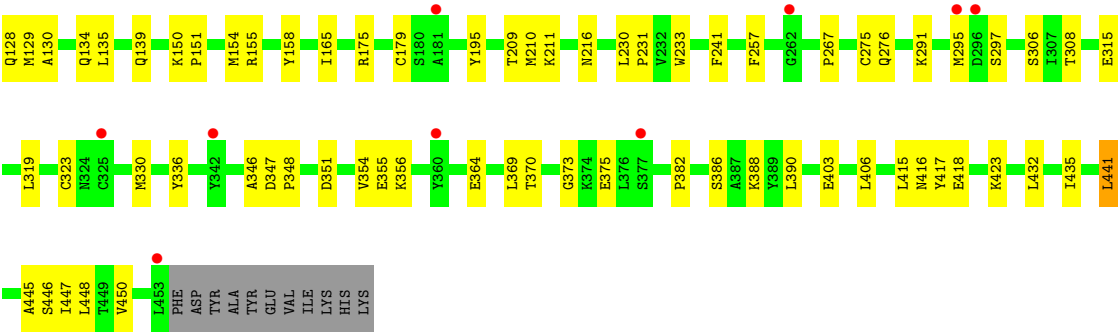


• Molecule 1: Acid-sensing ion channel 1



• Molecule 1: Acid-sensing ion channel 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.92Å 146.62Å 207.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 3.24 49.53 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.58-3.24) 99.8 (49.53-3.24)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.214 , 0.250 0.218 , 0.251	Depositor DCC
R_{free} test set	2031 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10321	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

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	0.63	0/3520	0.84	0/4759
1	B	0.63	0/3636	0.86	0/4918
1	C	0.65	0/3355	0.84	0/4538
All	All	0.64	0/10511	0.84	0/14215

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	GLY	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	3440	0	3336	87	0
1	B	3551	0	3439	79	2
1	C	3279	0	3175	78	0
2	A	14	0	13	3	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
All	All	10321	0	9989	210	2

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 10.

All (210) 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:392:LYS:NZ	1:C:129:MET:SD	1.97	1.36
1:B:20:LEU:O	1:B:21:PHE:CD2	2.20	0.94
1:A:352:PHE:CE2	1:A:357:ASP:HB2	2.03	0.92
1:B:17:LEU:O	1:B:21:PHE:HE2	1.53	0.91
1:B:23:GLY:O	1:B:28:HIS:HE1	1.52	0.91
1:B:384:LYS:NZ	1:C:403:GLU:OE1	2.07	0.88
1:B:17:LEU:O	1:B:21:PHE:CE2	2.30	0.84
1:B:23:GLY:O	1:B:28:HIS:CE1	2.32	0.81
1:B:20:LEU:C	1:B:21:PHE:CD2	2.54	0.80
1:A:49:CYS:CB	1:C:447:ILE:HD11	2.13	0.78
1:A:73:HIS:O	1:C:76:LYS:HE2	1.84	0.78
1:A:352:PHE:HE2	1:A:357:ASP:HB2	1.46	0.77
1:A:35:SER:O	1:A:39:LEU:HB2	1.88	0.74
1:B:211:LYS:HA	1:B:415:LEU:HD11	1.69	0.73
1:B:392:LYS:NZ	1:C:129:MET:CE	2.52	0.71
1:A:49:CYS:HB3	1:C:447:ILE:HD11	1.73	0.71
1:A:49:CYS:HB2	1:C:447:ILE:HD11	1.74	0.69
1:A:45:LEU:HD12	1:A:46:TRP:N	2.08	0.69
1:B:21:PHE:O	1:B:22:GLN:O	2.11	0.69
1:C:128:GLN:OE1	1:C:129:MET:HE2	1.94	0.67
1:C:61:CYS:O	1:C:65:VAL:HG23	1.94	0.67
1:C:127:THR:OG1	1:C:233:TRP:CD1	2.49	0.66
1:B:119:ASN:HD21	1:B:123:GLU:HG3	1.61	0.65
1:A:83:SER:HB2	1:B:358:GLN:CD	2.18	0.63
1:B:210:MET:HG2	1:C:355:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PHE:HB2	1:B:308:THR:HG23	1.82	0.62
1:B:447:ILE:HB	1:C:448:LEU:HD11	1.81	0.62
1:C:209:THR:CG2	1:C:211:LYS:O	2.49	0.60
1:B:210:MET:HG2	1:C:355:GLU:CB	2.31	0.60
1:A:209:THR:CG2	1:A:211:LYS:O	2.48	0.60
1:A:257:PHE:HB2	1:A:308:THR:HG23	1.83	0.60
1:C:369:LEU:HD12	1:C:370:THR:N	2.17	0.60
1:B:267:PRO:HA	1:B:406:LEU:HB3	1.82	0.60
1:A:80:VAL:CG2	1:A:417:TYR:CZ	2.85	0.60
1:B:17:LEU:HD22	1:B:20:LEU:HD12	1.85	0.59
1:C:127:THR:HG21	1:C:233:TRP:HB2	1.84	0.59
1:B:17:LEU:HA	1:B:20:LEU:HD12	1.84	0.59
1:A:83:SER:HB2	1:B:358:GLN:HG2	1.85	0.59
1:B:80:VAL:CG2	1:B:417:TYR:CZ	2.86	0.59
1:C:150:LYS:HB3	1:C:151:PRO:HD2	1.85	0.59
1:C:80:VAL:CG2	1:C:417:TYR:CZ	2.86	0.59
1:C:267:PRO:HA	1:C:406:LEU:HB3	1.84	0.58
1:C:369:LEU:HD12	1:C:369:LEU:C	2.23	0.58
1:A:83:SER:CB	1:B:358:GLN:HG2	2.33	0.58
1:C:257:PHE:HB2	1:C:308:THR:HG23	1.85	0.58
1:B:21:PHE:O	1:B:22:GLN:C	2.42	0.57
1:C:117:LEU:HA	1:C:233:TRP:CH2	2.39	0.57
1:A:150:LYS:HB3	1:A:151:PRO:HD2	1.87	0.57
1:A:444:GLY:O	1:A:448:LEU:HD23	2.04	0.57
1:C:85:LEU:HD12	1:C:415:LEU:HD23	1.86	0.57
1:A:267:PRO:HA	1:A:406:LEU:HB3	1.86	0.57
1:A:368:ASN:ND2	2:A:501:NAG:H83	2.20	0.56
1:B:135:LEU:HD21	1:B:139:GLN:NE2	2.19	0.56
1:B:64:ARG:HD3	1:B:434:ASP:HB3	1.86	0.56
1:A:35:SER:O	1:A:39:LEU:CB	2.53	0.56
1:A:268:GLY:C	1:A:381:ILE:HG22	2.26	0.56
1:A:441:LEU:C	1:A:441:LEU:HD12	2.26	0.56
1:A:184:PHE:CE1	1:A:197:PHE:HB2	2.41	0.56
1:A:80:VAL:HG23	1:A:417:TYR:CZ	2.41	0.56
1:B:319:LEU:HD11	1:B:346:ALA:HA	1.87	0.56
1:A:35:SER:HA	1:A:38:ARG:HB2	1.88	0.56
1:C:134:GLN:CD	1:C:231:PRO:HB3	2.27	0.55
1:B:77:LEU:HB2	1:C:75:THR:HG21	1.87	0.55
1:A:240:SER:OG	1:A:242:GLU:OE1	2.21	0.55
1:A:83:SER:HB2	1:B:358:GLN:CG	2.37	0.55
1:C:117:LEU:HA	1:C:233:TRP:HH2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TRP:CE2	1:A:424:LYS:HD3	2.42	0.55
1:A:74:VAL:HG21	1:C:74:VAL:CG2	2.38	0.54
1:A:191:TYR:HE1	1:A:259:ASP:HA	1.72	0.54
1:A:130:ALA:HB2	1:A:233:TRP:CB	2.37	0.54
1:B:80:VAL:HG22	1:B:417:TYR:CZ	2.43	0.54
1:B:17:LEU:HD22	1:B:20:LEU:CD1	2.38	0.54
1:C:128:GLN:C	1:C:129:MET:HG3	2.27	0.54
1:A:40:SER:HB2	1:A:43:ARG:HB2	1.89	0.54
1:C:209:THR:HG23	1:C:211:LYS:O	2.07	0.54
1:C:211:LYS:HB3	1:C:216:ASN:HD22	1.71	0.54
1:B:20:LEU:O	1:B:21:PHE:CG	2.60	0.54
1:C:80:VAL:HG22	1:C:417:TYR:CZ	2.44	0.53
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.07	0.53
1:C:355:GLU:HG2	1:C:356:LYS:N	2.24	0.53
1:A:73:HIS:O	1:C:76:LYS:CE	2.55	0.53
1:A:210:MET:C	1:A:415:LEU:HD11	2.29	0.53
1:B:61:CYS:SG	1:B:435:ILE:HG13	2.48	0.53
1:A:46:TRP:CD1	1:A:46:TRP:C	2.82	0.53
1:A:319:LEU:HD12	1:A:330:MET:CE	2.39	0.52
1:A:446:SER:O	1:A:450:VAL:HG23	2.09	0.52
1:A:74:VAL:HG21	1:C:74:VAL:HG23	1.92	0.52
1:C:127:THR:HG22	1:C:129:MET:N	2.24	0.52
1:A:382:PRO:HB3	1:A:390:LEU:HD12	1.92	0.51
1:C:441:LEU:O	1:C:445:ALA:N	2.42	0.51
1:B:236:THR:OG1	1:B:239:THR:HG23	2.10	0.51
1:A:269:PHE:N	1:A:381:ILE:HG22	2.26	0.51
1:B:80:VAL:HG21	1:B:417:TYR:CZ	2.45	0.51
1:C:80:VAL:HG21	1:C:417:TYR:CZ	2.45	0.51
1:C:446:SER:O	1:C:450:VAL:HG23	2.11	0.51
1:B:20:LEU:O	1:B:21:PHE:CE2	2.64	0.51
1:B:20:LEU:O	1:B:22:GLN:N	2.44	0.51
1:A:287:TRP:CZ2	1:A:424:LYS:HD3	2.46	0.50
1:A:448:LEU:HD11	1:B:46:TRP:HZ2	1.77	0.50
1:A:448:LEU:HD11	1:B:46:TRP:CZ2	2.47	0.50
1:B:446:SER:O	1:B:450:VAL:HG23	2.12	0.50
1:C:382:PRO:HB3	1:C:390:LEU:HD12	1.94	0.49
1:A:257:PHE:HB2	1:A:308:THR:CG2	2.43	0.49
1:A:190:ARG:NH2	1:A:315:GLU:OE1	2.45	0.49
1:A:83:SER:CB	1:B:358:GLN:CG	2.90	0.49
1:C:130:ALA:HB2	1:C:233:TRP:CB	2.42	0.49
1:A:231:PRO:HG2	1:A:233:TRP:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PHE:HB2	1:B:308:THR:CG2	2.42	0.49
1:C:128:GLN:O	1:C:129:MET:HG3	2.12	0.49
1:B:98:PHE:O	1:B:230:LEU:HD13	2.13	0.49
1:A:458:TYR:CD1	1:A:458:TYR:C	2.86	0.49
1:C:80:VAL:HG22	1:C:417:TYR:CE2	2.47	0.48
1:A:447:ILE:HG23	1:B:45:LEU:HD23	1.95	0.48
1:A:43:ARG:NH1	1:A:456:TYR:HD2	2.12	0.48
1:C:57:LEU:HD22	1:C:441:LEU:HD13	1.96	0.48
1:A:65:VAL:HG22	1:A:431:LEU:HD11	1.95	0.48
1:B:150:LYS:HB3	1:B:151:PRO:HD2	1.96	0.47
1:C:127:THR:CG2	1:C:233:TRP:HB2	2.44	0.47
1:B:80:VAL:HG22	1:B:417:TYR:CE2	2.50	0.47
1:A:75:THR:HG21	1:C:77:LEU:HB2	1.97	0.47
1:A:260:GLN:HG2	1:A:261:LEU:HD12	1.96	0.47
1:B:84:GLN:HE21	1:B:210:MET:CE	2.28	0.47
1:B:22:GLN:O	1:B:23:GLY:O	2.30	0.47
1:C:257:PHE:HB2	1:C:308:THR:CG2	2.45	0.47
1:B:128:GLN:N	1:B:128:GLN:OE1	2.38	0.47
1:B:234:GLY:O	1:B:239:THR:HG21	2.15	0.47
1:A:211:LYS:HB2	1:A:216:ASN:CG	2.35	0.47
1:B:343:LYS:HG2	1:B:344:GLU:HG2	1.96	0.47
1:A:77:LEU:HB2	1:B:75:THR:HG21	1.97	0.46
1:A:35:SER:O	1:A:39:LEU:N	2.42	0.46
1:B:432:LEU:HA	1:B:435:ILE:HG22	1.96	0.46
1:C:319:LEU:HD11	1:C:346:ALA:HA	1.98	0.46
1:A:368:ASN:OD1	2:A:501:NAG:O5	2.33	0.46
1:B:382:PRO:HB3	1:B:390:LEU:HD12	1.98	0.46
1:C:154:MET:HE3	1:C:158:TYR:CE2	2.51	0.46
1:C:165:ILE:HB	1:C:195:TYR:CE2	2.50	0.46
1:C:175:ARG:O	1:C:175:ARG:HG2	2.16	0.46
1:C:130:ALA:HB2	1:C:233:TRP:HB2	1.97	0.46
1:B:386:SER:HB2	1:C:241:PHE:HD1	1.80	0.46
1:A:319:LEU:O	1:A:323:CYS:N	2.48	0.46
1:C:275:CYS:HA	1:C:373:GLY:O	2.16	0.46
1:A:381:ILE:CD1	1:A:407:VAL:HG23	2.46	0.45
1:B:210:MET:O	1:B:210:MET:HG3	2.15	0.45
1:B:211:LYS:HD3	1:C:354:VAL:HG21	1.98	0.45
1:C:85:LEU:HD12	1:C:415:LEU:CD2	2.47	0.45
1:A:275:CYS:HA	1:A:373:GLY:O	2.17	0.45
1:C:128:GLN:HG3	1:C:129:MET:HE3	1.98	0.45
1:A:368:ASN:HD22	2:A:501:NAG:H83	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TRP:CH2	1:B:424:LYS:HE3	2.52	0.45
1:C:135:LEU:HD23	1:C:139:GLN:HG2	1.98	0.45
1:A:278:GLN:OE1	1:A:371:ARG:NH1	2.50	0.45
1:B:115:LEU:N	1:B:115:LEU:HD23	2.32	0.45
1:C:432:LEU:O	1:C:435:ILE:HG13	2.17	0.45
1:A:386:SER:HB3	1:B:232:VAL:HG11	1.99	0.44
1:A:130:ALA:HB2	1:A:233:TRP:HB3	1.99	0.44
1:A:241:PHE:HD1	1:C:386:SER:HB2	1.82	0.44
1:A:83:SER:CB	1:B:358:GLN:CD	2.86	0.44
1:A:115:LEU:HD23	1:A:115:LEU:N	2.32	0.44
1:C:210:MET:C	1:C:415:LEU:HD11	2.38	0.44
1:A:80:VAL:CG2	1:A:417:TYR:CE1	3.00	0.44
1:C:115:LEU:N	1:C:115:LEU:HD23	2.33	0.44
1:A:98:PHE:O	1:A:230:LEU:HD13	2.17	0.43
1:B:76:LYS:HE2	1:C:73:HIS:NE2	2.32	0.43
1:B:21:PHE:CE1	1:B:23:GLY:C	2.91	0.43
1:A:73:HIS:O	1:C:76:LYS:CD	2.67	0.43
1:A:123:GLU:CD	1:A:124:ILE:HD12	2.39	0.43
1:B:127:THR:OG1	1:B:233:TRP:CD1	2.70	0.43
1:A:185:LYS:HD2	1:A:201:ARG:HD2	2.01	0.43
1:C:351:ASP:O	1:C:355:GLU:OE1	2.37	0.43
1:A:84:GLN:HE21	1:A:210:MET:CE	2.31	0.43
1:C:347:ASP:N	1:C:348:PRO:HD2	2.33	0.43
1:C:76:LYS:CE	1:C:423:LYS:HG3	2.49	0.42
1:B:384:LYS:CE	1:C:403:GLU:OE1	2.67	0.42
1:B:270:GLN:HB2	1:B:270:GLN:HE21	1.62	0.42
1:B:275:CYS:HA	1:B:373:GLY:O	2.19	0.42
1:B:287:TRP:CH2	1:B:424:LYS:CE	3.02	0.42
1:A:319:LEU:HD12	1:A:330:MET:HE1	2.02	0.42
1:B:158:TYR:HB3	1:B:188:PHE:HE2	1.84	0.42
1:A:45:LEU:HD12	1:A:45:LEU:C	2.39	0.42
1:A:93:CYS:SG	1:A:258:ILE:HD13	2.60	0.42
1:C:98:PHE:O	1:C:230:LEU:HD13	2.20	0.42
1:B:210:MET:O	1:B:415:LEU:HD11	2.20	0.42
1:B:21:PHE:CD1	1:B:23:GLY:C	2.93	0.41
1:C:276:GLN:NE2	1:C:418:GLU:OE2	2.52	0.41
1:A:406:LEU:C	1:A:406:LEU:HD12	2.40	0.41
1:A:434:ASP:O	1:A:438:GLN:NE2	2.53	0.41
1:B:406:LEU:C	1:B:406:LEU:HD12	2.40	0.41
1:C:315:GLU:HB3	1:C:330:MET:CE	2.50	0.41
1:B:87:PHE:CG	1:B:88:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD21	1:A:139:GLN:NE2	2.35	0.41
1:A:209:THR:HG23	1:A:211:LYS:O	2.19	0.41
1:A:60:VAL:HG23	1:A:61:CYS:N	2.35	0.41
1:C:388:LYS:HA	1:C:388:LYS:HD2	1.85	0.41
1:C:406:LEU:HD12	1:C:406:LEU:C	2.41	0.41
1:C:76:LYS:HE3	1:C:423:LYS:HG3	2.02	0.41
1:A:386:SER:HB3	1:B:232:VAL:CG1	2.49	0.41
1:B:278:GLN:OE1	1:B:371:ARG:NH1	2.53	0.41
1:B:21:PHE:HD1	1:B:23:GLY:O	2.02	0.41
1:B:21:PHE:CE1	1:B:23:GLY:CA	3.04	0.41
1:C:319:LEU:O	1:C:323:CYS:N	2.49	0.41
1:B:80:VAL:CG2	1:B:417:TYR:CE2	3.04	0.41
1:A:87:PHE:CG	1:A:88:PRO:HD2	2.56	0.41
1:A:269:PHE:CA	1:A:381:ILE:HG22	2.51	0.40
1:A:381:ILE:HA	1:A:382:PRO:HA	1.90	0.40
1:A:437:GLY:HA3	1:B:438:GLN:HE22	1.86	0.40
1:C:155:ARG:HD2	1:C:336:TYR:CE2	2.56	0.40
1:A:282:TYR:CE2	1:A:365:MET:SD	3.14	0.40
1:C:80:VAL:CG2	1:C:417:TYR:CE2	3.04	0.40
1:C:135:LEU:C	1:C:135:LEU:HD23	2.42	0.40
1:C:295:MET:O	1:C:295:MET:SD	2.79	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:HIS:NE2	1:B:109:TYR:OH[2_555]	1.22	0.98
1:B:32:HIS:CE1	1:B:109:TYR:OH[2_555]	1.89	0.31

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	426/454 (94%)	403 (95%)	22 (5%)	1 (0%)	47	78
1	B	441/454 (97%)	417 (95%)	20 (4%)	4 (1%)	17	52
1	C	408/454 (90%)	387 (95%)	21 (5%)	0	100	100
All	All	1275/1362 (94%)	1207 (95%)	63 (5%)	5 (0%)	34	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	PHE
1	B	23	GLY
1	A	40	SER
1	B	22	GLN
1	B	127	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/394 (95%)	362 (96%)	13 (4%)	36	67
1	B	386/394 (98%)	377 (98%)	9 (2%)	50	76
1	C	358/394 (91%)	347 (97%)	11 (3%)	40	70
All	All	1119/1182 (95%)	1086 (97%)	33 (3%)	42	71

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	51	LEU
1	A	121	ARG
1	A	171	SER
1	A	179	CYS
1	A	183	ASP
1	A	239	THR
1	A	297	SER

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Mol	Chain	Res	Type
1	A	298	ASP
1	A	342	TYR
1	A	361	CYS
1	A	434	ASP
1	A	438	GLN
1	B	30	LEU
1	B	40	SER
1	B	53	SER
1	B	80	VAL
1	B	171	SER
1	B	179	CYS
1	B	297	SER
1	B	347	ASP
1	B	439	MET
1	C	58	LEU
1	C	80	VAL
1	C	126	ASP
1	C	179	CYS
1	C	291	LYS
1	C	297	SER
1	C	306	SER
1	C	364	GLU
1	C	375	GLU
1	C	416	ASN
1	C	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	270	GLN
1	A	322	ASN
1	A	358	GLN
1	B	28	HIS
1	B	84	GLN
1	B	270	GLN
1	B	276	GLN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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$
2	NAG	B	501	1	14,14,15	1.58	4 (28%)	17,19,21	3.06	10 (58%)
2	NAG	C	501	1	14,14,15	1.35	2 (14%)	17,19,21	1.55	4 (23%)
2	NAG	A	501	1	14,14,15	1.27	1 (7%)	17,19,21	2.00	6 (35%)

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
2	NAG	B	501	1	-	4/6/23/26	0/1/1/1
2	NAG	C	501	1	-	3/6/23/26	0/1/1/1
2	NAG	A	501	1	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	C1-C2	2.82	1.56	1.52
2	B	501	NAG	O5-C5	2.75	1.49	1.43
2	C	501	NAG	O5-C1	2.72	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAG	C1-C2	2.66	1.56	1.52
2	C	501	NAG	O5-C5	2.41	1.48	1.43
2	B	501	NAG	O5-C1	2.32	1.47	1.43
2	B	501	NAG	C3-C2	2.14	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	O5-C5-C6	7.00	118.18	107.20
2	B	501	NAG	C1-O5-C5	6.13	120.50	112.19
2	C	501	NAG	O5-C5-C6	4.16	113.73	107.20
2	A	501	NAG	C8-C7-N2	4.16	123.15	116.10
2	B	501	NAG	O5-C1-C2	3.71	117.15	111.29
2	A	501	NAG	C2-N2-C7	3.52	127.92	122.90
2	B	501	NAG	C2-N2-C7	3.10	127.32	122.90
2	B	501	NAG	C3-C4-C5	3.01	115.61	110.24
2	B	501	NAG	C4-C3-C2	2.99	115.41	111.02
2	B	501	NAG	C6-C5-C4	-2.85	106.34	113.00
2	A	501	NAG	O7-C7-N2	-2.82	116.76	121.95
2	A	501	NAG	C1-O5-C5	2.77	115.95	112.19
2	B	501	NAG	O7-C7-N2	-2.74	116.92	121.95
2	A	501	NAG	O5-C5-C6	-2.69	102.98	107.20
2	A	501	NAG	C3-C4-C5	2.58	114.83	110.24
2	C	501	NAG	O4-C4-C3	-2.57	104.41	110.35
2	B	501	NAG	C8-C7-N2	2.35	120.08	116.10
2	C	501	NAG	C4-C3-C2	2.15	114.17	111.02
2	C	501	NAG	O4-C4-C5	2.09	114.48	109.30
2	B	501	NAG	O6-C6-C5	2.06	118.36	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAG	C8-C7-N2-C2
2	A	501	NAG	O7-C7-N2-C2
2	B	501	NAG	O5-C5-C6-O6
2	C	501	NAG	C8-C7-N2-C2
2	B	501	NAG	C8-C7-N2-C2
2	B	501	NAG	O7-C7-N2-C2
2	B	501	NAG	C4-C5-C6-O6
2	C	501	NAG	O7-C7-N2-C2
2	A	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	501	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	3	0

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	428/454 (94%)	-0.02	11 (2%) 56 44	58, 93, 149, 207	0
1	B	443/454 (97%)	0.03	17 (3%) 40 29	61, 96, 161, 206	0
1	C	410/454 (90%)	-0.03	9 (2%) 62 52	62, 99, 152, 199	0
All	All	1281/1362 (94%)	-0.01	37 (2%) 51 40	58, 96, 154, 207	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	ASP	4.8
1	A	133	LYS	4.3
1	B	134	GLN	3.6
1	C	295	MET	3.5
1	C	377	SER	3.4
1	A	128	GLN	3.4
1	C	325	CYS	3.3
1	A	127	THR	3.3
1	B	445	ALA	3.2
1	A	375	GLU	3.1
1	B	126	ASP	3.0
1	A	129	MET	3.0
1	A	131	ASP	3.0
1	C	360	TYR	2.9
1	A	132	GLU	2.7
1	B	456	TYR	2.7
1	B	132	GLU	2.6
1	B	130	ALA	2.6
1	B	83	SER	2.5
1	B	133	LYS	2.5
1	A	126	ASP	2.5
1	C	181	ALA	2.5
1	A	130	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	129	MET	2.4
1	B	377	SER	2.3
1	C	342	TYR	2.3
1	B	446	SER	2.3
1	A	233	TRP	2.3
1	B	233	TRP	2.3
1	B	447	ILE	2.2
1	B	128	GLN	2.2
1	B	109	TYR	2.2
1	A	202	ASP	2.2
1	C	296	ASP	2.1
1	C	262	GLY	2.1
1	B	364	GLU	2.1
1	C	453	LEU	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
2	NAG	A	501	14/15	0.82	0.34	107,132,149,150	0
2	NAG	C	501	14/15	0.88	0.33	98,123,134,135	0
2	NAG	B	501	14/15	0.88	0.32	108,132,140,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.