



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2021 – 10:10 AM JST

PDB ID : 6L6N
Title : hASIC1a co-crystallized with Nafamostat
Authors : Lei, F.; Jian, S.
Deposited on : 2019-10-29
Resolution : 2.86 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 : 2.16
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) : 2.16

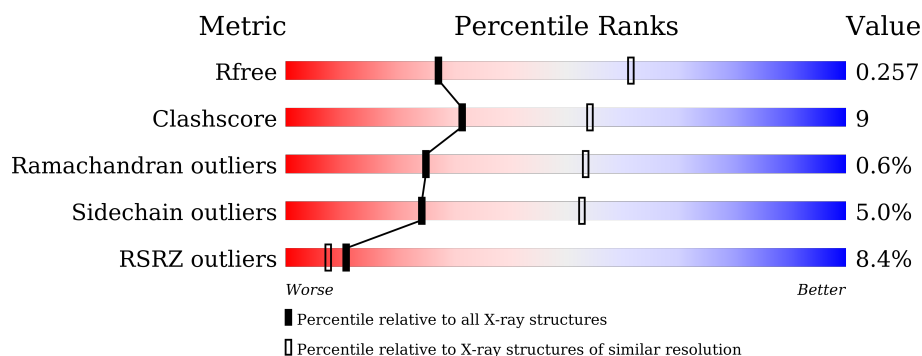
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	454	<div> <div>11%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	454	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	454	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9786 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	405	Total	C	N	O	S	0	0	0
			3242	2070	532	611	29			
1	B	403	Total	C	N	O	S	0	0	0
			3220	2053	529	609	29			
1	C	401	Total	C	N	O	S	0	0	0
			3205	2043	527	606	29			

There are 42 discrepancies between the modelled and reference sequences:

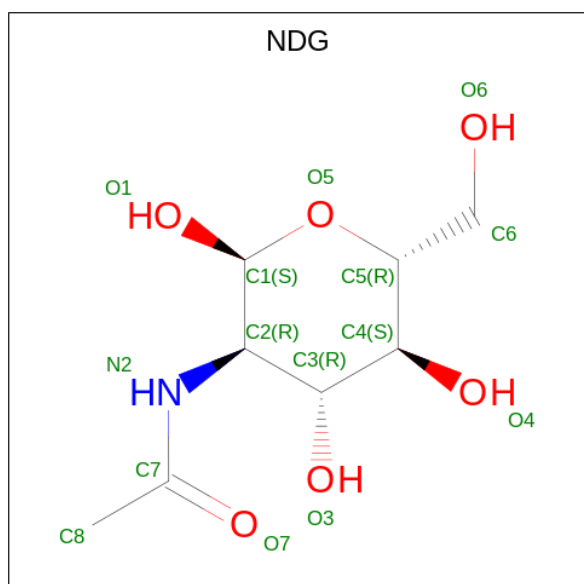
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP P78348
A	12	SER	-	expression tag	UNP P78348
A	13	GLY	-	expression tag	UNP P78348
A	14	GLY	-	expression tag	UNP P78348
A	15	SER	-	expression tag	UNP P78348
A	16	GLY	-	expression tag	UNP P78348
A	17	LEU	-	expression tag	UNP P78348
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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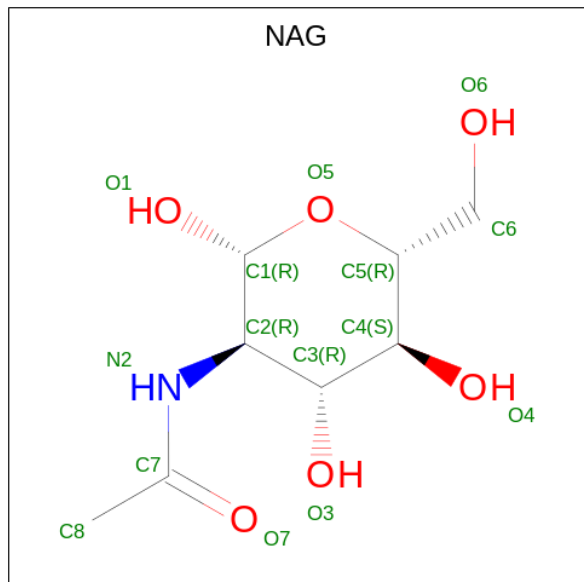
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	LEU	-	expression tag	UNP P78348
B	21	PHE	-	expression tag	UNP P78348
B	22	GLN	-	expression tag	UNP P78348
B	23	GLY	-	expression tag	UNP P78348
B	24	PRO	-	expression tag	UNP P78348
C	11	GLY	-	expression tag	UNP P78348
C	12	SER	-	expression tag	UNP P78348
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-alpha-D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

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

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

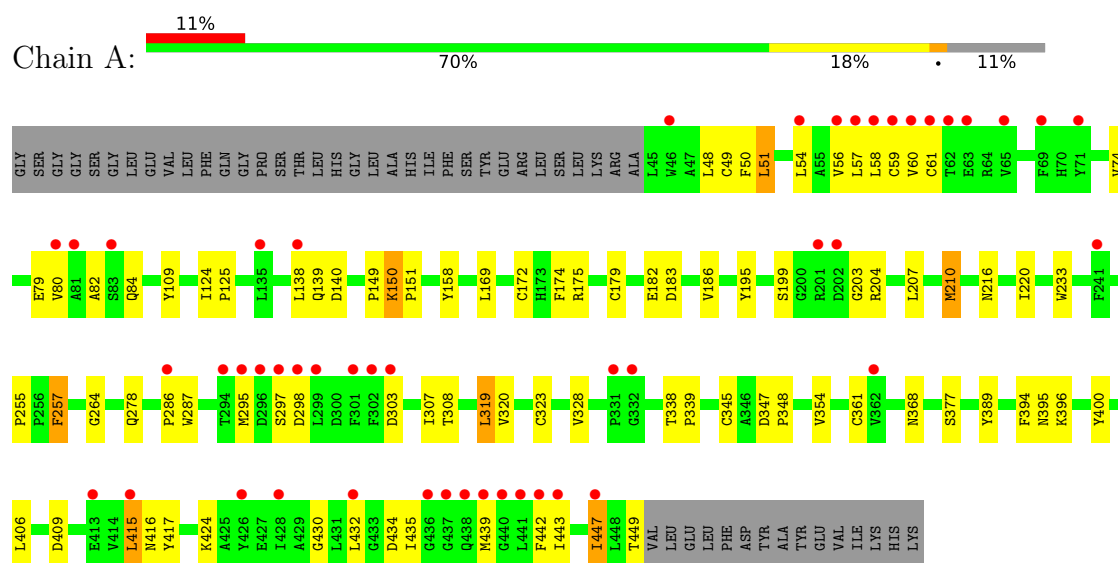
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	21	Total	O	0	0
			21	21		
6	C	16	Total	O	0	0
			16	16		

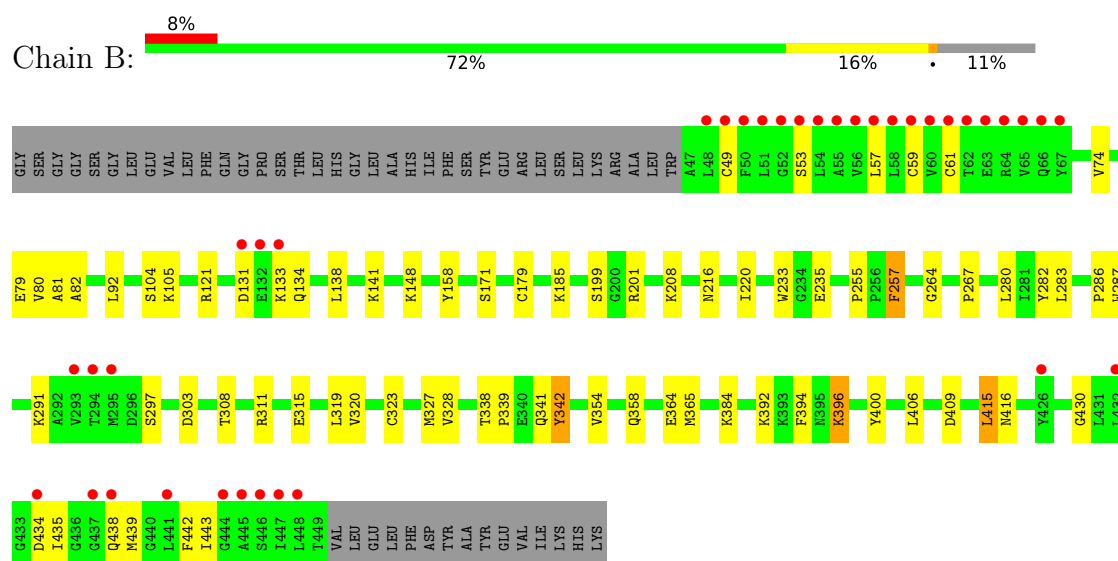
3 Residue-property plots [i](#)

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.

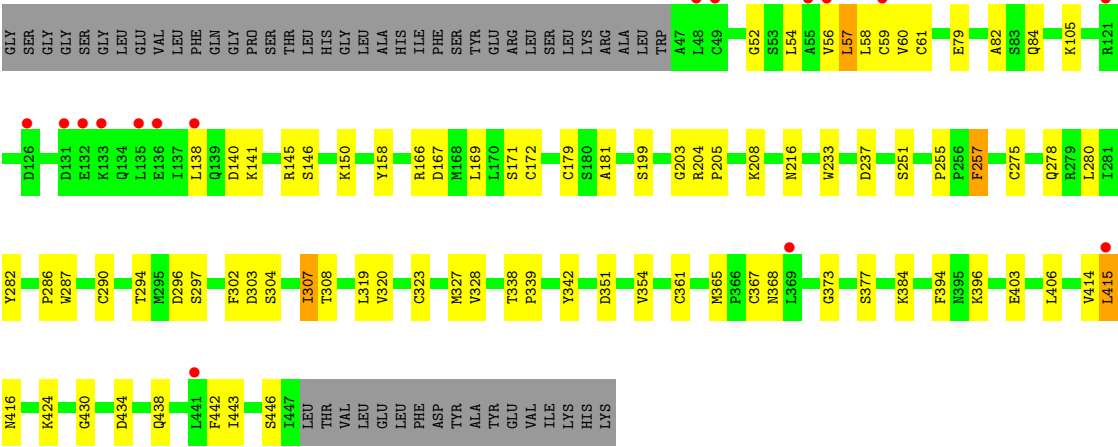
• Molecule 1: Acid-sensing ion channel 1



• 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	83.65Å 142.71Å 221.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.17 – 2.86 72.17 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.17-2.86) 99.8 (72.17-2.86)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.210 , 0.247 0.221 , 0.257	Depositor DCC
R_{free} test set	3099 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9786	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 3.12% 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: CL, EDO, NDG, 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	0.67	0/3318	0.84	0/4487
1	B	0.67	0/3294	0.86	0/4453
1	C	0.66	0/3279	0.84	1/4432 (0.0%)
All	All	0.67	0/9891	0.85	1/13372 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ASP	CB-CA-C	-5.42	99.56	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3242	0	3134	80	0
1	B	3220	0	3114	48	0
1	C	3205	0	3097	53	0
2	A	14	0	12	0	0
3	A	14	0	13	1	0
3	B	14	0	13	0	0
3	C	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	4	0	6	1	0
6	A	6	0	0	1	0
6	B	21	0	0	1	0
6	C	16	0	0	1	0
All	All	9786	0	9415	172	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 9.

All (172) 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:54:LEU:HD13	1:A:442:PHE:CE2	1.92	1.03
1:A:54:LEU:HD13	1:A:442:PHE:CZ	1.95	1.01
1:A:54:LEU:HD13	1:A:442:PHE:CD2	2.04	0.93
1:A:48:LEU:O	1:A:48:LEU:HD23	1.73	0.88
1:A:54:LEU:HD13	1:A:442:PHE:CE1	2.10	0.86
1:C:61:CYS:SG	1:C:438:GLN:OE1	2.36	0.84
1:B:311:ARG:O	1:B:315:GLU:HG3	1.80	0.81
1:A:54:LEU:HD13	1:A:442:PHE:CG	2.17	0.79
1:A:54:LEU:CD1	1:A:442:PHE:CD2	2.65	0.79
1:C:57:LEU:HD11	1:C:438:GLN:O	1.82	0.79
1:C:290:CYS:HG	1:C:367:CYS:HG	0.78	0.78
1:C:294:THR:OG1	1:C:296:ASP:OD1	2.02	0.77
1:A:54:LEU:HD13	1:A:442:PHE:CD1	2.22	0.75
1:A:84:GLN:HE21	1:A:210:MET:CE	2.02	0.73
1:A:54:LEU:CD1	1:A:442:PHE:CE2	2.70	0.73
1:A:48:LEU:HG	1:A:51:LEU:CD2	2.19	0.72
1:C:297:SER:OG	1:C:302:PHE:O	2.06	0.72
1:A:57:LEU:CD2	1:A:442:PHE:HB2	2.20	0.71
1:B:435:ILE:O	1:B:439:MET:HG2	1.92	0.70
1:A:54:LEU:CD1	1:A:442:PHE:CG	2.76	0.69
1:C:54:LEU:HB2	1:C:442:PHE:CE1	2.27	0.69
1:B:82:ALA:O	1:B:415:LEU:HB3	1.93	0.68
1:A:84:GLN:HE21	1:A:210:MET:HE3	1.58	0.68
1:A:287:TRP:CH2	1:A:424:LYS:HE2	2.28	0.68
1:A:257:PHE:HB2	1:A:308:THR:HG23	1.75	0.68
1:B:257:PHE:HB2	1:B:308:THR:HG23	1.77	0.67
1:B:430:GLY:O	1:B:434:ASP:OD1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HG	1:A:51:LEU:HD23	1.77	0.67
1:C:430:GLY:O	1:C:434:ASP:OD1	2.14	0.66
1:A:82:ALA:O	1:A:415:LEU:HB3	1.94	0.66
1:A:216:ASN:ND2	1:B:354:VAL:O	2.30	0.64
1:A:50:PHE:CZ	1:A:442:PHE:CE1	2.84	0.64
1:C:257:PHE:HB2	1:C:308:THR:HG23	1.78	0.64
1:B:79:GLU:HB3	1:B:416:ASN:HD21	1.63	0.64
1:C:82:ALA:O	1:C:415:LEU:HB3	1.98	0.64
1:A:175:ARG:HH22	1:B:358:GLN:NE2	1.94	0.63
1:A:51:LEU:C	1:A:51:LEU:HD12	2.18	0.63
1:C:278:GLN:HE21	1:C:280:LEU:HD11	1.62	0.63
1:A:57:LEU:CD2	1:A:442:PHE:CB	2.77	0.62
1:C:368:ASN:HD22	3:C:501:NAG:C7	2.12	0.62
1:B:133:LYS:HD2	1:B:133:LYS:O	1.98	0.62
1:A:57:LEU:HD21	1:A:442:PHE:CB	2.30	0.61
1:C:204:ARG:HG2	1:C:205:PRO:HD2	1.82	0.61
1:A:395:ASN:HD22	3:A:502:NAG:H83	1.65	0.61
1:B:338:THR:OG1	1:B:341:GLN:HG3	2.00	0.60
1:B:282:TYR:CZ	1:B:365:MET:CE	2.84	0.59
1:C:282:TYR:CZ	1:C:365:MET:HE3	2.37	0.59
1:A:54:LEU:HB2	1:A:442:PHE:CE1	2.38	0.59
1:C:297:SER:HB3	1:C:303:ASP:C	2.24	0.58
1:C:396:LYS:HE2	6:C:614:HOH:O	2.04	0.58
1:A:345:CYS:O	1:A:348:PRO:HG2	2.04	0.58
1:C:282:TYR:CZ	1:C:365:MET:CE	2.88	0.56
1:B:384:LYS:HE3	1:C:403:GLU:OE1	2.06	0.56
1:C:138:LEU:HD13	1:C:233:TRP:CH2	2.41	0.56
1:A:174:PHE:CD2	1:A:207:LEU:HD23	2.41	0.56
1:A:138:LEU:HD13	1:A:233:TRP:CH2	2.42	0.55
1:A:57:LEU:HD12	1:A:58:LEU:N	2.21	0.55
1:C:57:LEU:CD1	1:C:438:GLN:O	2.55	0.54
1:A:109:TYR:CE2	1:A:149:PRO:HG3	2.43	0.54
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.08	0.54
1:A:443:ILE:O	1:A:447:ILE:HD13	2.09	0.53
1:A:48:LEU:HG	1:A:51:LEU:HD21	1.87	0.53
1:B:396:LYS:HG2	1:B:400:TYR:CE1	2.43	0.53
1:A:57:LEU:HD23	1:A:442:PHE:HB2	1.90	0.52
1:C:79:GLU:HA	1:C:79:GLU:OE1	2.10	0.52
1:A:84:GLN:HE21	1:A:210:MET:HE2	1.74	0.52
1:A:406:LEU:HD12	1:A:406:LEU:C	2.30	0.51
1:B:280:LEU:HB3	1:B:282:TYR:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:SER:HB3	1:B:303:ASP:O	2.11	0.51
1:B:255:PRO:O	1:B:308:THR:HG21	2.10	0.51
1:B:396:LYS:HG2	1:B:400:TYR:CD1	2.46	0.51
1:A:56:VAL:HA	1:A:59:CYS:SG	2.51	0.51
1:A:255:PRO:O	1:A:308:THR:HG21	2.11	0.51
1:A:48:LEU:C	1:A:48:LEU:HD23	2.31	0.51
1:B:49:CYS:O	1:B:53:SER:HB3	2.11	0.51
1:C:158:TYR:CD2	1:C:328:VAL:HG21	2.46	0.51
1:C:414:VAL:HG12	1:C:416:ASN:HB2	1.93	0.51
1:C:255:PRO:O	1:C:308:THR:HG21	2.11	0.50
1:C:406:LEU:HD12	1:C:406:LEU:C	2.32	0.50
1:A:435:ILE:O	1:A:439:MET:HG3	2.11	0.50
1:C:290:CYS:HG	1:C:367:CYS:CB	2.25	0.50
1:B:406:LEU:HD12	1:B:406:LEU:C	2.32	0.50
1:C:52:GLY:O	1:C:56:VAL:HG23	2.12	0.50
1:A:158:TYR:CD2	1:A:328:VAL:HG21	2.47	0.50
1:B:138:LEU:HD13	1:B:233:TRP:CH2	2.47	0.49
1:B:158:TYR:CD2	1:B:328:VAL:HG21	2.47	0.49
1:A:50:PHE:CZ	1:A:442:PHE:CZ	3.00	0.49
1:A:287:TRP:CZ2	1:A:424:LYS:HE2	2.48	0.49
1:B:57:LEU:CD1	1:B:438:GLN:O	2.61	0.49
1:A:57:LEU:O	1:A:61:CYS:HB2	2.13	0.48
1:C:84:GLN:HE22	1:C:208:LYS:HD2	1.79	0.48
1:C:307:ILE:HD12	1:C:307:ILE:H	1.78	0.48
1:A:389:TYR:OH	1:B:235:GLU:HG3	2.14	0.47
1:C:166:ARG:HG3	1:C:181:ALA:CB	2.44	0.47
1:A:54:LEU:CD1	1:A:442:PHE:CD1	2.96	0.47
1:B:282:TYR:CZ	1:B:365:MET:HE2	2.50	0.47
1:B:257:PHE:HB2	1:B:308:THR:CG2	2.45	0.47
1:B:57:LEU:O	1:B:61:CYS:HB2	2.13	0.47
1:C:297:SER:CB	1:C:302:PHE:O	2.62	0.46
1:A:297:SER:HB3	1:A:303:ASP:O	2.15	0.46
1:B:131:ASP:HB3	1:B:134:GLN:HG3	1.96	0.46
1:B:81:ALA:HB2	1:C:365:MET:HG3	1.97	0.46
1:C:204:ARG:HG2	1:C:205:PRO:CD	2.45	0.46
1:B:327:MET:HG2	1:B:342:TYR:CE1	2.51	0.46
1:C:169:LEU:HD11	1:C:172:CYS:HB2	1.98	0.46
1:B:286:PRO:HD2	1:B:287:TRP:CE3	2.51	0.46
1:A:139:GLN:HA	1:A:139:GLN:OE1	2.16	0.45
1:A:57:LEU:C	1:A:57:LEU:HD12	2.37	0.45
1:B:104:SER:HA	5:B:503:EDO:H11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:O	1:A:323:CYS:HB2	2.17	0.45
1:C:145:ARG:O	1:C:146:SER:OG	2.24	0.45
1:C:286:PRO:HD2	1:C:287:TRP:CZ3	2.52	0.44
1:A:257:PHE:HB2	1:A:308:THR:CG2	2.44	0.44
1:C:297:SER:HB3	1:C:303:ASP:O	2.17	0.44
1:A:264:GLY:H	1:C:377:SER:HB2	1.81	0.44
1:A:150:LYS:HB3	1:A:151:PRO:HD2	1.99	0.44
1:A:432:LEU:HA	1:A:435:ILE:HG13	2.00	0.44
1:A:58:LEU:C	1:A:58:LEU:HD12	2.37	0.44
1:C:54:LEU:HB2	1:C:442:PHE:HE1	1.79	0.44
1:A:297:SER:O	1:A:298:ASP:HB3	2.18	0.44
1:C:237:ASP:OD2	1:C:351:ASP:OD2	2.36	0.44
1:C:287:TRP:CZ2	1:C:424:LYS:HE2	2.52	0.44
1:C:54:LEU:CD1	1:C:58:LEU:HD23	2.47	0.44
1:A:295:MET:HG2	1:A:295:MET:O	2.17	0.44
1:A:286:PRO:HD2	1:A:287:TRP:CE3	2.53	0.44
1:A:286:PRO:HD2	1:A:287:TRP:CZ3	2.52	0.44
1:B:319:LEU:O	1:B:323:CYS:HB2	2.18	0.43
1:B:286:PRO:HD2	1:B:287:TRP:CZ3	2.52	0.43
1:C:58:LEU:HD12	1:C:58:LEU:C	2.38	0.43
1:B:105:LYS:HG3	1:B:141:LYS:O	2.17	0.43
1:C:286:PRO:HD2	1:C:287:TRP:CE3	2.53	0.43
1:C:319:LEU:O	1:C:323:CYS:HB2	2.19	0.43
1:A:186:VAL:HG22	1:A:195:TYR:CE1	2.54	0.43
1:A:377:SER:HA	6:A:604:HOH:O	2.19	0.43
1:A:439:MET:O	1:A:443:ILE:HG12	2.18	0.43
1:B:185:LYS:HD3	1:B:201:ARG:HD2	2.00	0.43
1:A:347:ASP:N	1:A:348:PRO:HD2	2.34	0.43
1:B:394:PHE:O	1:B:396:LYS:HD3	2.18	0.43
1:B:439:MET:O	1:B:443:ILE:HG12	2.18	0.43
1:B:291:LYS:HA	6:B:617:HOH:O	2.19	0.42
1:A:307:ILE:H	1:A:307:ILE:HD12	1.83	0.42
1:A:394:PHE:O	1:A:396:LYS:HG2	2.19	0.42
1:C:327:MET:HG2	1:C:342:TYR:CE1	2.54	0.42
1:A:295:MET:HG3	1:A:303:ASP:OD1	2.19	0.42
1:A:354:VAL:O	1:C:216:ASN:ND2	2.49	0.42
1:A:169:LEU:HD11	1:A:172:CYS:HB2	2.02	0.41
1:C:257:PHE:HB2	1:C:308:THR:CG2	2.47	0.41
1:A:396:LYS:HD2	1:A:400:TYR:CE1	2.55	0.41
1:B:57:LEU:HD11	1:B:438:GLN:O	2.20	0.41
1:A:183:ASP:HA	1:A:204:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:SER:HB2	1:B:264:GLY:H	1.85	0.41
1:A:48:LEU:O	1:A:51:LEU:HG	2.21	0.41
1:A:57:LEU:CD2	1:A:442:PHE:HB3	2.50	0.41
1:A:84:GLN:NE2	1:A:210:MET:HE3	2.31	0.41
1:B:57:LEU:HD12	1:B:438:GLN:O	2.20	0.41
1:B:338:THR:O	1:B:339:PRO:C	2.59	0.41
1:A:430:GLY:O	1:A:434:ASP:OD2	2.38	0.41
1:A:57:LEU:HD21	1:A:442:PHE:HB3	2.01	0.41
1:B:216:ASN:ND2	1:C:354:VAL:O	2.48	0.41
1:A:338:THR:O	1:A:339:PRO:C	2.59	0.41
1:B:57:LEU:CD1	1:B:442:PHE:CD2	3.03	0.41
1:A:124:ILE:HA	1:A:125:PRO:HD3	1.93	0.41
1:C:394:PHE:O	1:C:396:LYS:HG2	2.20	0.41
1:A:80:VAL:HG21	1:A:417:TYR:CZ	2.56	0.41
1:C:275:CYS:HA	1:C:373:GLY:O	2.21	0.41
1:C:338:THR:O	1:C:339:PRO:C	2.58	0.40
1:B:267:PRO:HA	1:B:406:LEU:HB3	2.03	0.40
1:B:92:LEU:C	1:B:92:LEU:HD12	2.42	0.40
1:C:105:LYS:HG3	1:C:141:LYS:O	2.21	0.40
1:B:148:LYS:HA	1:B:148:LYS:HD2	1.90	0.40
1:B:435:ILE:O	1:B:439:MET:CG	2.66	0.40
1:C:287:TRP:CH2	1:C:424:LYS:CE	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/454 (89%)	385 (96%)	15 (4%)	3 (1%)	22	50
1	B	401/454 (88%)	382 (95%)	18 (4%)	1 (0%)	47	75
1	C	399/454 (88%)	380 (95%)	16 (4%)	3 (1%)	19	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1203/1362 (88%)	1147 (95%)	49 (4%)	7 (1%)	25	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	LEU
1	C	415	LEU
1	B	415	LEU
1	A	140	ASP
1	C	140	ASP
1	A	203	GLY
1	C	203	GLY

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	354/394 (90%)	334 (94%)	20 (6%)	21	47
1	B	352/394 (89%)	335 (95%)	17 (5%)	25	55
1	C	350/394 (89%)	334 (95%)	16 (5%)	27	56
All	All	1056/1182 (89%)	1003 (95%)	53 (5%)	24	53

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	51	LEU
1	A	60	VAL
1	A	74	VAL
1	A	150	LYS
1	A	179	CYS
1	A	182	GLU
1	A	199	SER
1	A	210	MET

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Mol	Chain	Res	Type
1	A	220	ILE
1	A	257	PHE
1	A	278	GLN
1	A	319	LEU
1	A	320	VAL
1	A	361	CYS
1	A	368	ASN
1	A	409	ASP
1	A	416	ASN
1	A	447	ILE
1	A	449	THR
1	B	59	CYS
1	B	74	VAL
1	B	80	VAL
1	B	121	ARG
1	B	171	SER
1	B	179	CYS
1	B	199	SER
1	B	208	LYS
1	B	220	ILE
1	B	257	PHE
1	B	283	LEU
1	B	320	VAL
1	B	342	TYR
1	B	364	GLU
1	B	392	LYS
1	B	396	LYS
1	B	409	ASP
1	C	57	LEU
1	C	59	CYS
1	C	60	VAL
1	C	150	LYS
1	C	171	SER
1	C	179	CYS
1	C	199	SER
1	C	251	SER
1	C	257	PHE
1	C	304	SER
1	C	307	ILE
1	C	320	VAL
1	C	361	CYS
1	C	384	LYS

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Mol	Chain	Res	Type
1	C	443	ILE
1	C	446	SER

Sometimes 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	416	ASN
1	B	358	GLN
1	B	416	ASN
1	C	84	GLN
1	C	278	GLN
1	C	399	GLN
1	C	416	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	A	502	1	14,14,15	0.84	0	17,19,21	2.45	4 (23%)
3	NAG	C	502	1	14,14,15	0.63	0	17,19,21	1.38	2 (11%)
3	NAG	B	501	1	14,14,15	0.97	0	17,19,21	2.07	4 (23%)
3	NAG	C	501	1	14,14,15	0.44	0	17,19,21	1.32	3 (17%)
2	NDG	A	501	-	14,14,15	0.69	0	17,19,21	2.09	5 (29%)
5	EDO	B	503	-	3,3,3	0.09	0	2,2,2	0.21	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	A	502	1	-	4/6/23/26	0/1/1/1
3	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	1/6/23/26	0/1/1/1
3	NAG	C	501	1	-	2/6/23/26	0/1/1/1
2	NDG	A	501	-	-	3/6/23/26	0/1/1/1
5	EDO	B	503	-	-	1/1/1/1	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C1-O5-C5	6.89	121.52	112.19
3	B	501	NAG	C1-C2-N2	5.03	119.08	110.49
2	A	501	NDG	C1-C2-N2	4.55	118.26	110.49
3	A	502	NAG	C8-C7-N2	4.34	123.44	116.10
2	A	501	NDG	C2-N2-C7	3.76	128.26	122.90
2	A	501	NDG	O5-C1-C2	-3.60	105.60	111.29
3	B	501	NAG	C2-N2-C7	3.54	127.94	122.90
3	A	502	NAG	O5-C1-C2	-3.19	106.25	111.29
2	A	501	NDG	C1-O5-C5	3.12	116.43	112.19
3	B	501	NAG	C4-C3-C2	3.05	115.49	111.02
3	C	502	NAG	C1-C2-N2	-2.71	105.85	110.49
3	B	501	NAG	C3-C4-C5	2.63	114.94	110.24
3	C	501	NAG	C1-C2-N2	-2.51	106.20	110.49
3	C	501	NAG	C4-C3-C2	2.39	114.52	111.02
3	C	502	NAG	O5-C5-C4	-2.29	105.26	110.83
3	C	501	NAG	C1-O5-C5	2.18	115.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NDG	O5-C5-C6	2.16	110.58	107.20
3	A	502	NAG	O7-C7-N2	-2.10	118.09	121.95

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAG	C4-C5-C6-O6
3	A	502	NAG	C8-C7-N2-C2
3	A	502	NAG	O7-C7-N2-C2
3	A	502	NAG	O5-C5-C6-O6
2	A	501	NDG	C4-C5-C6-O6
2	A	501	NDG	O5-C5-C6-O6
5	B	503	EDO	O1-C1-C2-O2
3	B	501	NAG	C3-C2-N2-C7
3	C	501	NAG	C4-C5-C6-O6
3	C	502	NAG	C4-C5-C6-O6
3	C	501	NAG	O5-C5-C6-O6
2	A	501	NDG	C1-C2-N2-C7
3	C	502	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
3	C	501	NAG	1	0
5	B	503	EDO	1	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	405/454 (89%)	0.66	48 (11%) 4 3	51, 93, 192, 271	0
1	B	403/454 (88%)	0.48	37 (9%) 9 6	53, 84, 185, 241	0
1	C	401/454 (88%)	0.31	16 (3%) 38 32	51, 86, 185, 231	0
All	All	1209/1362 (88%)	0.49	101 (8%) 11 7	51, 88, 188, 271	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	ILE	7.8
1	B	49	CYS	7.0
1	B	56	VAL	6.8
1	A	302	PHE	5.8
1	A	438	GLN	5.6
1	A	295	MET	5.5
1	A	441	LEU	5.5
1	A	297	SER	5.5
1	A	301	PHE	5.4
1	A	80	VAL	5.0
1	A	81	ALA	4.9
1	A	303	ASP	4.8
1	A	60	VAL	4.8
1	B	448	LEU	4.8
1	B	60	VAL	4.7
1	B	295	MET	4.6
1	B	445	ALA	4.5
1	B	446	SER	4.5
1	A	443	ILE	4.4
1	B	64	ARG	4.4
1	A	440	GLY	4.4
1	A	296	ASP	4.2
1	B	63	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	55	ALA	4.1
1	A	69	PHE	4.1
1	C	56	VAL	4.1
1	B	441	LEU	4.1
1	B	132	GLU	3.9
1	C	126	ASP	3.9
1	A	299	LEU	3.9
1	C	132	GLU	3.9
1	B	58	LEU	3.9
1	C	48	LEU	3.8
1	B	48	LEU	3.8
1	B	53	SER	3.8
1	A	439	MET	3.7
1	B	59	CYS	3.7
1	A	62	THR	3.7
1	A	61	CYS	3.7
1	A	442	PHE	3.7
1	A	298	ASP	3.6
1	A	56	VAL	3.6
1	A	202	ASP	3.6
1	B	438	GLN	3.6
1	C	135	LEU	3.5
1	A	71	TYR	3.5
1	A	332	GLY	3.5
1	A	426	TYR	3.4
1	B	52	GLY	3.2
1	B	434	ASP	3.2
1	B	66	GLN	3.1
1	A	437	GLY	3.1
1	A	63	GLU	3.1
1	B	61	CYS	3.1
1	B	65	VAL	3.0
1	A	294	THR	3.0
1	A	138	LEU	3.0
1	A	59	CYS	2.9
1	A	331	PRO	2.9
1	B	50	PHE	2.9
1	A	436	GLY	2.8
1	A	46	TRP	2.8
1	B	67	TYR	2.7
1	C	133	LYS	2.7
1	A	432	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	133	LYS	2.6
1	A	362	VAL	2.6
1	A	428	ILE	2.6
1	C	138	LEU	2.6
1	B	62	THR	2.5
1	B	293	VAL	2.5
1	C	121	ARG	2.5
1	C	136	GLU	2.5
1	A	447	ILE	2.4
1	A	58	LEU	2.4
1	B	131	ASP	2.4
1	A	241	PHE	2.4
1	B	294	THR	2.4
1	C	441	LEU	2.4
1	B	444	GLY	2.3
1	C	55	ALA	2.3
1	B	432	LEU	2.3
1	A	65	VAL	2.3
1	C	49	CYS	2.3
1	B	426	TYR	2.3
1	A	415	LEU	2.2
1	A	286	PRO	2.2
1	B	51	LEU	2.2
1	C	131	ASP	2.2
1	C	59	CYS	2.2
1	C	415	LEU	2.2
1	B	54	LEU	2.2
1	A	54	LEU	2.1
1	A	83	SER	2.1
1	A	201	ARG	2.1
1	B	437	GLY	2.1
1	A	135	LEU	2.1
1	B	57	LEU	2.1
1	C	369	LEU	2.1
1	A	57	LEU	2.1
1	A	413	GLU	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 [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
3	NAG	A	502	14/15	0.70	0.37	113,164,181,181	0
3	NAG	C	501	14/15	0.76	0.29	143,166,187,203	0
3	NAG	B	501	14/15	0.83	0.25	122,161,183,185	0
3	NAG	C	502	14/15	0.83	0.15	137,155,164,166	0
2	NDG	A	501	14/15	0.89	0.24	117,145,163,166	0
4	CL	B	502	1/1	0.90	0.16	91,91,91,91	0
5	EDO	B	503	4/4	0.91	0.11	91,93,96,104	0
4	CL	C	503	1/1	0.94	0.19	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.