



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:10 PM UTC

PDB ID : 6L6N / pdb_00006l6n
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 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

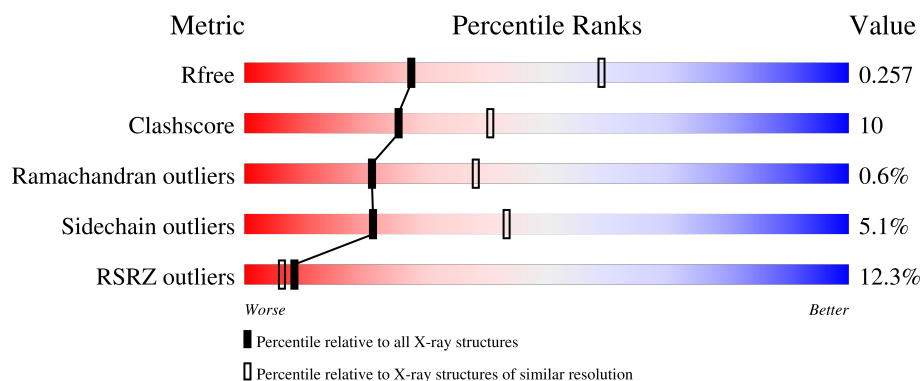
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	12% 68% 20% • 11%
1	B	454	11% 71% 17% • 11%
1	C	454	10% 68% 19% • 12%

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:

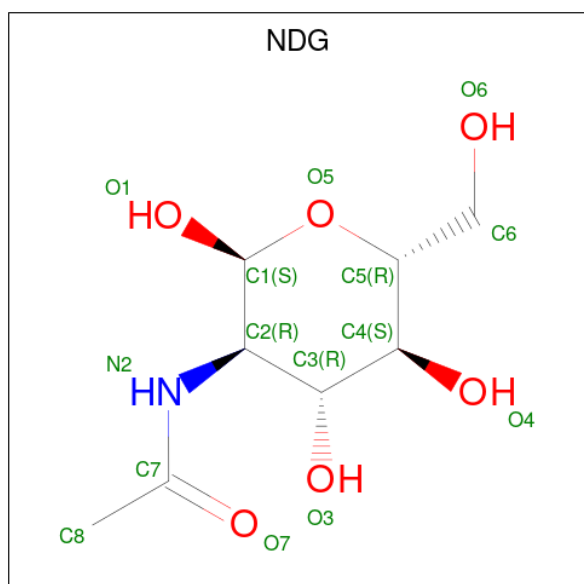
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP P78348
A	12	SER	-	expression tag	UNP P78348
A	13	GLY	-	expression tag	UNP P78348
A	14	GLY	-	expression tag	UNP P78348
A	15	SER	-	expression tag	UNP P78348
A	16	GLY	-	expression tag	UNP P78348
A	17	LEU	-	expression tag	UNP P78348
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 (CCD ID: NDG) (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		

- 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	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 (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



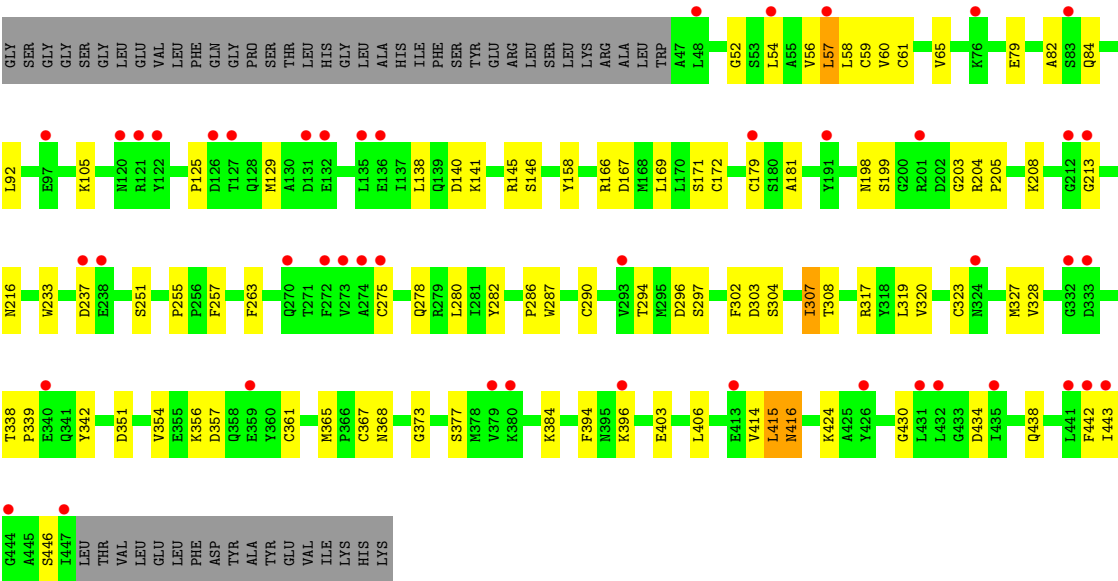
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- 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		

HIS
LYS

● 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 (4.98%)	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)	0.32 , 72.8	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

5.1 Standard geometry

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

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	1.01	1/3318 (0.0%)	1.40	9/4487 (0.2%)
1	B	1.00	0/3294	1.41	4/4453 (0.1%)
1	C	0.99	0/3279	1.40	8/4432 (0.2%)
All	All	1.00	1/9891 (0.0%)	1.40	21/13372 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	ASN	C-O	6.09	1.31	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ASP	CA-CB-CG	6.92	119.52	112.60
1	C	167	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	125	PRO	CA-C-N	5.86	130.51	121.19
1	A	125	PRO	C-N-CA	5.86	130.51	121.19
1	C	213	GLY	CA-C-O	-5.71	118.01	122.52
1	A	57	LEU	CA-C-O	-5.63	114.45	120.42
1	C	125	PRO	CA-C-N	5.61	129.24	120.82
1	C	125	PRO	C-N-CA	5.61	129.24	120.82
1	B	213	GLY	CA-C-O	-5.61	118.09	122.52
1	B	198	ASN	CA-C-N	5.57	128.01	120.38
1	B	198	ASN	C-N-CA	5.57	128.01	120.38
1	A	198	ASN	CA-C-N	5.56	127.73	120.28
1	A	198	ASN	C-N-CA	5.56	127.73	120.28
1	C	263	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	49	CYS	N-CA-C	-5.29	106.09	112.54
1	A	127	THR	CA-CB-OG1	-5.22	101.78	109.60
1	C	198	ASN	CA-C-N	5.16	127.19	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	ASN	C-N-CA	5.16	127.19	120.28
1	A	296	ASP	CA-C-N	5.04	127.04	120.28
1	A	296	ASP	C-N-CA	5.04	127.04	120.28
1	C	167	ASP	CB-CA-C	-5.03	99.56	109.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	83	0
1	B	3220	0	3114	51	0
1	C	3205	0	3097	59	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
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	183	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 10.

All (183) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD23	1:A:48:LEU:O	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:A:84:GLN:HE21	1:A:210:MET:HE3	1.47	0.78
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: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:84:GLN:HE21	1:A:210:MET:CE	2.02	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:C:327:MET:HE3	1:C:342:TYR:HE1	1.58	0.69
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:A:51:LEU:HD12	1:A:51:LEU:C	2.18	0.68
1:B:82:ALA:O	1:B:415:LEU:HB3	1.93	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
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:C:282:TYR:CZ	1:C:365:MET:HE3	2.31	0.66
1:A:50:PHE:CZ	1:A:442:PHE:CE1	2.84	0.64
1:A:216:ASN:ND2	1:B:354:VAL:O	2.30	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:C:278:GLN:HE21	1:C:280:LEU:HD11	1.62	0.63
1:C:297:SER:HB3	1:C:303:ASP:C	2.24	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:O	1:B:133:LYS:HD2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:54:LEU:HB2	1:A:442:PHE:CE1	2.38	0.59
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:A:406:LEU:C	1:A:406:LEU:HD12	2.30	0.56
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:48:LEU:HD23	1:A:48:LEU:C	2.31	0.55
1:A:138:LEU:HD13	1:A:233:TRP:CH2	2.42	0.55
1:C:406:LEU:C	1:C:406:LEU:HD12	2.32	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:B:406:LEU:HD12	1:B:406:LEU:C	2.32	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:B:280:LEU:HB3	1:B:282:TYR:HE1	1.75	0.51
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:B:49:CYS:O	1:B:53:SER:HB3	2.11	0.51
1:C:327:MET:HE3	1:C:342:TYR:CE1	2.42	0.51
1:A:84:GLN:NE2	1:A:210:MET:HE3	2.22	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: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:C:52:GLY:O	1:C:56:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD12	1:A:57:LEU:C	2.37	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:58:LEU:C	1:A:58:LEU:HD12	2.37	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:58:LEU:C	1:C:58:LEU:HD12	2.38	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: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:B:389:TYR:CD1	1:C:129:MET:HE3	2.50	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:81:ALA:HB2	1:C:365:MET:HG3	1.97	0.46
1:B:131:ASP:HB3	1:B:134:GLN:HG3	1.96	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:B:338:THR:O	1:B:339:PRO:C	2.59	0.46
1:A:338:THR:O	1:A:339:PRO:C	2.59	0.45
1:B:282:TYR:CZ	1:B:365:MET:HE2	2.51	0.45
1:C:338:THR:O	1:C:339:PRO:C	2.58	0.45
1:A:139:GLN:HA	1:A:139:GLN:OE1	2.16	0.45
1:B:92:LEU:C	1:B:92:LEU:HD12	2.42	0.45
1:B:104:SER:HA	5:B:503:EDO:H11	1.98	0.45
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:282:TYR:CE2	1:C:365:MET:HE3	2.52	0.45
1:A:92:LEU:C	1:A:92:LEU:HD12	2.42	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:LEU:HA	1:A:435:ILE:HG13	2.00	0.44
1:C:92:LEU:C	1:C:92:LEU:HD12	2.42	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:54:LEU:CD1	1:C:58:LEU:HD23	2.47	0.44
1:C:287:TRP:CZ2	1:C:424:LYS:HE2	2.52	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:C:297:SER:HB3	1:C:303:ASP:O	2.17	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: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:48:LEU:C	1:A:48:LEU:CD2	2.92	0.43
1:A:439:MET:O	1:A:443:ILE:HG12	2.18	0.43
1:B:327:MET:HE2	1:B:342:TYR:HE1	1.83	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:A:297:SER:HB3	1:A:303:ASP:C	2.43	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:HD12	1:A:307:ILE:H	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:356:LYS:O	1:A:357:ASP:C	2.63	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
1:C:356:LYS:O	1:C:357:ASP:C	2.62	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

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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:B:57:LEU:HD12	1:B:438:GLN:O	2.20	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:124:ILE:HA	1:A:125:PRO:HD3	1.93	0.41
1:B:57:LEU:CD1	1:B:442:PHE:CD2	3.03	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:B:267:PRO:HA	1:B:406:LEU:HB3	2.03	0.40
1:B:356:LYS:O	1:B:357:ASP:C	2.63	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 ⓘ

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	403/454 (89%)	385 (96%)	15 (4%)	3 (1%)	18	35
1	B	401/454 (88%)	382 (95%)	18 (4%)	1 (0%)	43	62
1	C	399/454 (88%)	380 (95%)	16 (4%)	3 (1%)	16	31
All	All	1203/1362 (88%)	1147 (95%)	49 (4%)	7 (1%)	21	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	LEU

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Mol	Chain	Res	Type
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%)	19	40
1	B	352/394 (89%)	335 (95%)	17 (5%)	23	46
1	C	350/394 (89%)	333 (95%)	17 (5%)	22	45
All	All	1056/1182 (89%)	1002 (95%)	54 (5%)	21	43

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	60	VAL
1	A	65	VAL
1	A	74	VAL
1	A	154	MET
1	A	179	CYS
1	A	182	GLU
1	A	199	SER
1	A	209	THR
1	A	210	MET
1	A	211	LYS
1	A	220	ILE
1	A	278	GLN
1	A	291	LYS
1	A	319	LEU
1	A	320	VAL

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Mol	Chain	Res	Type
1	A	361	CYS
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	137	ILE
1	B	171	SER
1	B	179	CYS
1	B	199	SER
1	B	208	LYS
1	B	220	ILE
1	B	283	LEU
1	B	311	ARG
1	B	320	VAL
1	B	364	GLU
1	B	384	LYS
1	B	392	LYS
1	B	396	LYS
1	C	57	LEU
1	C	59	CYS
1	C	60	VAL
1	C	65	VAL
1	C	171	SER
1	C	179	CYS
1	C	199	SER
1	C	251	SER
1	C	304	SER
1	C	307	ILE
1	C	317	ARG
1	C	320	VAL
1	C	361	CYS
1	C	384	LYS
1	C	416	ASN
1	C	443	ILE
1	C	446	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	73	HIS
1	A	84	GLN
1	A	329	HIS
1	A	416	ASN
1	B	73	HIS
1	B	84	GLN
1	B	134	GLN
1	B	260	GLN
1	B	270	GLN
1	B	416	ASN
1	C	70	HIS
1	C	84	GLN
1	C	134	GLN
1	C	143	ASN
1	C	270	GLN
1	C	278	GLN
1	C	329	HIS
1	C	399	GLN
1	C	416	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	502	1	14,14,15	0.64	0	17,19,21	1.38	2 (11%)
5	EDO	B	503	-	3,3,3	0.08	0	2,2,2	0.15	0
3	NAG	A	502	1	14,14,15	0.84	0	17,19,21	2.49	5 (29%)
3	NAG	C	501	1	14,14,15	0.45	0	17,19,21	1.30	3 (17%)
2	NDG	A	501	-	14,14,15	0.71	0	17,19,21	2.15	4 (23%)
3	NAG	B	501	1	14,14,15	1.00	0	17,19,21	2.14	4 (23%)

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	C	502	1	-	2/6/23/26	0/1/1/1
5	EDO	B	503	-	-	1/1/1/1	-
3	NAG	A	502	1	-	4/6/23/26	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
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1

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	6.97	121.52	112.19
3	B	501	NAG	C1-C2-N2	5.49	119.08	110.43
2	A	501	NDG	C1-C2-N2	4.96	118.26	110.43
3	A	502	NAG	C8-C7-N2	4.42	123.44	116.12
2	A	501	NDG	C2-N2-C7	4.00	128.26	122.90
3	B	501	NAG	C2-N2-C7	3.76	127.94	122.90
2	A	501	NDG	O5-C1-C2	-3.68	105.60	111.29
3	A	502	NAG	O5-C1-C2	-3.26	106.25	111.29
2	A	501	NDG	C1-O5-C5	3.16	116.43	112.19
3	B	501	NAG	C4-C3-C2	3.05	115.49	111.02
3	C	502	NAG	C1-C2-N2	-2.91	105.85	110.43
3	C	501	NAG	C1-C2-N2	-2.68	106.20	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAG	C3-C4-C5	2.59	114.94	110.23
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	2.21	115.15	112.19
3	A	502	NAG	O7-C7-N2	-2.20	118.09	121.98
3	A	502	NAG	O7-C7-C8	-2.02	118.46	122.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDG	C1-C2-N2-C7
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	C	501	NAG	C4-C5-C6-O6
3	C	502	NAG	C4-C5-C6-O6
3	C	501	NAG	O5-C5-C6-O6
3	B	501	NAG	C1-C2-N2-C7
3	B	501	NAG	C3-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
5	B	503	EDO	1	0
3	A	502	NAG	1	0
3	C	501	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.70	54 (13%) 7 5	51, 93, 192, 271	0
1	B	403/454 (88%)	0.50	49 (12%) 8 6	53, 84, 185, 241	0
1	C	401/454 (88%)	0.66	46 (11%) 9 7	51, 86, 185, 231	0
All	All	1209/1362 (88%)	0.62	149 (12%) 8 6	51, 88, 188, 271	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	VAL	6.2
1	B	293	VAL	5.8
1	A	48	LEU	5.2
1	B	127	THR	5.1
1	A	448	LEU	4.9
1	A	81	ALA	4.8
1	A	298	ASP	4.7
1	A	135	LEU	4.6
1	B	447	ILE	4.6
1	A	413	GLU	4.4
1	C	132	GLU	4.4
1	C	413	GLU	4.3
1	C	122	TYR	4.2
1	B	237	ASP	4.2
1	A	421	GLU	4.0
1	A	83	SER	4.0
1	C	447	ILE	4.0
1	C	275	CYS	4.0
1	C	443	ILE	4.0
1	A	449	THR	4.0
1	A	45	LEU	3.9
1	B	133	LYS	3.9
1	C	238	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	212	GLY	3.9
1	A	441	LEU	3.7
1	C	324	ASN	3.7
1	A	139	GLN	3.7
1	B	131	ASP	3.7
1	A	417	TYR	3.7
1	C	444	GLY	3.7
1	C	83	SER	3.6
1	A	46	TRP	3.6
1	B	125	PRO	3.5
1	A	302	PHE	3.5
1	C	359	GLU	3.4
1	C	131	ASP	3.4
1	B	59	CYS	3.4
1	B	303	ASP	3.4
1	C	237	ASP	3.4
1	C	213	GLY	3.3
1	C	126	ASP	3.3
1	B	204	ARG	3.3
1	B	47	ALA	3.3
1	A	52	GLY	3.3
1	A	202	ASP	3.2
1	C	135	LEU	3.2
1	B	438	GLN	3.2
1	B	362	VAL	3.2
1	A	297	SER	3.1
1	C	333	ASP	3.1
1	C	442	PHE	3.1
1	B	56	VAL	3.1
1	A	51	LEU	3.1
1	A	344	GLU	3.1
1	C	272	PHE	3.0
1	C	293	VAL	3.0
1	C	136	GLU	3.0
1	A	47	ALA	3.0
1	A	138	LEU	3.0
1	B	50	PHE	3.0
1	C	426	TYR	3.0
1	B	415	LEU	2.9
1	B	53	SER	2.9
1	B	295	MET	2.9
1	B	429	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	64	ARG	2.9
1	C	270	GLN	2.9
1	C	435	ILE	2.9
1	A	142	ALA	2.9
1	A	213	GLY	2.8
1	B	134	GLN	2.8
1	A	293	VAL	2.8
1	A	49	CYS	2.8
1	C	54	LEU	2.8
1	C	76	LYS	2.8
1	C	201	ARG	2.7
1	B	61	CYS	2.7
1	A	146	SER	2.7
1	B	442	PHE	2.7
1	A	141	LYS	2.7
1	A	212	GLY	2.7
1	B	60	VAL	2.7
1	B	443	ILE	2.7
1	C	120	ASN	2.7
1	A	227	ASP	2.7
1	B	182	GLU	2.6
1	C	379	VAL	2.6
1	B	292	ALA	2.6
1	A	331	PRO	2.6
1	B	261	LEU	2.6
1	B	414	VAL	2.6
1	B	432	LEU	2.6
1	A	414	VAL	2.6
1	A	435	ILE	2.6
1	A	123	GLU	2.6
1	A	415	LEU	2.5
1	C	431	LEU	2.5
1	B	49	CYS	2.5
1	A	129	MET	2.5
1	C	179	CYS	2.5
1	A	53	SER	2.5
1	B	446	SER	2.5
1	B	294	THR	2.5
1	B	69	PHE	2.5
1	B	409	ASP	2.4
1	A	109	TYR	2.4
1	A	431	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	441	LEU	2.4
1	B	205	PRO	2.4
1	B	201	ARG	2.4
1	B	441	LEU	2.4
1	A	74	VAL	2.4
1	C	380	LYS	2.4
1	B	227	ASP	2.3
1	B	449	THR	2.3
1	C	191	TYR	2.3
1	C	121	ARG	2.3
1	C	340	GLU	2.3
1	A	79	GLU	2.3
1	B	129	MET	2.3
1	C	127	THR	2.3
1	A	113	GLU	2.3
1	A	292	ALA	2.3
1	A	347	ASP	2.3
1	A	133	LYS	2.3
1	B	55	ALA	2.2
1	B	238	GLU	2.2
1	B	51	LEU	2.2
1	C	274	ALA	2.2
1	A	204	ARG	2.2
1	B	71	TYR	2.2
1	A	145	ARG	2.2
1	C	273	VAL	2.2
1	A	233	TRP	2.2
1	C	332	GLY	2.2
1	C	48	LEU	2.2
1	B	321	GLU	2.2
1	C	97	GLU	2.2
1	B	126	ASP	2.1
1	A	126	ASP	2.1
1	B	54	LEU	2.1
1	C	57	LEU	2.1
1	A	60	VAL	2.1
1	A	120	ASN	2.1
1	B	324	ASN	2.1
1	C	432	LEU	2.1
1	A	56	VAL	2.1
1	C	396	LYS	2.1
1	A	432	LEU	2.1

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($\text{\AA}^2$)	Q<0.9
3	NAG	A	502	14/15	0.30	0.16	113,164,181,181	0
3	NAG	C	501	14/15	0.54	0.20	143,166,187,203	0
2	NDG	A	501	14/15	0.66	0.14	117,145,163,166	0
3	NAG	C	502	14/15	0.72	0.12	137,155,164,166	0
3	NAG	B	501	14/15	0.73	0.14	122,161,183,185	0
5	EDO	B	503	4/4	0.76	0.29	91,93,96,104	0
4	CL	C	503	1/1	0.93	0.18	91,91,91,91	0
4	CL	B	502	1/1	0.95	0.14	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.