



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 PM UTC

PDB ID : 4GJR / pdb_00004gjr
Title : Crystal structure of the TAL effector dHax3 bound to methylated dsDNA
Authors : Yan, N.; Deng, D.; Yan, C.Y.; Yin, P.; Pan, X.J.; Shi, Y.G.
Deposited on : 2012-08-10
Resolution : 1.85 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

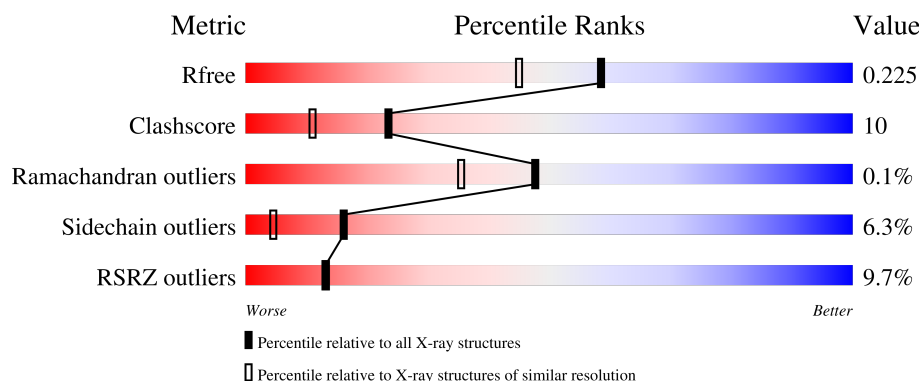
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	499	12% 76% 20% ..
1	B	499	7% 81% 16% ..
2	G	17	6% 71% 24% 6%
2	I	17	12% 71% 29%
3	H	17	6% 71% 29%

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Mol	Chain	Length	Quality of chain
3	J	17	6% 53% 47%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9340 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 Hax3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	1	0
			3546	2220	656	658	12			
1	B	487	Total	C	N	O	S	0	7	0
			3575	2232	666	664	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	-	expression tag	UNP Q3ZD72
A	300	HIS	ASN	engineered mutation	UNP Q3ZD72
A	301	ASP	ILE	engineered mutation	UNP Q3ZD72
A	368	HIS	ASN	engineered mutation	UNP Q3ZD72
A	369	ASP	ILE	engineered mutation	UNP Q3ZD72
A	402	ASN	HIS	engineered mutation	UNP Q3ZD72
A	403	GLY	ASP	engineered mutation	UNP Q3ZD72
A	436	ASN	HIS	engineered mutation	UNP Q3ZD72
A	437	GLY	ASP	engineered mutation	UNP Q3ZD72
A	470	ASN	HIS	engineered mutation	UNP Q3ZD72
A	471	GLY	ASP	engineered mutation	UNP Q3ZD72
A	539	GLY	SER	engineered mutation	UNP Q3ZD72
A	572	HIS	ASN	engineered mutation	UNP Q3ZD72
A	573	ASP	SER	engineered mutation	UNP Q3ZD72
A	606	ASN	HIS	engineered mutation	UNP Q3ZD72
A	607	GLY	ASP	engineered mutation	UNP Q3ZD72
A	640	HIS	ASN	engineered mutation	UNP Q3ZD72
A	641	ASP	ILE	engineered mutation	UNP Q3ZD72
A	721	LEU	-	expression tag	UNP Q3ZD72
A	722	GLU	-	expression tag	UNP Q3ZD72
A	723	HIS	-	expression tag	UNP Q3ZD72
A	724	HIS	-	expression tag	UNP Q3ZD72
A	725	HIS	-	expression tag	UNP Q3ZD72
A	726	HIS	-	expression tag	UNP Q3ZD72
A	727	HIS	-	expression tag	UNP Q3ZD72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	728	HIS	-	expression tag	UNP Q3ZD72
B	230	MET	-	expression tag	UNP Q3ZD72
B	300	HIS	ASN	engineered mutation	UNP Q3ZD72
B	301	ASP	ILE	engineered mutation	UNP Q3ZD72
B	368	HIS	ASN	engineered mutation	UNP Q3ZD72
B	369	ASP	ILE	engineered mutation	UNP Q3ZD72
B	402	ASN	HIS	engineered mutation	UNP Q3ZD72
B	403	GLY	ASP	engineered mutation	UNP Q3ZD72
B	436	ASN	HIS	engineered mutation	UNP Q3ZD72
B	437	GLY	ASP	engineered mutation	UNP Q3ZD72
B	470	ASN	HIS	engineered mutation	UNP Q3ZD72
B	471	GLY	ASP	engineered mutation	UNP Q3ZD72
B	539	GLY	SER	engineered mutation	UNP Q3ZD72
B	572	HIS	ASN	engineered mutation	UNP Q3ZD72
B	573	ASP	SER	engineered mutation	UNP Q3ZD72
B	606	ASN	HIS	engineered mutation	UNP Q3ZD72
B	607	GLY	ASP	engineered mutation	UNP Q3ZD72
B	640	HIS	ASN	engineered mutation	UNP Q3ZD72
B	641	ASP	ILE	engineered mutation	UNP Q3ZD72
B	721	LEU	-	expression tag	UNP Q3ZD72
B	722	GLU	-	expression tag	UNP Q3ZD72
B	723	HIS	-	expression tag	UNP Q3ZD72
B	724	HIS	-	expression tag	UNP Q3ZD72
B	725	HIS	-	expression tag	UNP Q3ZD72
B	726	HIS	-	expression tag	UNP Q3ZD72
B	727	HIS	-	expression tag	UNP Q3ZD72
B	728	HIS	-	expression tag	UNP Q3ZD72

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*(5CM)P*TP*AP*(5CM)P*CP*TP*CP*(5CM)P*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			334	164	49	105	16			
2	G	17	Total	C	N	O	P	0	0	0
			333	163	49	105	16			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*GP*GP*AP*GP*GP*TP*AP*GP*AP*GP*GP*GP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	17	Total 360	C 169	N 80	O 95	P 16	0	0	0
3	H	17	Total 360	C 169	N 80	O 95	P 16	0	0	0

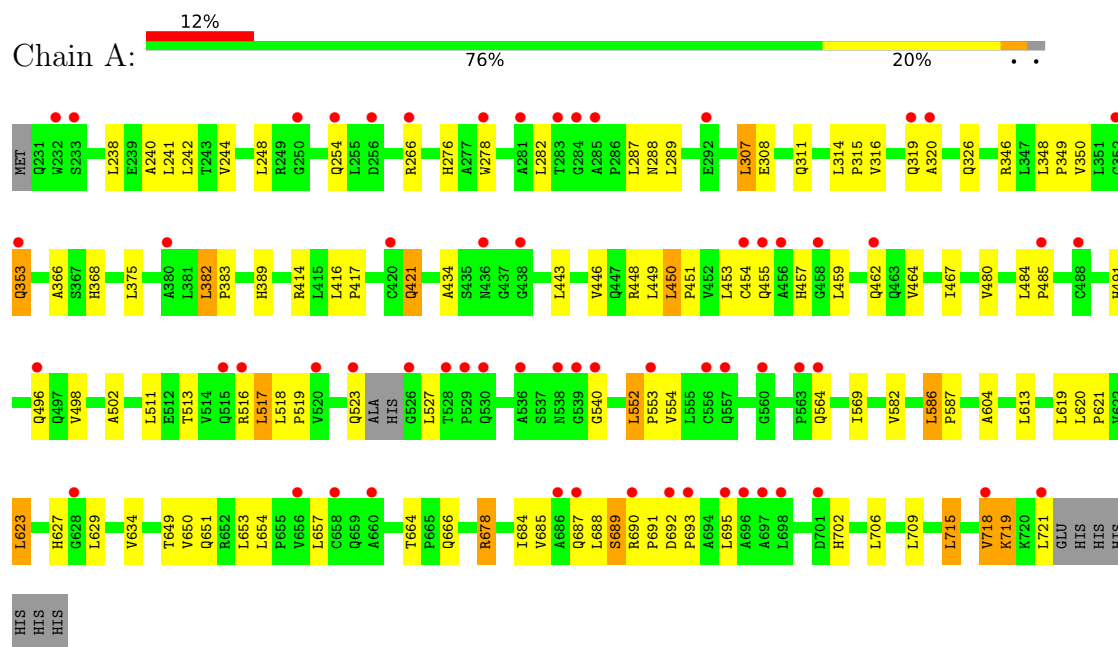
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	296	Total 296	O 296	0	0
4	I	52	Total 52	O 52	0	0
4	J	49	Total 49	O 49	0	0
4	B	321	Total 321	O 321	0	0
4	G	62	Total 62	O 62	0	0
4	H	52	Total 52	O 52	0	0

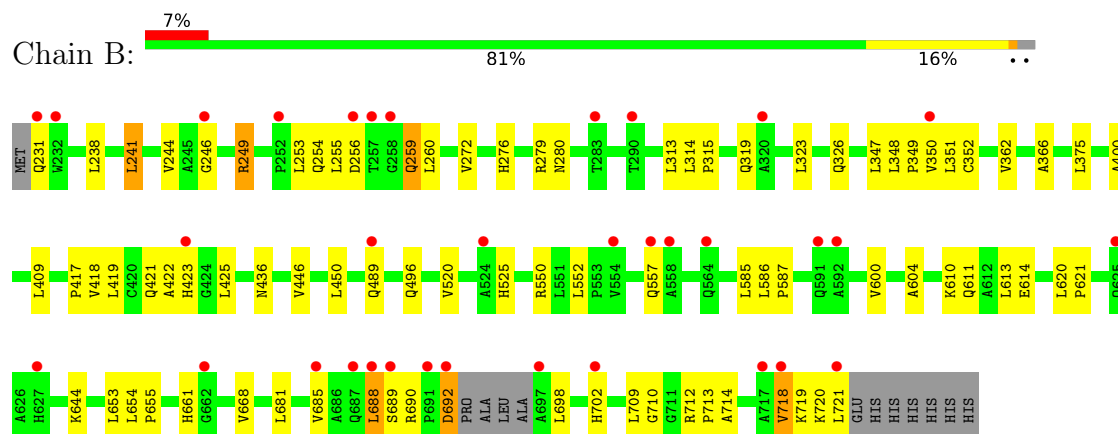
3 Residue-property plots

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: Hax3



• Molecule 1: Hax3



• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*(5CM)P*TP*AP*(5CM)P*CP*TP*CP*(5CM)P*CP*T)-3')





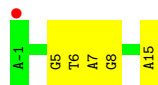
- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*(5CM)P*TP*AP*(5CM)P*CP*TP*CP*(5CM)P*CP*T)-3')



- Molecule 3: DNA (5'-D(*AP*GP*GP*GP*AP*GP*GP*TP*AP*GP*AP*GP*GP*GP*AP*CP*A)-3')



- Molecule 3: DNA (5'-D(*AP*GP*GP*GP*AP*GP*GP*TP*AP*GP*AP*GP*GP*GP*AP*CP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.84Å 87.62Å 88.45Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	32.37 – 1.85 32.37 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (32.37-1.85) 99.3 (32.37-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.198 , 0.230 0.195 , 0.225	Depositor DCC
R_{free} test set	5156 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	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	0.96	EDS
Total number of atoms	9340	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: 5CM

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	0.45	0/3597	0.75	0/4913
1	B	0.48	0/3625	0.75	1/4947 (0.0%)
2	G	0.33	0/299	0.93	0/450
2	I	0.32	0/300	0.97	0/452
3	H	0.25	0/408	0.77	0/631
3	J	0.25	0/408	0.79	1/631 (0.2%)
All	All	0.44	0/8637	0.77	2/12024 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ASN	N-CA-C	6.89	121.39	112.92
3	J	8	DG	C4'-C3'-O3'	-5.19	102.22	110.00

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	3546	0	3692	98	0
1	B	3575	0	3715	64	0
2	G	333	0	198	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	334	0	201	1	0
3	H	360	0	190	8	0
3	J	360	0	190	6	0
4	A	296	0	0	9	1
4	B	321	0	0	4	1
4	G	62	0	0	1	0
4	H	52	0	0	2	0
4	I	52	0	0	0	0
4	J	49	0	0	4	0
All	All	9340	0	8186	167	1

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 (167) 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:692:ASP:OD1	1:A:693:PRO:HD2	1.47	1.15
1:A:484:LEU:HB3	1:A:485:PRO:HD3	1.49	0.93
1:A:721:LEU:HD12	1:B:709:LEU:HD21	1.50	0.92
1:A:552:LEU:O	1:A:552:LEU:HD13	1.69	0.91
1:A:709:LEU:HD23	1:B:721:LEU:CD1	2.06	0.86
1:A:552:LEU:C	1:A:552:LEU:CD1	2.50	0.85
1:A:709:LEU:HD23	1:B:721:LEU:HD13	1.60	0.82
1:A:346:ARG:NH2	4:A:1059:HOH:O	2.13	0.82
1:B:423[B]:HIS:O	1:B:450:LEU:CD2	2.31	0.79
3:J:-1:DA:N3	4:J:121:HOH:O	2.15	0.79
3:J:5:DG:N3	4:J:114:HOH:O	2.17	0.76
1:A:552:LEU:O	1:A:552:LEU:CD1	2.35	0.74
2:G:1:DT:O5'	4:G:158:HOH:O	2.06	0.73
1:A:692:ASP:OD1	1:A:693:PRO:CD	2.33	0.73
1:A:496:GLN:OE1	4:A:928:HOH:O	2.08	0.71
1:A:417:PRO:O	1:A:421:GLN:HG3	1.91	0.71
1:B:423[B]:HIS:O	1:B:450:LEU:HD23	1.90	0.71
1:B:698:LEU:HG	1:B:702:HIS:CD2	2.26	0.70
1:A:721:LEU:HD12	1:B:709:LEU:CD2	2.22	0.70
1:B:550:ARG:NH1	4:B:915:HOH:O	2.26	0.69
1:A:552:LEU:HD13	1:A:552:LEU:C	2.14	0.69
1:A:314:LEU:HB3	1:A:315:PRO:HD3	1.75	0.68
1:A:450:LEU:HB3	1:A:451:PRO:HD3	1.78	0.65
1:A:702:HIS:HE1	4:B:1081:HOH:O	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD23	1:B:362:VAL:HG11	1.79	0.65
3:H:8:DG:N3	4:H:134:HOH:O	2.30	0.64
2:G:1:DT:N3	3:H:15:DA:C2	2.65	0.64
1:A:552:LEU:N	1:A:553:PRO:HD2	2.13	0.64
1:A:709:LEU:CD2	1:B:721:LEU:HB3	2.28	0.63
1:B:423[B]:HIS:O	1:B:450:LEU:HD21	1.98	0.63
1:A:552:LEU:C	1:A:552:LEU:HD12	2.23	0.63
1:A:241:LEU:C	1:A:241:LEU:HD23	2.24	0.63
2:G:1:DT:O2	3:H:15:DA:H2	1.82	0.62
1:B:314:LEU:HB3	1:B:315:PRO:HD3	1.84	0.60
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.85	0.59
1:A:238:LEU:O	1:A:242:LEU:HG	2.03	0.59
1:A:692:ASP:OD2	1:A:719:LYS:HG3	2.04	0.58
1:A:709:LEU:HD23	1:B:721:LEU:HB3	1.84	0.58
1:B:489:GLN:HB3	4:B:1021:HOH:O	2.02	0.57
1:B:654:LEU:HD13	1:B:668:VAL:HG11	1.86	0.57
1:A:416:LEU:HB3	1:A:417:PRO:HD3	1.86	0.57
1:A:348:LEU:HB3	1:A:349:PRO:HD3	1.85	0.56
3:J:14:DC:H2''	3:J:15:DA:C8	2.40	0.56
1:A:414:ARG:NH1	4:A:969:HOH:O	2.34	0.56
1:A:484:LEU:HD12	1:A:498:VAL:HG21	1.88	0.55
1:A:484:LEU:HB3	1:A:485:PRO:CD	2.31	0.55
1:A:685:VAL:O	1:A:689:SER:HB2	2.07	0.54
1:B:692:ASP:OD2	1:B:692:ASP:N	2.38	0.54
1:A:623:LEU:HG	1:A:629:LEU:HD12	1.88	0.54
1:B:698:LEU:HG	1:B:702:HIS:HD2	1.73	0.54
1:A:657:LEU:HD21	1:A:685:VAL:HG22	1.89	0.53
3:H:6:DT:H2'	3:H:7:DA:C8	2.42	0.53
1:A:350:VAL:HB	4:A:1028:HOH:O	2.09	0.52
1:B:418:VAL:O	1:B:422[B]:ALA:HB3	2.09	0.52
1:A:462:GLN:NE2	4:A:1001:HOH:O	2.43	0.52
1:B:653:LEU:HD13	1:B:685:VAL:HG21	1.92	0.52
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.92	0.52
1:A:721:LEU:CD1	1:B:709:LEU:CD2	2.86	0.52
1:A:448:ARG:NH1	1:A:449:LEU:HD21	2.24	0.52
1:A:620:LEU:HD13	1:A:634:VAL:HG11	1.91	0.51
1:B:689:SER:C	1:B:690:ARG:HG3	2.34	0.51
1:A:684:ILE:HG12	1:A:715:LEU:HD21	1.91	0.51
1:A:666:GLN:H	1:A:666:GLN:CD	2.18	0.51
2:I:1:DT:H2''	2:I:2:DG:C8	2.46	0.51
1:B:366:ALA:HB2	1:B:375:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:C	1:A:314:LEU:HD23	2.36	0.50
1:A:687:GLN:HB2	1:A:695:LEU:HD22	1.94	0.50
1:A:282:LEU:HD22	1:A:289:LEU:HD12	1.94	0.50
1:A:687:GLN:HG3	1:A:688:LEU:HD23	1.92	0.50
1:B:254:GLN:O	1:B:255:LEU:HD23	2.12	0.50
1:A:651:GLN:OE1	4:A:1061:HOH:O	2.20	0.49
1:A:586:LEU:N	1:A:587:PRO:HD2	2.27	0.49
1:A:569:ILE:HD13	1:A:582:VAL:HG21	1.93	0.49
1:B:348:LEU:HD22	1:B:352:CYS:SG	2.52	0.49
1:A:450:LEU:HD13	1:A:464:VAL:HG11	1.95	0.49
1:A:702:HIS:HB3	1:B:702:HIS:CE1	2.49	0.48
1:B:241:LEU:CD2	1:B:272:VAL:HG11	2.43	0.48
1:B:654:LEU:HB3	1:B:655:PRO:HD3	1.95	0.48
2:G:1:DT:C2	3:H:15:DA:H2	2.32	0.48
1:A:348:LEU:C	1:A:348:LEU:HD23	2.38	0.48
1:A:450:LEU:HD12	1:A:454:CYS:SG	2.53	0.48
1:B:417:PRO:O	1:B:421[B]:GLN:HG2	2.14	0.48
1:A:368:HIS:HE1	4:J:132:HOH:O	1.96	0.47
1:A:467:ILE:HD13	1:A:480:VAL:HG21	1.96	0.47
1:A:417:PRO:O	1:A:421:GLN:CG	2.62	0.47
1:A:604:ALA:HB2	1:A:613:LEU:HD11	1.97	0.47
1:B:348:LEU:HB3	1:B:349:PRO:HD3	1.97	0.47
1:B:710:GLY:HA3	1:B:714:ALA:HB2	1.97	0.47
1:A:240:ALA:O	1:A:244:VAL:HG23	2.14	0.46
1:A:287:LEU:HD11	1:A:311:GLN:HA	1.96	0.46
1:A:695:LEU:HD12	1:A:718:VAL:HG12	1.96	0.46
1:A:664:THR:HB	1:A:666:GLN:OE1	2.16	0.46
1:A:552:LEU:N	1:A:553:PRO:CD	2.78	0.46
1:B:718:VAL:O	1:B:721:LEU:HB2	2.16	0.46
1:A:518:LEU:HB3	1:A:519:PRO:HD3	1.98	0.46
1:B:620:LEU:C	1:B:620:LEU:HD13	2.41	0.46
1:A:241:LEU:HD23	1:A:241:LEU:O	2.15	0.46
1:A:248:LEU:HD21	1:A:276:HIS:HA	1.98	0.46
1:A:666:GLN:HG3	4:A:897:HOH:O	2.16	0.46
1:B:244:VAL:HG13	1:B:276:HIS:HB2	1.98	0.45
1:B:610:LYS:NZ	4:B:1016:HOH:O	2.49	0.45
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.98	0.45
1:B:586:LEU:HB3	1:B:587:PRO:HD3	1.98	0.45
1:B:610:LYS:O	1:B:614:GLU:HG3	2.16	0.45
1:A:316:VAL:O	1:A:320:ALA:HB3	2.16	0.45
1:A:389:HIS:HB3	1:A:416:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LEU:HD23	1:B:721:LEU:HD12	1.92	0.45
1:B:620:LEU:N	1:B:621:PRO:HD2	2.32	0.45
1:B:419:LEU:HA	1:B:423[B]:HIS:HB2	1.99	0.45
1:B:681:LEU:O	1:B:685:VAL:HG23	2.16	0.45
1:B:246:GLY:O	1:B:249:ARG:CG	2.65	0.45
1:B:425[A]:LEU:HD11	1:B:446:VAL:HG11	1.97	0.45
1:A:695:LEU:CD1	1:A:718:VAL:HG12	2.48	0.44
1:A:457:HIS:HB3	1:A:484:LEU:HD23	1.98	0.44
1:A:278[A]:TRP:CE3	1:A:307:LEU:HB3	2.53	0.44
3:J:11:DG:H1'	4:J:129:HOH:O	2.16	0.44
2:G:1:DT:C2	3:H:15:DA:C2	3.05	0.44
1:A:278[A]:TRP:NE1	4:A:907:HOH:O	2.38	0.44
1:A:620:LEU:HB3	1:A:621:PRO:HD3	1.98	0.44
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.87	0.44
1:B:279:ARG:HG2	1:B:280:ASN:N	2.33	0.43
1:B:256:ASP:OD1	1:B:259:GLN:NE2	2.48	0.43
1:B:315:PRO:O	1:B:319:GLN:HG2	2.18	0.43
1:B:712:ARG:N	1:B:713:PRO:CD	2.81	0.43
1:A:484:LEU:CD1	1:A:498:VAL:HG21	2.48	0.43
1:B:654:LEU:N	1:B:655:PRO:CD	2.82	0.43
3:J:11:DG:H2''	3:J:12:DG:H8	1.84	0.43
1:B:400:ALA:HB2	1:B:409:LEU:HD11	2.00	0.43
1:B:710:GLY:O	1:B:713:PRO:HD2	2.19	0.43
1:A:308:GLU:O	1:A:311:GLN:HG3	2.19	0.43
1:A:513:THR:O	1:A:517:LEU:HB2	2.19	0.43
1:A:266:ARG:NH1	3:J:9:DA:OP2	2.52	0.43
1:B:425[B]:LEU:HD11	1:B:446:VAL:HG11	1.99	0.43
1:A:434:ALA:HB2	1:A:443:LEU:HD11	2.01	0.42
1:A:450:LEU:CD1	1:A:454:CYS:SG	3.07	0.42
1:A:518:LEU:C	1:A:518:LEU:HD23	2.43	0.42
2:G:14:DC:H2''	2:G:15:5CM:H6	2.00	0.42
1:A:709:LEU:HD23	1:B:721:LEU:CB	2.49	0.42
1:A:326:GLN:H	1:A:326:GLN:CD	2.27	0.42
1:A:627:HIS:HB3	1:A:654:LEU:HD13	2.01	0.42
1:A:382:LEU:N	1:A:383:PRO:CD	2.83	0.42
1:B:276:HIS:CD2	1:B:279:ARG:NH2	2.88	0.42
3:H:8:DG:H1'	4:H:134:HOH:O	2.19	0.42
1:A:484:LEU:CB	1:A:485:PRO:HD3	2.31	0.42
1:A:241:LEU:C	1:A:241:LEU:CD2	2.93	0.42
1:B:276:HIS:NE2	1:B:279:ARG:NH2	2.68	0.42
1:A:491:HIS:HD2	1:A:518:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLY:N	4:A:845:HOH:O	2.49	0.41
1:A:650:VAL:O	1:A:654:LEU:HB2	2.21	0.41
1:B:719:LYS:HE3	1:B:719:LYS:HB2	1.88	0.41
3:H:5:DG:H2'	3:H:6:DT:C6	2.55	0.41
1:A:709:LEU:CD2	1:B:721:LEU:CB	2.98	0.41
1:B:661:HIS:ND1	1:B:688:LEU:HB3	2.35	0.41
1:B:688:LEU:HD12	1:B:688:LEU:HA	1.89	0.41
1:A:278[A]:TRP:HE3	1:A:307:LEU:HB3	1.86	0.41
1:A:446:VAL:O	1:A:450:LEU:HB2	2.20	0.41
1:A:684:ILE:O	1:A:688:LEU:HG	2.20	0.41
1:B:246:GLY:O	1:B:249:ARG:HG3	2.21	0.41
1:B:604:ALA:HB2	1:B:613:LEU:HD11	2.01	0.41
1:B:496:GLN:NE2	1:B:496:GLN:H	2.18	0.41
1:B:525:HIS:HB3	1:B:552:LEU:HD22	2.03	0.41
1:A:649:THR:OG1	1:A:678:ARG:HD3	2.21	0.40
1:A:349:PRO:O	1:A:353:GLN:HB2	2.22	0.40
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.40
1:A:502:ALA:HB2	1:A:511:LEU:HD11	2.03	0.40
1:A:654:LEU:C	1:A:654:LEU:HD23	2.46	0.40
1:A:366:ALA:HB2	1:A:375:LEU:HD11	2.04	0.40

All (1) 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)
4:A:947:HOH:O	4:B:888:HOH:O[1_656]	2.07	0.13

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	486/499 (97%)	467 (96%)	18 (4%)	1 (0%)	43 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	490/499 (98%)	479 (98%)	11 (2%)	0	100	100
All	All	976/998 (98%)	946 (97%)	29 (3%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	691	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	374/383 (98%)	346 (92%)	28 (8%)	12	3
1	B	377/383 (98%)	358 (95%)	19 (5%)	22	8
All	All	751/766 (98%)	704 (94%)	47 (6%)	16	4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	288	ASN
1	A	307	LEU
1	A	319	GLN
1	A	353	GLN
1	A	382	LEU
1	A	421	GLN
1	A	450	LEU
1	A	453	LEU
1	A	455	GLN
1	A	459	LEU
1	A	516	ARG
1	A	517	LEU
1	A	523	GLN
1	A	527	LEU

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Mol	Chain	Res	Type
1	A	552	LEU
1	A	554	VAL
1	A	564	GLN
1	A	586	LEU
1	A	619	LEU
1	A	623	LEU
1	A	678	ARG
1	A	689	SER
1	A	690	ARG
1	A	706	LEU
1	A	715	LEU
1	A	718	VAL
1	A	719	LYS
1	B	231	GLN
1	B	238	LEU
1	B	241	LEU
1	B	249	ARG
1	B	259	GLN
1	B	260	LEU
1	B	313	LEU
1	B	323	LEU
1	B	326	GLN
1	B	347	LEU
1	B	350	VAL
1	B	351	LEU
1	B	520	VAL
1	B	557	GLN
1	B	585	LEU
1	B	688	LEU
1	B	692	ASP
1	B	718	VAL
1	B	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	HIS
1	A	339	GLN
1	A	402	ASN
1	A	462	GLN
1	A	491	HIS
1	A	543	GLN

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Mol	Chain	Res	Type
1	A	577	GLN
1	A	606	ASN
1	A	611	GLN
1	A	640	HIS
1	A	645	GLN
1	A	702	HIS
1	B	339	GLN
1	B	373	GLN
1	B	407	GLN
1	B	441	GLN
1	B	457	HIS
1	B	475	GLN
1	B	509	GLN
1	B	543	GLN
1	B	572	HIS
1	B	577	GLN
1	B	591	GLN
1	B	627	HIS
1	B	640	HIS
1	B	687	GLN
1	B	702	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	5CM	G	11	2,3	18,21,22	1.67	3 (16%)	24,30,33	1.24	2 (8%)
2	5CM	G	8	2,3	18,21,22	1.72	3 (16%)	24,30,33	1.19	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5CM	I	11	2,3	18,21,22	1.62	3 (16%)	24,30,33	1.21	2 (8%)
2	5CM	I	8	2,3	18,21,22	1.71	3 (16%)	24,30,33	1.20	2 (8%)
2	5CM	G	15	2,3	18,21,22	1.66	3 (16%)	24,30,33	1.16	2 (8%)
2	5CM	I	15	2,3	18,21,22	1.66	3 (16%)	24,30,33	1.18	2 (8%)

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	5CM	G	11	2,3	-	0/7/21/22	0/2/2/2
2	5CM	G	8	2,3	-	0/7/21/22	0/2/2/2
2	5CM	I	11	2,3	-	0/7/21/22	0/2/2/2
2	5CM	I	8	2,3	-	0/7/21/22	0/2/2/2
2	5CM	G	15	2,3	-	0/7/21/22	0/2/2/2
2	5CM	I	15	2,3	-	0/7/21/22	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	8	5CM	C5-C4	6.13	1.48	1.44
2	I	8	5CM	C5-C4	6.05	1.48	1.44
2	G	11	5CM	C5-C4	5.85	1.48	1.44
2	I	15	5CM	C5-C4	5.75	1.48	1.44
2	G	15	5CM	C5-C4	5.71	1.48	1.44
2	I	11	5CM	C5-C4	5.49	1.48	1.44
2	I	15	5CM	C6-C5	2.76	1.39	1.34
2	I	8	5CM	C6-C5	2.74	1.39	1.34
2	I	11	5CM	C6-C5	2.73	1.39	1.34
2	G	11	5CM	C6-C5	2.69	1.39	1.34
2	G	8	5CM	C6-C5	2.67	1.39	1.34
2	G	15	5CM	C6-C5	2.60	1.38	1.34
2	G	15	5CM	C6-N1	-2.52	1.33	1.38
2	I	11	5CM	C6-N1	-2.45	1.33	1.38
2	G	11	5CM	C6-N1	-2.39	1.33	1.38
2	I	8	5CM	C6-N1	-2.35	1.34	1.38
2	I	15	5CM	C6-N1	-2.32	1.34	1.38
2	G	8	5CM	C6-N1	-2.31	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	15	5CM	C5-C6-N1	-3.62	119.38	123.31
2	G	11	5CM	C5-C6-N1	-3.56	119.45	123.31
2	I	8	5CM	C5-C6-N1	-3.51	119.50	123.31
2	I	15	5CM	C5-C6-N1	-3.48	119.53	123.31
2	G	8	5CM	C5-C6-N1	-3.45	119.57	123.31
2	I	11	5CM	C5-C6-N1	-3.32	119.71	123.31
2	G	8	5CM	C5-C4-N3	-2.80	118.89	121.75
2	I	15	5CM	C5-C4-N3	-2.70	118.98	121.75
2	I	11	5CM	C5-C4-N3	-2.68	119.01	121.75
2	G	11	5CM	C5-C4-N3	-2.66	119.03	121.75
2	I	8	5CM	C5-C4-N3	-2.64	119.05	121.75
2	G	15	5CM	C5-C4-N3	-2.44	119.25	121.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	15	5CM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	489/499 (97%)	0.70	62 (12%) 8 7	16, 33, 59, 102	1 (0%)
1	B	487/499 (97%)	0.35	34 (6%) 22 24	13, 29, 55, 88	7 (1%)
2	G	14/17 (82%)	-0.27	1 (7%) 22 24	17, 22, 48, 80	0
2	I	14/17 (82%)	-0.33	2 (14%) 6 6	19, 21, 62, 70	0
3	H	17/17 (100%)	0.44	1 (5%) 28 31	27, 32, 79, 86	0
3	J	17/17 (100%)	0.52	1 (5%) 28 31	23, 34, 65, 71	0
All	All	1038/1066 (97%)	0.50	101 (9%) 13 13	13, 30, 59, 102	8 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	695	LEU	6.8
1	A	697	ALA	5.4
1	B	697	ALA	4.9
1	A	284	GLY	4.9
1	A	696	ALA	4.6
1	A	319	GLN	4.4
1	B	691	PRO	4.4
1	A	488	CYS	4.2
1	A	250	GLY	4.0
1	B	689	SER	4.0
1	A	557	GLN	3.9
1	B	257	THR	3.8
1	A	256	ASP	3.8
1	A	693	PRO	3.8
1	A	278[A]	TRP	3.7
1	A	721	LEU	3.6
1	A	690	ARG	3.5
1	B	721	LEU	3.5
2	G	17	DT	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	685	VAL	3.3
1	A	462	GLN	3.2
1	A	254	GLN	3.2
1	B	558	ALA	3.1
1	A	438	GLY	3.1
1	A	523	GLN	3.1
1	A	232	TRP	3.0
1	B	232	TRP	3.0
1	A	660	ALA	3.0
1	A	496	GLN	2.9
1	A	528	THR	2.9
1	B	256	ASP	2.9
1	A	285	ALA	2.8
1	A	539	GLY	2.8
1	B	231	GLN	2.8
1	A	485	PRO	2.8
1	B	246	GLY	2.8
1	A	687	GLN	2.8
1	A	281	ALA	2.7
1	A	283	THR	2.7
1	B	283	THR	2.7
1	A	530	GLN	2.7
1	B	320	ALA	2.7
1	A	686	ALA	2.7
1	A	553	PRO	2.7
3	H	-1	DA	2.6
3	J	-1	DA	2.6
1	A	292	GLU	2.6
1	A	692	ASP	2.6
1	A	526	GLY	2.6
1	B	524	ALA	2.6
1	B	423[A]	HIS	2.5
1	A	516	ARG	2.5
1	B	625	GLN	2.5
1	A	380	ALA	2.5
1	B	592	ALA	2.5
1	A	515	GLN	2.5
1	A	456	ALA	2.5
1	B	290	THR	2.5
1	A	656	VAL	2.5
1	B	591	GLN	2.4
1	A	556	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	320	ALA	2.4
1	B	718	VAL	2.4
1	B	489	GLN	2.4
1	A	628	GLY	2.4
1	A	658	CYS	2.4
2	I	1	DT	2.4
1	B	258	GLY	2.4
1	B	557	GLN	2.3
1	A	560	GLY	2.3
1	A	454	CYS	2.3
1	A	564	GLN	2.3
1	A	529	PRO	2.3
1	B	564	GLN	2.2
1	B	687	GLN	2.2
2	I	17	DT	2.2
1	A	563	PRO	2.2
1	B	717	ALA	2.2
1	A	352	CYS	2.2
1	B	662	GLY	2.2
1	B	252	PRO	2.2
1	A	701	ASP	2.2
1	A	698	LEU	2.2
1	B	688	LEU	2.2
1	A	266	ARG	2.2
1	B	350	VAL	2.1
1	B	554	VAL	2.1
1	B	692	ASP	2.1
1	A	718	VAL	2.1
1	A	538	ASN	2.1
1	A	458	GLY	2.1
1	A	520	VAL	2.1
1	A	353	GLN	2.1
1	A	455	GLN	2.1
1	A	536	ALA	2.1
1	A	233	SER	2.0
1	B	702	HIS	2.0
1	A	420	CYS	2.0
1	B	627	HIS	2.0
1	A	436	ASN	2.0
1	A	540	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	5CM	G	15	20/21	0.94	0.10	29,30,35,38	0
2	5CM	I	15	20/21	0.95	0.09	29,30,33,36	0
2	5CM	I	8	20/21	0.97	0.06	18,19,20,21	0
2	5CM	G	8	20/21	0.98	0.06	16,17,18,20	0
2	5CM	G	11	20/21	0.98	0.06	17,20,22,23	0
2	5CM	I	11	20/21	0.98	0.06	19,22,24,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.