



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:55 AM UTC

PDB ID : 5LY2 / pdb_00005ly2
Title : JMJD2A/ KDM4A COMPLEXED WITH NI(II), NOG AND Macrocytic PEPTIDE Inhibitor CP2_R6Kme3 (13-mer)
Authors : Chowdhury, R.; Madden, S.K.; Hopkinson, R.; Schofield, C.J.
Deposited on : 2016-09-23
Resolution : 2.43 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

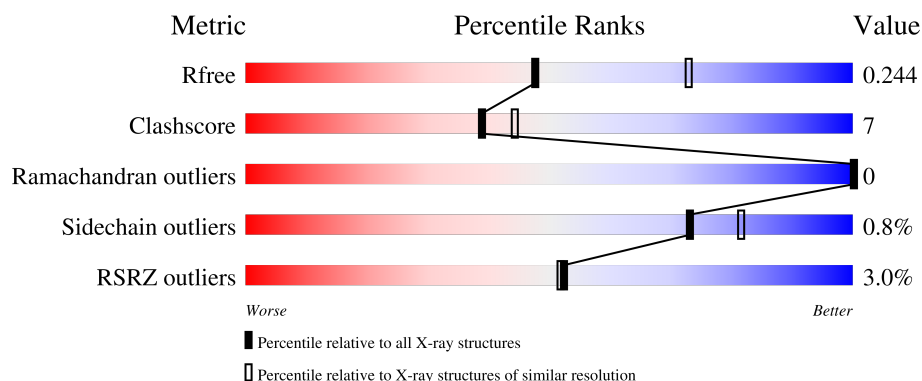
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	381	 2% 80% 11% 9%
1	B	381	 2% 78% 12% 9%
1	C	381	 2% 77% 13% 10%
1	D	381	 3% 77% 14% 9%
2	E	14	 14% 50% 43% 7%

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Mol	Chain	Length	Quality of chain
2	F	14	14% 29% 29% 43%
2	G	14	29% 50% 43% 7%
2	H	14	14% 29% 29% 43%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12172 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	4	0
			2810	1824	460	511	15			
1	B	345	Total	C	N	O	S	0	4	0
			2793	1811	455	511	16			
1	C	342	Total	C	N	O	S	0	2	0
			2778	1800	468	496	14			
1	D	347	Total	C	N	O	S	0	1	0
			2787	1807	462	503	15			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP O75164
A	-20	HIS	-	expression tag	UNP O75164
A	-19	HIS	-	expression tag	UNP O75164
A	-18	HIS	-	expression tag	UNP O75164
A	-17	HIS	-	expression tag	UNP O75164
A	-16	HIS	-	expression tag	UNP O75164
A	-15	HIS	-	expression tag	UNP O75164
A	-14	SER	-	expression tag	UNP O75164
A	-13	SER	-	expression tag	UNP O75164
A	-12	GLY	-	expression tag	UNP O75164
A	-11	VAL	-	expression tag	UNP O75164
A	-10	ASP	-	expression tag	UNP O75164
A	-9	LEU	-	expression tag	UNP O75164
A	-8	GLY	-	expression tag	UNP O75164
A	-7	THR	-	expression tag	UNP O75164
A	-6	GLU	-	expression tag	UNP O75164
A	-5	ASN	-	expression tag	UNP O75164
A	-4	LEU	-	expression tag	UNP O75164
A	-3	TYR	-	expression tag	UNP O75164
A	-2	PHE	-	expression tag	UNP O75164
A	-1	GLN	-	expression tag	UNP O75164

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75164
B	-21	MET	-	expression tag	UNP O75164
B	-20	HIS	-	expression tag	UNP O75164
B	-19	HIS	-	expression tag	UNP O75164
B	-18	HIS	-	expression tag	UNP O75164
B	-17	HIS	-	expression tag	UNP O75164
B	-16	HIS	-	expression tag	UNP O75164
B	-15	HIS	-	expression tag	UNP O75164
B	-14	SER	-	expression tag	UNP O75164
B	-13	SER	-	expression tag	UNP O75164
B	-12	GLY	-	expression tag	UNP O75164
B	-11	VAL	-	expression tag	UNP O75164
B	-10	ASP	-	expression tag	UNP O75164
B	-9	LEU	-	expression tag	UNP O75164
B	-8	GLY	-	expression tag	UNP O75164
B	-7	THR	-	expression tag	UNP O75164
B	-6	GLU	-	expression tag	UNP O75164
B	-5	ASN	-	expression tag	UNP O75164
B	-4	LEU	-	expression tag	UNP O75164
B	-3	TYR	-	expression tag	UNP O75164
B	-2	PHE	-	expression tag	UNP O75164
B	-1	GLN	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164
C	-21	MET	-	expression tag	UNP O75164
C	-20	HIS	-	expression tag	UNP O75164
C	-19	HIS	-	expression tag	UNP O75164
C	-18	HIS	-	expression tag	UNP O75164
C	-17	HIS	-	expression tag	UNP O75164
C	-16	HIS	-	expression tag	UNP O75164
C	-15	HIS	-	expression tag	UNP O75164
C	-14	SER	-	expression tag	UNP O75164
C	-13	SER	-	expression tag	UNP O75164
C	-12	GLY	-	expression tag	UNP O75164
C	-11	VAL	-	expression tag	UNP O75164
C	-10	ASP	-	expression tag	UNP O75164
C	-9	LEU	-	expression tag	UNP O75164
C	-8	GLY	-	expression tag	UNP O75164
C	-7	THR	-	expression tag	UNP O75164
C	-6	GLU	-	expression tag	UNP O75164
C	-5	ASN	-	expression tag	UNP O75164
C	-4	LEU	-	expression tag	UNP O75164
C	-3	TYR	-	expression tag	UNP O75164

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP O75164
C	-1	GLN	-	expression tag	UNP O75164
C	0	SER	-	expression tag	UNP O75164
D	-21	MET	-	expression tag	UNP O75164
D	-20	HIS	-	expression tag	UNP O75164
D	-19	HIS	-	expression tag	UNP O75164
D	-18	HIS	-	expression tag	UNP O75164
D	-17	HIS	-	expression tag	UNP O75164
D	-16	HIS	-	expression tag	UNP O75164
D	-15	HIS	-	expression tag	UNP O75164
D	-14	SER	-	expression tag	UNP O75164
D	-13	SER	-	expression tag	UNP O75164
D	-12	GLY	-	expression tag	UNP O75164
D	-11	VAL	-	expression tag	UNP O75164
D	-10	ASP	-	expression tag	UNP O75164
D	-9	LEU	-	expression tag	UNP O75164
D	-8	GLY	-	expression tag	UNP O75164
D	-7	THR	-	expression tag	UNP O75164
D	-6	GLU	-	expression tag	UNP O75164
D	-5	ASN	-	expression tag	UNP O75164
D	-4	LEU	-	expression tag	UNP O75164
D	-3	TYR	-	expression tag	UNP O75164
D	-2	PHE	-	expression tag	UNP O75164
D	-1	GLN	-	expression tag	UNP O75164
D	0	SER	-	expression tag	UNP O75164

- Molecule 2 is a protein called CP2_R6Kme3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	S	0	0	0
			136	91	22	22	1			
2	F	8	Total	C	N	O		0	0	0
			74	48	14	12				
2	G	14	Total	C	N	O	S	0	0	0
			134	89	22	22	1			
2	H	8	Total	C	N	O		0	0	0
			74	48	14	12				

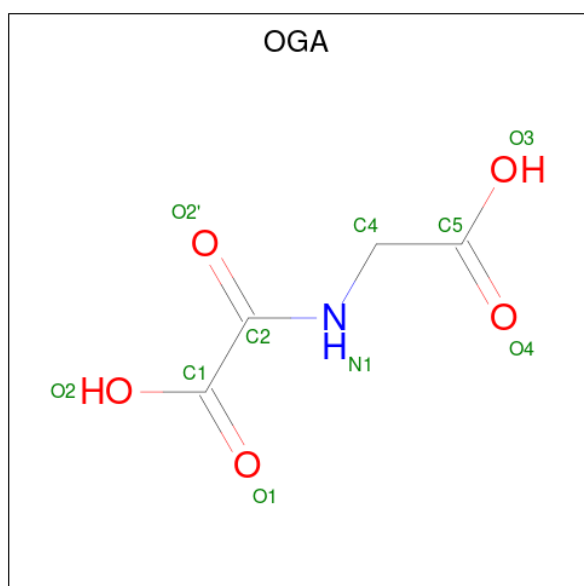
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	B	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	D	1	Total Ni 1 1	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



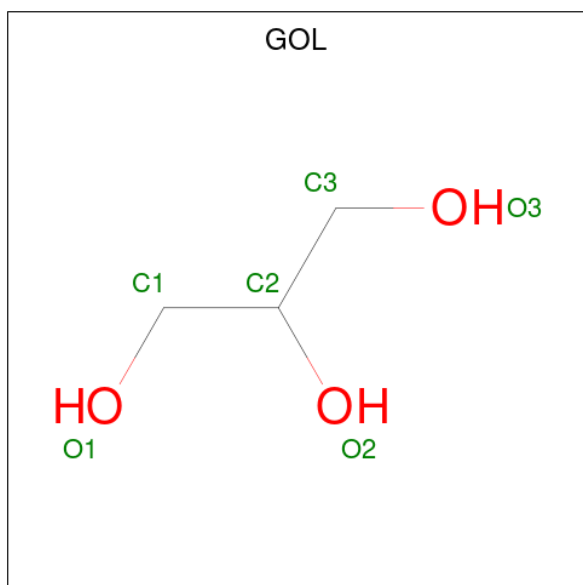
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 10 4 1 5	0	0
5	B	1	Total C N O 10 4 1 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			10	4	1	5		
5	D	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Cl	0	0
			2	2		
7	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Cl	0	0
			2	2		

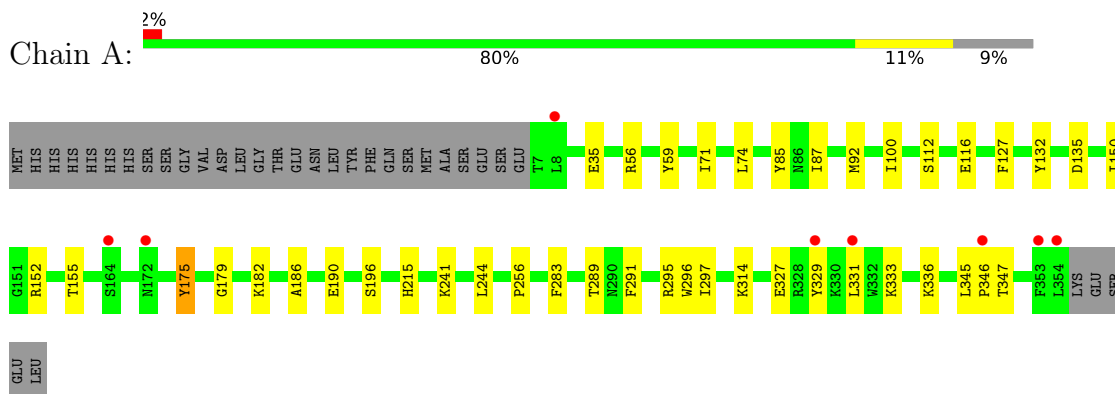
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	126	Total	O	0	0
			126	126		
8	B	122	Total	O	0	0
			122	122		
8	C	130	Total	O	0	0
			130	130		
8	D	110	Total	O	0	0
			110	110		
8	E	5	Total	O	0	0
			5	5		
8	F	2	Total	O	0	0
			2	2		
8	G	4	Total	O	0	0
			4	4		
8	H	4	Total	O	0	0
			4	4		

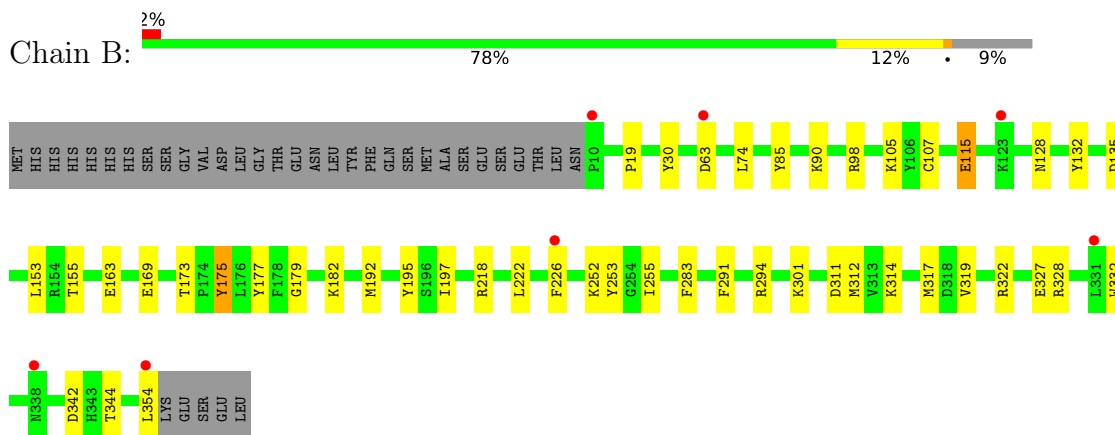
3 Residue-property plots

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.

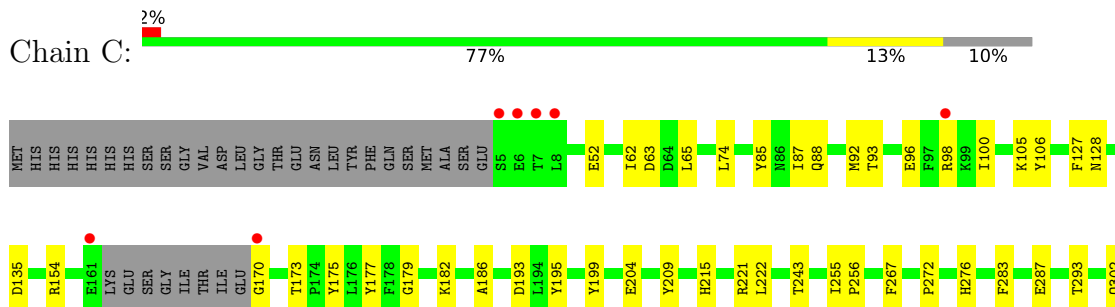
- Molecule 1: Lysine-specific demethylase 4A



- Molecule 1: Lysine-specific demethylase 4A

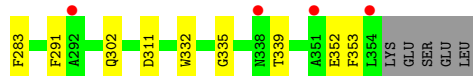
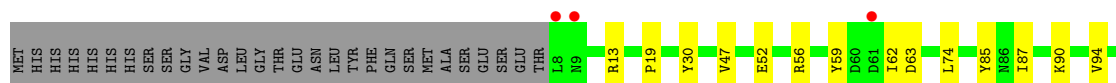
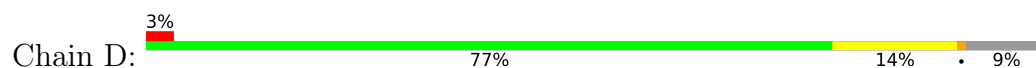


- Molecule 1: Lysine-specific demethylase 4A

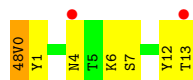




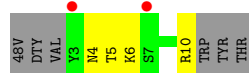
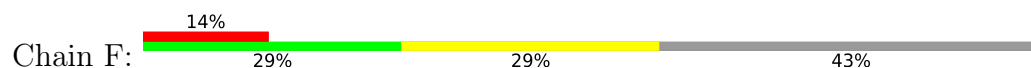
- Molecule 1: Lysine-specific demethylase 4A



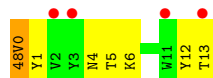
- Molecule 2: CP2_R6Kme3



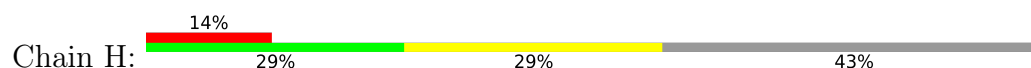
- Molecule 2: CP2_R6Kme3



- Molecule 2: CP2_R6Kme3



- Molecule 2: CP2_R6Kme3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.31Å 103.75Å 142.37Å 90.00° 99.14° 90.00°	Depositor
Resolution (Å)	48.67 – 2.43 48.67 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.67-2.43) 98.3 (48.67-2.43)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.219 , 0.245 0.221 , 0.244	Depositor DCC
R_{free} test set	3236 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12172	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.89% 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: NI, 48V, DTY, M3L, OGA, CL, GOL, ZN

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	0.18	0/2897	0.39	0/3939
1	B	0.19	0/2880	0.41	0/3914
1	C	0.20	0/2864	0.43	0/3888
1	D	0.20	0/2874	0.42	0/3908
2	E	1.48	0/107	1.15	1/147 (0.7%)
2	F	1.19	0/64	1.09	0/86
2	G	1.17	0/105	0.96	0/144
2	H	1.03	0/64	1.05	0/86
All	All	0.28	0/11855	0.44	1/16112 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	ASN	N-CA-C	6.45	120.10	107.98

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	2810	0	2632	30	0
1	B	2793	0	2624	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2778	0	2645	35	0
1	D	2787	0	2617	42	0
2	E	136	0	123	8	0
2	F	74	0	71	7	0
2	G	134	0	115	15	0
2	H	74	0	71	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	10	0	3	0	0
5	B	10	0	3	1	0
5	C	10	0	3	0	0
5	D	10	0	3	0	0
6	A	12	0	16	0	0
6	B	18	0	24	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
8	A	126	0	0	2	0
8	B	122	0	0	5	0
8	C	130	0	0	4	0
8	D	110	0	0	4	0
8	E	5	0	0	0	0
8	F	2	0	0	0	0
8	G	4	0	0	0	0
8	H	4	0	0	0	0
All	All	12172	0	10950	153	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 7.

All (153) 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:C:135:ASP:OD2	2:G:5:THR:HG22	1.52	1.09
1:C:135:ASP:OD2	2:G:5:THR:CG2	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASP:OD2	2:F:5:THR:CG2	2.26	0.83
1:B:115:GLU:N	1:B:115:GLU:OE2	2.20	0.75
1:A:241:LYS:NZ	2:E:6:M3L:O	2.20	0.72
1:A:327:GLU:N	1:A:327:GLU:OE2	2.23	0.71
1:B:135:ASP:OD2	2:F:5:THR:HG22	1.89	0.71
1:B:311:ASP:OD1	2:F:4:ASN:ND2	2.21	0.69
2:G:13:THR:HG21	2:H:10:ARG:C	2.18	0.69
1:B:107:CYS:SG	8:B:604:HOH:O	2.51	0.67
1:D:182:LYS:NZ	8:D:503:HOH:O	2.29	0.66
1:C:85:TYR:CD1	1:D:74:LEU:HD21	2.31	0.66
2:G:5:THR:HG22	2:G:6:M3L:N	2.11	0.66
1:C:345:LEU:HD23	1:C:346:PRO:O	1.97	0.65
1:D:168:ILE:HB	1:D:171:VAL:CG2	2.27	0.65
2:E:0:48V:H10	2:E:12:TYR:CE2	2.32	0.65
1:D:135:ASP:OD2	2:H:5:THR:HG22	1.97	0.64
1:A:331:LEU:HD12	1:A:336:LYS:HB2	1.80	0.64
1:A:74:LEU:HD21	1:B:85:TYR:CD2	2.34	0.63
1:D:252:LYS:NZ	8:D:505:HOH:O	2.31	0.62
1:B:192:MET:HE2	1:B:317:MET:HE1	1.82	0.61
1:A:85:TYR:CD1	1:B:74:LEU:HD21	2.36	0.61
1:D:63:ASP:HA	1:D:94:VAL:CG2	2.32	0.59
1:B:342:ASP:OD2	1:B:344:THR:OG1	2.21	0.59
1:D:135:ASP:HA	1:D:175:TYR:CD2	2.39	0.58
1:B:179:GLY:O	1:B:283:PHE:HA	2.04	0.58
1:B:135:ASP:OD2	2:F:5:THR:HG21	2.03	0.57
1:B:177:TYR:OH	2:F:6:M3L:HM22	2.04	0.57
1:D:146:ASP:OD1	1:D:152:ARG:NH1	2.30	0.57
1:C:302:GLN:NE2	1:C:339:THR:O	2.38	0.57
1:D:177:TYR:OH	2:H:6:M3L:HM13	2.05	0.56
1:B:252:LYS:NZ	8:B:510:HOH:O	2.37	0.56
1:A:155:THR:HG21	1:A:291:PHE:HB2	1.88	0.56
1:D:63:ASP:HA	1:D:94:VAL:HG23	1.88	0.56
1:B:132:TYR:OH	5:B:405:OGA:O4	2.20	0.56
1:D:63:ASP:OD2	1:D:98:ARG:NH1	2.36	0.55
1:B:312:MET:SD	1:B:314:LYS:HG3	2.47	0.54
1:B:163:GLU:OE2	1:B:322:ARG:NH2	2.40	0.54
1:A:329:TYR:O	1:A:333:LYS:CB	2.56	0.54
1:B:218:ARG:HG2	1:B:255:ILE:CD1	2.38	0.54
1:D:135:ASP:OD2	2:H:5:THR:CG2	2.56	0.54
1:D:74:LEU:HD13	1:D:87:ILE:HD12	1.90	0.54
1:C:328:ARG:NH2	1:C:337:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD22	1:A:87:ILE:HD11	1.89	0.53
1:B:98:ARG:NH1	8:B:517:HOH:O	2.42	0.53
2:E:0:48V:N05	2:E:0:48V:S07	2.80	0.53
1:C:98[A]:ARG:HG3	1:C:283:PHE:CE2	2.44	0.53
1:B:63:ASP:OD1	1:B:98:ARG:NH2	2.26	0.52
1:A:345:LEU:HD12	1:A:346:PRO:HD2	1.92	0.52
1:C:179:GLY:O	1:C:283:PHE:HA	2.09	0.52
1:C:312:MET:HA	2:G:4:ASN:HD22	1.75	0.52
1:D:155:THR:CG2	1:D:157:LEU:HD22	2.40	0.52
1:D:169:GLU:HB3	1:D:175:TYR:CE1	2.45	0.51
1:C:222:LEU:HD22	1:C:255:ILE:CD1	2.41	0.51
1:C:177:TYR:OH	2:G:6:M3L:HM23	2.11	0.51
1:C:74:LEU:HD12	1:C:87:ILE:CD1	2.42	0.50
1:B:153:LEU:HD11	1:B:197:ILE:HG21	1.94	0.50
1:B:192:MET:CE	1:B:317:MET:HE1	2.42	0.49
1:A:92:MET:HE1	1:A:100:ILE:HD12	1.93	0.49
1:A:179:GLY:O	1:A:283:PHE:HA	2.13	0.49
1:D:191:ASP:OD1	8:D:501:HOH:O	2.20	0.49
1:C:215:HIS:CD2	1:C:256:PRO:HG2	2.47	0.49
1:B:222:LEU:HD11	1:B:226:PHE:CE2	2.48	0.49
1:A:186:ALA:HA	1:A:244:LEU:HD23	1.95	0.49
1:D:153:LEU:HD11	1:D:197:ILE:HG21	1.95	0.48
1:A:127:PHE:O	1:A:182:LYS:NZ	2.44	0.48
1:B:195:TYR:HB2	1:B:291:PHE:O	2.13	0.48
1:D:195:TYR:HB2	1:D:291:PHE:O	2.14	0.48
1:A:314:LYS:NZ	8:A:611:HOH:O	2.46	0.48
1:D:241:LYS:NZ	2:H:6:M3L:O	2.33	0.48
2:G:5:THR:CG2	2:G:6:M3L:N	2.76	0.47
2:G:5:THR:HG22	2:G:6:M3L:H	1.74	0.47
2:G:0:48V:N01	2:G:0:48V:C08	2.78	0.47
1:B:19:PRO:HB3	1:B:30:TYR:CE1	2.49	0.47
1:A:112:SER:OG	1:A:116:GLU:OE1	2.29	0.46
1:A:241:LYS:HZ3	2:E:6:M3L:C	2.22	0.46
1:D:62:ILE:O	1:D:94:VAL:HG21	2.16	0.46
1:A:329:TYR:O	1:A:333:LYS:HB2	2.15	0.46
1:C:88:GLN:OE1	2:G:12:TYR:HB3	2.16	0.46
1:D:103:SER:O	1:D:107:CYS:HB3	2.15	0.46
1:A:135:ASP:HA	1:A:175:TYR:CD2	2.51	0.46
1:D:90:LYS:HB2	2:G:1:DTY:CZ	2.46	0.46
1:A:135:ASP:OD2	2:E:7:SER:HB2	2.16	0.46
1:D:90:LYS:HE2	2:G:1:DTY:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:THR:CG2	2:G:6:M3L:H	2.29	0.45
1:D:47:VAL:HG11	1:D:148:TRP:CH2	2.52	0.45
1:B:218:ARG:HG2	1:B:255:ILE:HD13	1.97	0.45
1:C:74:LEU:HD11	1:D:85:TYR:CG	2.51	0.45
1:D:332:TRP:O	1:D:335:GLY:N	2.50	0.45
1:B:327:GLU:HG2	1:B:328:ARG:HG3	1.99	0.45
1:B:135:ASP:HA	1:B:175:TYR:CD2	2.52	0.45
2:H:6:M3L:HM13	2:H:6:M3L:HD3	1.69	0.44
1:B:105:LYS:O	1:B:128:ASN:ND2	2.48	0.44
1:C:209:TYR:O	1:C:276:HIS:HA	2.17	0.44
1:D:155:THR:HG21	1:D:291:PHE:HB2	1.99	0.44
1:C:93:THR:OG1	1:C:96:GLU:HG3	2.18	0.44
1:B:294:ARG:NH2	8:B:520:HOH:O	2.44	0.44
1:C:195:TYR:CE1	1:C:293:THR:HG22	2.53	0.44
1:D:241:LYS:HD2	2:H:6:M3L:O	2.18	0.44
1:C:312:MET:HA	2:G:4:ASN:ND2	2.31	0.44
1:C:128:ASN:OD1	8:C:601:HOH:O	2.21	0.43
1:D:159:LEU:O	1:D:163:GLU:CB	2.66	0.43
1:D:226:PHE:HZ	1:D:253:TYR:CZ	2.36	0.43
1:C:199:TYR:HB2	1:C:267:PHE:CE1	2.53	0.43
1:C:222:LEU:HD22	1:C:255:ILE:HD12	2.01	0.43
1:C:105:LYS:HE3	1:C:106:TYR:CE2	2.53	0.43
2:E:13:THR:HG21	2:F:10:ARG:C	2.44	0.43
1:C:63:ASP:OD1	1:C:98[A]:ARG:NH2	2.52	0.43
1:C:128:ASN:ND2	8:C:618:HOH:O	2.49	0.43
1:B:169:GLU:HA	1:B:173:THR:OG1	2.18	0.42
1:D:56:ARG:HD3	1:D:59:TYR:CD1	2.54	0.42
1:D:186:ALA:HB1	1:D:243:THR:O	2.19	0.42
1:A:190:GLU:HG3	1:A:196:SER:HB2	2.01	0.42
1:C:204:GLU:OE2	8:C:602:HOH:O	2.22	0.42
1:D:19:PRO:HB3	1:D:30:TYR:CZ	2.54	0.42
1:D:13:ARG:NH2	8:D:519:HOH:O	2.47	0.42
1:B:301:LYS:HE3	1:B:332:TRP:CD1	2.54	0.42
1:C:193:ASP:O	1:C:272:PRO:HB3	2.20	0.42
1:A:71:ILE:HG13	1:A:132:TYR:HB3	2.01	0.42
1:B:155:THR:HG21	1:B:291:PHE:HB2	2.02	0.42
1:D:159:LEU:O	1:D:163:GLU:N	2.46	0.42
1:D:190:GLU:O	1:D:239:ARG:NH1	2.52	0.42
1:D:352:GLU:HG3	1:D:353:PHE:CD2	2.55	0.42
1:A:152:ARG:NH1	8:A:614:HOH:O	2.53	0.41
1:C:170:GLY:O	1:C:173:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:ND1	1:A:256:PRO:HG2	2.35	0.41
1:A:329:TYR:O	1:A:333:LYS:HB3	2.19	0.41
1:B:90:LYS:HB2	2:E:1:DTY:CE1	2.50	0.41
1:A:295:ARG:HB2	1:A:347:THR:HA	2.02	0.41
2:F:6:M3L:HD2	2:F:6:M3L:HM13	1.84	0.41
1:A:150:ILE:HG23	1:A:289:THR:HG22	2.03	0.41
1:B:182:LYS:NZ	8:B:522:HOH:O	2.44	0.41
1:D:185:PHE:CD1	1:D:185:PHE:N	2.88	0.41
1:A:74:LEU:HD21	1:B:85:TYR:CG	2.55	0.41
1:C:74:LEU:HD12	1:C:87:ILE:HD12	2.03	0.41
1:D:302:GLN:NE2	1:D:339:THR:O	2.54	0.41
1:B:163:GLU:OE1	1:B:319:VAL:HG12	2.21	0.41
1:C:92:MET:HE1	1:C:100:ILE:HD12	2.02	0.41
1:C:154:ARG:NH1	8:C:617:HOH:O	2.48	0.41
2:E:0:48V:H9	2:E:0:48V:N01	2.35	0.41
1:A:296:TRP:O	1:A:297:ILE:C	2.63	0.41
1:C:62:ILE:HB	1:C:65:LEU:HD22	2.03	0.41
1:C:127:PHE:O	1:C:182:LYS:NZ	2.48	0.41
1:C:175:TYR:O	1:C:287:GLU:HA	2.20	0.41
1:D:171:VAL:HG23	1:D:172:ASN:H	1.85	0.41
1:D:179:GLY:O	1:D:283:PHE:HA	2.20	0.41
1:A:35:GLU:OE1	1:A:347:THR:HB	2.21	0.41
1:B:226:PHE:HZ	1:B:253:TYR:CZ	2.39	0.41
1:C:186:ALA:HB1	1:C:243:THR:O	2.21	0.41
1:A:56:ARG:HD3	1:A:59:TYR:CD1	2.57	0.40
2:G:13:THR:HG21	2:H:10:ARG:O	2.20	0.40
1:B:354:LEU:N	1:B:354:LEU:HD12	2.37	0.40
1:D:311:ASP:C	2:H:4:ASN:HD22	2.29	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	350/381 (92%)	344 (98%)	6 (2%)	0	100	100
1	B	347/381 (91%)	340 (98%)	7 (2%)	0	100	100
1	C	340/381 (89%)	335 (98%)	5 (2%)	0	100	100
1	D	346/381 (91%)	338 (98%)	8 (2%)	0	100	100
2	E	10/14 (71%)	10 (100%)	0	0	100	100
2	F	5/14 (36%)	5 (100%)	0	0	100	100
2	G	10/14 (71%)	10 (100%)	0	0	100	100
2	H	5/14 (36%)	5 (100%)	0	0	100	100
All	All	1413/1580 (89%)	1387 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	283/335 (84%)	282 (100%)	1 (0%)	84	89
1	B	286/335 (85%)	284 (99%)	2 (1%)	76	83
1	C	286/335 (85%)	284 (99%)	2 (1%)	76	83
1	D	281/335 (84%)	277 (99%)	4 (1%)	59	70
2	E	10/10 (100%)	10 (100%)	0	100	100
2	F	6/10 (60%)	6 (100%)	0	100	100
2	G	9/10 (90%)	9 (100%)	0	100	100
2	H	6/10 (60%)	6 (100%)	0	100	100
All	All	1167/1380 (85%)	1158 (99%)	9 (1%)	73	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	TYR
1	B	115	GLU

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Mol	Chain	Res	Type
1	B	175	TYR
1	C	52	GLU
1	C	221	ARG
1	D	52	GLU
1	D	157	LEU
1	D	175	TYR
1	D	185	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	ASN
1	A	72	GLN
1	A	84	GLN
1	A	86	ASN
1	C	72	GLN
1	C	86	ASN
1	C	124	ASN
1	C	215	HIS
1	D	37	GLN
1	D	124	ASN
2	H	4	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	M3L	F	6	2	10,11,12	1.21	0	9,14,16	0.56	0
2	M3L	E	6	2	10,11,12	1.15	0	9,14,16	0.45	0
2	48V	G	0	2	9,9,10	1.49	1 (11%)	8,10,12	2.69	3 (37%)
2	M3L	H	6	2	10,11,12	1.11	0	9,14,16	0.52	0
2	48V	E	0	2	9,9,10	1.63	2 (22%)	8,10,12	2.32	2 (25%)
2	M3L	G	6	2	10,11,12	0.80	0	9,14,16	0.30	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
2	M3L	F	6	2	-	2/9/10/12	-
2	M3L	E	6	2	-	2/9/10/12	-
2	48V	G	0	2	-	0/8/9/10	-
2	M3L	H	6	2	-	6/9/10/12	-
2	48V	E	0	2	-	3/8/9/10	-
2	M3L	G	6	2	-	5/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	0	48V	O04-C03	2.48	1.28	1.23
2	G	0	48V	C02-N01	-2.31	1.36	1.48
2	E	0	48V	C02-N01	-2.28	1.37	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	0	48V	C02-C03-N05	4.79	124.94	116.75
2	G	0	48V	C02-C03-N05	4.69	124.75	116.75
2	G	0	48V	O04-C03-C02	-4.18	114.02	120.25
2	E	0	48V	O04-C03-C02	-4.14	114.08	120.25
2	G	0	48V	C06-C02-C03	-4.00	100.61	109.43

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	0	48V	N01-C02-C03-N05
2	E	0	48V	C06-C02-C03-O04
2	E	0	48V	C06-C02-C03-N05
2	E	6	M3L	N-CA-CB-CG
2	E	6	M3L	C-CA-CB-CG
2	H	6	M3L	CG-CD-CE-NZ
2	H	6	M3L	CA-CB-CG-CD
2	H	6	M3L	CD-CE-NZ-CM1
2	H	6	M3L	CD-CE-NZ-CM3
2	H	6	M3L	CE-CD-CG-CB
2	H	6	M3L	CD-CE-NZ-CM2
2	G	6	M3L	CD-CE-NZ-CM2
2	G	6	M3L	CD-CE-NZ-CM1
2	G	6	M3L	CD-CE-NZ-CM3
2	G	6	M3L	CA-CB-CG-CD
2	G	6	M3L	CE-CD-CG-CB
2	F	6	M3L	CE-CD-CG-CB
2	F	6	M3L	CA-CB-CG-CD

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	6	M3L	2	0
2	E	6	M3L	2	0
2	G	0	48V	1	0
2	H	6	M3L	4	0
2	E	0	48V	3	0
2	G	6	M3L	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 13 are monoatomic - leaving 9 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
5	OGA	A	503	3	9,9,9	2.35	1 (11%)	8,11,11	0.95	0
5	OGA	B	405	3	9,9,9	2.34	1 (11%)	8,11,11	0.95	0
5	OGA	C	504	3	9,9,9	2.36	1 (11%)	8,11,11	0.86	0
6	GOL	B	406	-	5,5,5	0.43	0	5,5,5	0.30	0
5	OGA	D	405	3	9,9,9	2.34	1 (11%)	8,11,11	0.85	0
6	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.24	0
6	GOL	A	505	-	5,5,5	0.37	0	5,5,5	0.27	0
6	GOL	B	407	-	5,5,5	0.38	0	5,5,5	0.27	0
6	GOL	B	408	-	5,5,5	0.34	0	5,5,5	0.30	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
5	OGA	A	503	3	-	0/8/9/9	-
5	OGA	B	405	3	-	0/8/9/9	-
5	OGA	C	504	3	-	0/8/9/9	-
6	GOL	B	406	-	-	0/4/4/4	-
5	OGA	D	405	3	-	0/8/9/9	-
6	GOL	A	504	-	-	0/4/4/4	-
6	GOL	A	505	-	-	0/4/4/4	-
6	GOL	B	407	-	-	0/4/4/4	-
6	GOL	B	408	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	504	OGA	C2-C1	-6.41	1.46	1.54
5	A	503	OGA	C2-C1	-6.40	1.46	1.54
5	D	405	OGA	C2-C1	-6.38	1.46	1.54
5	B	405	OGA	C2-C1	-6.37	1.46	1.54

There are no bond angle outliers.

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
5	B	405	OGA	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	348/381 (91%)	0.40	8 (2%) 61 62	22, 41, 71, 83	4 (1%)
1	B	345/381 (90%)	0.36	7 (2%) 65 66	21, 42, 68, 83	4 (1%)
1	C	342/381 (89%)	0.16	8 (2%) 61 62	21, 38, 53, 73	2 (0%)
1	D	347/381 (91%)	0.49	10 (2%) 53 53	19, 44, 71, 89	1 (0%)
2	E	11/14 (78%)	1.41	2 (18%) 3 2	47, 52, 60, 61	0
2	F	7/14 (50%)	1.43	2 (28%) 1 1	51, 57, 65, 65	0
2	G	11/14 (78%)	1.32	4 (36%) 1 0	43, 55, 61, 62	0
2	H	7/14 (50%)	1.74	2 (28%) 1 1	60, 66, 77, 79	0
All	All	1418/1580 (89%)	0.38	43 (3%) 52 52	19, 41, 69, 89	11 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	LEU	3.7
2	E	13	THR	3.4
1	D	351	ALA	3.3
1	B	354	LEU	3.3
1	D	9	ASN	2.9
1	D	354	LEU	2.7
1	D	8	LEU	2.7
1	C	6	GLU	2.6
1	B	331	LEU	2.5
1	C	8	LEU	2.5
1	B	338	ASN	2.5
1	A	164	SER	2.5
1	B	63	ASP	2.5
1	D	168	ILE	2.5
2	H	5	THR	2.5
1	C	161	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	2.4
2	G	2	VAL	2.4
2	F	7	SER	2.4
1	D	292	ALA	2.4
2	G	11	TRP	2.3
1	C	354	LEU	2.3
1	D	61	ASP	2.3
1	A	353	PHE	2.3
2	E	4	ASN	2.2
1	D	171	VAL	2.2
1	D	113	GLU	2.2
1	B	123[A]	LYS	2.2
1	C	170	GLY	2.2
1	C	98[A]	ARG	2.2
1	A	346	PRO	2.2
1	B	10	PRO	2.2
2	G	3	TYR	2.2
1	B	226	PHE	2.2
1	A	329	TYR	2.1
2	H	4	ASN	2.1
1	D	338	ASN	2.1
1	C	7	THR	2.1
2	G	13	THR	2.1
1	C	5	SER	2.1
1	A	172	ASN	2.1
2	F	3	TYR	2.0
1	A	331	LEU	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	48V	E	0	10/11	0.71	0.17	55,60,63,71	0
2	48V	G	0	10/11	0.76	0.12	58,64,68,69	0
2	DTY	E	1	12/13	0.81	0.14	53,54,58,59	0
2	M3L	F	6	12/13	0.82	0.17	53,57,62,63	0
2	M3L	G	6	12/13	0.82	0.16	35,38,43,44	0
2	M3L	H	6	12/13	0.84	0.15	57,62,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	M3L	E	6	12/13	0.86	0.14	41,45,50,55	0
2	DTY	G	1	12/13	0.88	0.12	54,57,58,60	0

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
6	GOL	A	504	6/6	0.78	0.17	62,67,67,70	0
6	GOL	B	407	6/6	0.78	0.24	47,48,52,52	0
6	GOL	A	505	6/6	0.80	0.15	45,48,49,51	0
6	GOL	B	408	6/6	0.80	0.16	34,39,44,46	0
6	GOL	B	406	6/6	0.81	0.14	47,49,51,52	0
5	OGA	D	405	10/10	0.82	0.15	44,48,52,55	0
7	CL	C	503	1/1	0.84	0.20	91,91,91,91	0
5	OGA	B	405	10/10	0.89	0.12	41,44,48,50	0
5	OGA	A	503	10/10	0.92	0.10	36,38,41,41	0
5	OGA	C	504	10/10	0.93	0.08	38,44,45,46	0
7	CL	D	404	1/1	0.94	0.09	55,55,55,55	0
7	CL	B	401	1/1	0.96	0.08	48,48,48,48	0
7	CL	B	404	1/1	0.96	0.08	55,55,55,55	0
7	CL	D	401	1/1	0.98	0.10	43,43,43,43	0
4	ZN	C	502	1/1	0.99	0.02	36,36,36,36	0
4	ZN	D	403	1/1	0.99	0.03	46,46,46,46	0
3	NI	A	501	1/1	0.99	0.03	38,38,38,38	0
3	NI	C	501	1/1	0.99	0.03	37,37,37,37	0
3	NI	B	402	1/1	1.00	0.02	40,40,40,40	0
3	NI	D	402	1/1	1.00	0.01	42,42,42,42	0
4	ZN	A	502	1/1	1.00	0.05	37,37,37,37	0
4	ZN	B	403	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.