



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:03 AM UTC

PDB ID : 1X9Z / pdb_00001x9z
Title : Crystal structure of the MutL C-terminal domain
Authors : Guarne, A.; Ramon-Maiques, S.; Wolff, E.M.; Ghirlando, R.; Hu, X.; Miller, J.H.; Yang, W.
Deposited on : 2004-08-24
Resolution : 2.10 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

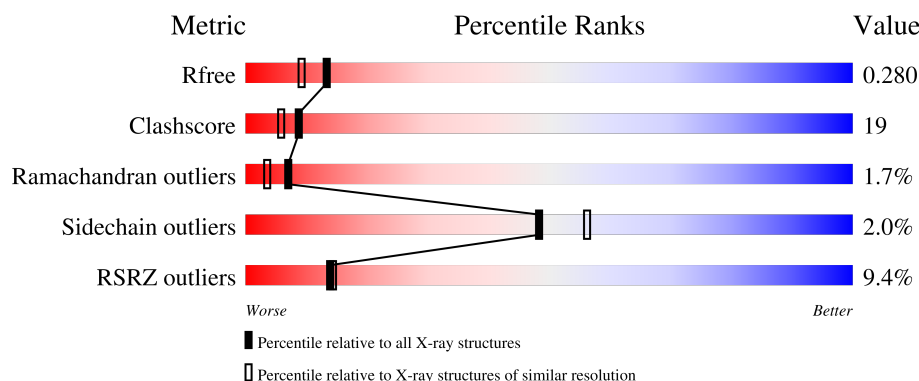
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	188	7% 72% 20% • • •
1	B	188	11% 66% 28% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	423	-	-	-	X
4	GOL	B	402	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3140 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 DNA mismatch repair protein mutL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	Se	0	1	0
			1409	898	250	256	3	2			
1	B	182	Total	C	N	O	S	Se	0	4	0
			1418	904	251	256	4	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	GLY	-	cloning artifact	UNP P23367
A	429	SER	-	cloning artifact	UNP P23367
A	430	HIS	-	cloning artifact	UNP P23367
A	431	MET	-	cloning artifact	UNP P23367
A	566	MSE	MET	modified residue	UNP P23367
A	574	MSE	MET	modified residue	UNP P23367
B	428	GLY	-	cloning artifact	UNP P23367
B	429	SER	-	cloning artifact	UNP P23367
B	430	HIS	-	cloning artifact	UNP P23367
B	431	MET	-	cloning artifact	UNP P23367
B	566	MSE	MET	modified residue	UNP P23367
B	574	MSE	MET	modified residue	UNP P23367

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

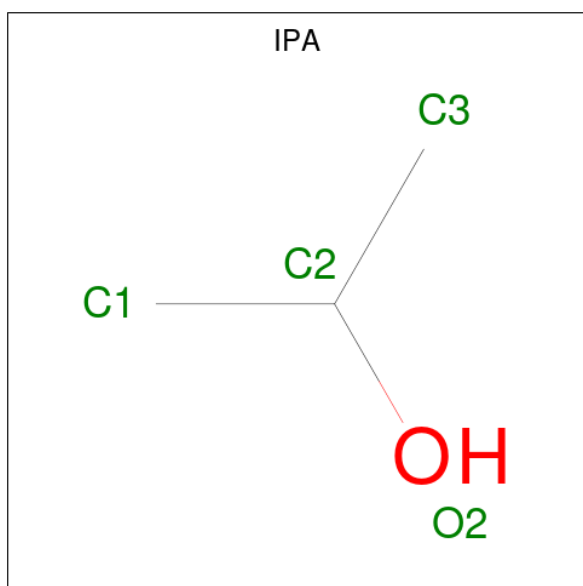
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	3	1		

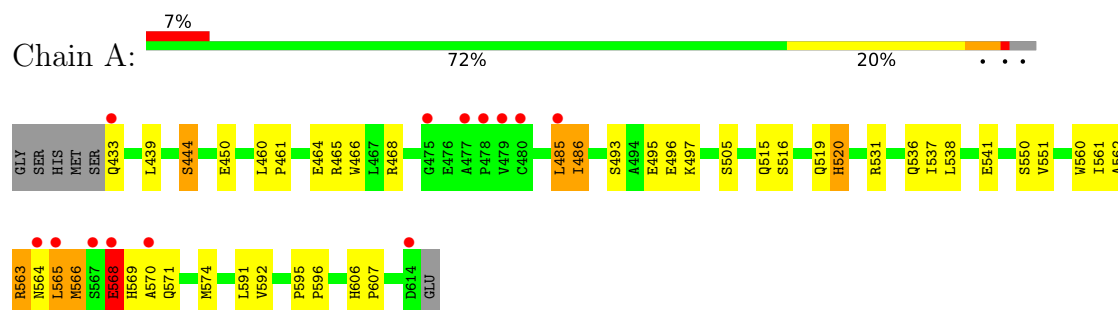
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	154	Total	O	0	0
			154	154		
6	B	136	Total	O	0	0
			136	136		

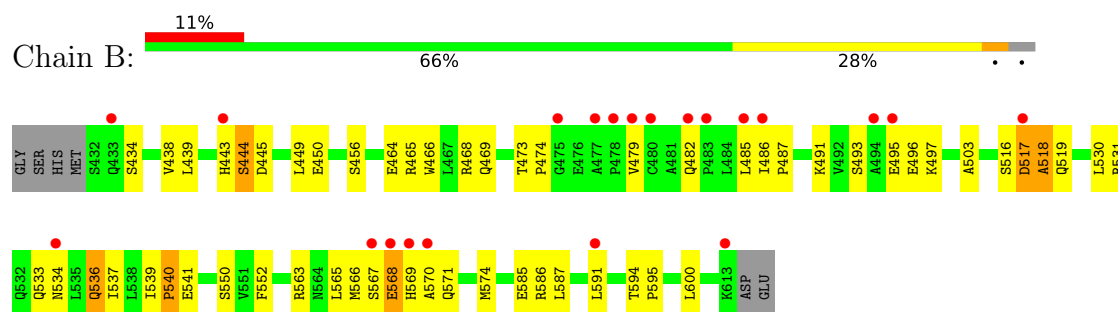
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA mismatch repair protein mutL



- Molecule 1: DNA mismatch repair protein mutL



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.99Å 95.99Å 140.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.61 – 2.10 19.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.61-2.10) 94.3 (19.61-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.09Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.278 0.239 , 0.280	Depositor DCC
R_{free} test set	3678 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3140	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9372e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IPA, CL, NA, GOL

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	0.53	0/1437	0.97	9/1953 (0.5%)
1	B	0.50	0/1458	0.93	2/1980 (0.1%)
All	All	0.52	0/2895	0.95	11/3933 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	MSE	N-CA-C	8.54	123.15	110.52
1	A	564	ASN	N-CA-C	6.92	121.77	113.12
1	A	550	SER	N-CA-C	-6.90	105.39	113.88
1	A	520	HIS	N-CA-C	6.66	119.53	109.41
1	A	485	LEU	N-CA-C	-6.48	103.90	110.97
1	B	550	SER	N-CA-C	-6.45	106.04	114.04
1	A	565	LEU	N-CA-C	6.16	120.79	113.28
1	A	563	ARG	N-CA-C	5.76	117.64	111.36
1	A	515	GLN	N-CA-C	-5.66	100.75	109.52
1	A	568	GLU	N-CA-C	-5.52	103.62	110.41
1	B	517	ASP	N-CA-C	-5.21	101.53	109.65

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	1409	0	1465	53	0
1	B	1418	0	1476	58	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	7	6	0
5	A	4	0	8	2	0
5	B	4	0	8	0	0
6	A	154	0	0	9	0
6	B	136	0	0	15	0
All	All	3140	0	2972	109	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 19.

All (109) 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:464:GLU:HG2	5:A:411:IPA:H32	1.44	0.95
1:B:479:VAL:HG12	4:B:402:GOL:O1	1.71	0.89
1:A:562:ALA:HA	1:A:566:MSE:CE	2.03	0.89
1:B:456:SER:HB3	1:B:600:LEU:HD11	1.55	0.86
1:A:562:ALA:HA	1:A:566:MSE:HE3	1.60	0.81
1:A:568:GLU:HA	6:A:230:HOH:O	1.87	0.75
1:A:468:ARG:HB3	1:A:566:MSE:HE1	1.71	0.72
1:A:551:VAL:HA	6:A:323:HOH:O	1.89	0.71
1:A:485:LEU:HG	1:A:531:ARG:HH22	1.57	0.70
1:B:456:SER:CB	1:B:600:LEU:HD11	2.21	0.70
1:B:536:GLN:H	1:B:536:GLN:HE21	1.43	0.66
1:A:538:LEU:CD1	1:A:565:LEU:HB3	2.27	0.65
1:A:568:GLU:H	1:A:568:GLU:CD	2.02	0.65
1:B:566:MSE:HE3	6:B:312:HOH:O	1.95	0.65
1:B:517:ASP:HB3	6:B:303:HOH:O	1.96	0.65
1:A:465[A]:ARG:HD2	1:A:563:ARG:HG2	1.80	0.64
1:A:560:TRP:HZ3	1:A:565:LEU:HD11	1.62	0.64
1:A:465[A]:ARG:HD3	1:A:563:ARG:HA	1.80	0.64
1:A:465[B]:ARG:HD2	1:A:563:ARG:HG2	1.80	0.64
1:B:503:ALA:HB2	1:B:552:PHE:CD2	2.33	0.64
1:A:486:ILE:O	1:A:486:ILE:HG13	1.99	0.63
1:B:479:VAL:HB	4:B:402:GOL:H12	1.79	0.63
1:B:569:HIS:HB3	6:B:319:HOH:O	1.97	0.63
1:B:479:VAL:HB	4:B:402:GOL:C1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ALA:HA	1:A:566:MSE:HE2	1.81	0.62
1:A:538:LEU:HD12	1:A:565:LEU:HB3	1.80	0.62
1:B:444:SER:HA	1:B:571:GLN:HE22	1.67	0.59
1:B:486:ILE:HG23	1:B:486:ILE:O	2.03	0.59
1:B:536:GLN:H	1:B:536:GLN:NE2	2.01	0.58
1:B:539:ILE:HB	1:B:540:PRO:HD3	1.85	0.57
1:B:465[B]:ARG:HH21	1:B:469:GLN:NE2	2.03	0.56
1:B:465[B]:ARG:HH21	1:B:469:GLN:HE22	1.53	0.56
1:A:466:TRP:CG	1:A:591:LEU:HD11	2.40	0.56
1:A:495:GLU:HG2	6:A:181:HOH:O	2.07	0.55
1:B:586:ARG:HH11	1:B:587:LEU:HG	1.70	0.55
1:B:465[B]:ARG:NH2	1:B:469:GLN:HE22	2.05	0.55
1:A:536:GLN:NE2	1:B:491:LYS:H	2.03	0.55
1:B:456:SER:HB3	1:B:600:LEU:CD1	2.34	0.54
1:A:541:GLU:HB3	1:A:565:LEU:CD2	2.38	0.54
1:A:433:GLN:HB2	1:A:592:VAL:HG11	1.90	0.54
1:A:538:LEU:HD12	1:A:565:LEU:HD13	1.89	0.53
1:B:434:SER:HB2	1:B:585:GLU:OE2	2.08	0.53
1:B:493:SER:OG	1:B:496:GLU:HG3	2.08	0.53
1:B:465[B]:ARG:HD2	1:B:563:ARG:HG2	1.91	0.53
1:B:439:LEU:HD11	1:B:450:GLU:HB2	1.91	0.53
1:B:479:VAL:CG1	4:B:402:GOL:O1	2.52	0.53
1:B:586:ARG:NH1	1:B:587:LEU:HG	2.24	0.52
6:A:107:HOH:O	1:B:496:GLU:HG2	2.10	0.52
1:B:465[A]:ARG:NE	6:B:305:HOH:O	2.43	0.52
1:A:516:SER:HB2	1:A:520:HIS:O	2.10	0.51
1:B:464:GLU:OE1	1:B:568:GLU:HG2	2.09	0.51
1:B:469:GLN:HG2	6:B:157:HOH:O	2.10	0.51
1:A:444:SER:HA	1:A:571:GLN:OE1	2.11	0.51
1:B:466:TRP:CG	1:B:591:LEU:HD11	2.45	0.51
1:A:468:ARG:HB3	1:A:566:MSE:CE	2.41	0.50
1:A:560:TRP:CZ3	1:A:565:LEU:HG	2.47	0.50
1:B:444:SER:HA	1:B:571:GLN:NE2	2.26	0.50
1:B:567:SER:N	6:B:312:HOH:O	2.45	0.50
1:B:465[B]:ARG:HD2	6:B:308:HOH:O	2.12	0.49
1:B:465[B]:ARG:HD3	6:B:293:HOH:O	2.11	0.49
1:A:433:GLN:HB3	6:A:264:HOH:O	2.12	0.49
1:A:444:SER:HB3	1:A:571:GLN:HE22	1.77	0.49
1:B:595:PRO:HG3	6:B:318:HOH:O	2.13	0.49
1:A:592:VAL:O	1:A:595:PRO:HD3	2.12	0.49
1:B:468:ARG:NH1	6:B:306:HOH:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ARG:HH11	1:B:586:ARG:HG3	1.78	0.48
1:A:466:TRP:CB	1:A:591:LEU:HD11	2.43	0.48
1:B:465[A]:ARG:NH1	6:B:292:HOH:O	2.47	0.48
1:B:534:ASN:HB3	1:B:536:GLN:HE22	1.79	0.47
1:B:537:ILE:O	1:B:541:GLU:HG3	2.15	0.47
1:B:443:HIS:O	1:B:445:ASP:N	2.47	0.47
1:B:518:ALA:N	6:B:303:HOH:O	2.47	0.47
1:B:534:ASN:CA	1:B:536:GLN:HE22	2.28	0.46
1:B:438:VAL:HA	1:B:449:LEU:HD23	1.96	0.46
1:B:479:VAL:CG1	4:B:402:GOL:C1	2.94	0.46
1:A:569:HIS:HB2	5:A:411:IPA:H31	1.96	0.45
1:A:493:SER:OG	1:A:496:GLU:HG3	2.17	0.45
1:A:485:LEU:CG	1:A:531:ARG:HH22	2.28	0.45
1:A:541:GLU:HB3	1:A:565:LEU:HD22	1.98	0.45
1:A:560:TRP:HZ3	1:A:565:LEU:CD1	2.29	0.45
1:B:519:GLN:N	6:B:303:HOH:O	2.50	0.44
1:A:439:LEU:O	1:A:574:MSE:HE1	2.17	0.44
1:A:538:LEU:CD1	1:A:565:LEU:CB	2.94	0.44
1:A:596:PRO:HB2	6:A:134:HOH:O	2.17	0.44
1:B:486:ILE:O	1:B:487:PRO:C	2.60	0.43
1:A:541:GLU:HB3	1:A:565:LEU:HD21	2.00	0.43
1:B:438:VAL:HG12	1:B:574[B]:MSE:SE	2.70	0.42
1:A:460:LEU:N	1:A:461:PRO:CD	2.82	0.42
1:A:497:LYS:HE3	1:A:516:SER:OG	2.19	0.42
1:A:537:ILE:O	1:A:541:GLU:HG3	2.20	0.42
1:A:560:TRP:CZ3	1:A:565:LEU:CG	3.03	0.42
1:B:473:THR:HA	1:B:474:PRO:HD3	1.92	0.42
1:B:497:LYS:HE3	1:B:516:SER:HB2	2.01	0.42
1:B:479:VAL:CB	4:B:402:GOL:C1	2.95	0.42
1:A:541:GLU:CB	1:A:565:LEU:HD22	2.50	0.41
1:A:606:HIS:HB2	1:A:607:PRO:HD3	2.03	0.41
1:B:566:MSE:HB3	6:B:312:HOH:O	2.20	0.41
1:B:482:GLN:HG3	1:B:531:ARG:NH2	2.36	0.41
1:A:486:ILE:O	1:A:486:ILE:CG1	2.67	0.41
1:A:505:SER:HB2	6:A:34:HOH:O	2.19	0.41
1:A:561:ILE:HG22	1:A:566:MSE:HE2	2.03	0.41
1:A:465[B]:ARG:HD3	6:A:268:HOH:O	2.21	0.41
1:B:530:LEU:CD2	1:B:565:LEU:HD21	2.51	0.41
1:B:533:GLN:HG2	6:B:296:HOH:O	2.20	0.40
1:A:568:GLU:CD	6:A:107:HOH:O	2.64	0.40
1:A:595:PRO:HA	1:A:596:PRO:HD2	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:HD11	1:A:450:GLU:HB2	2.04	0.40
1:A:568:GLU:HB2	1:B:495:GLU:HG2	2.03	0.40
1:B:485:LEU:HA	1:B:485:LEU:HD23	1.60	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	181/188 (96%)	173 (96%)	6 (3%)	2 (1%)	11	8
1	B	184/188 (98%)	176 (96%)	4 (2%)	4 (2%)	5	2
All	All	365/376 (97%)	349 (96%)	10 (3%)	6 (2%)	7	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	SER
1	B	444	SER
1	B	518	ALA
1	B	570	ALA
1	B	568	GLU
1	A	570	ALA

5.3.2 Protein sidechains [i](#)

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	154/156 (99%)	151 (98%)	3 (2%)	50	58
1	B	157/156 (101%)	154 (98%)	3 (2%)	50	58
All	All	311/312 (100%)	305 (98%)	6 (2%)	48	58

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	486	ILE
1	A	519	GLN
1	A	568	GLU
1	B	536	GLN
1	B	540	PRO
1	B	594	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	GLN
1	A	532	GLN
1	A	536	GLN
1	A	571	GLN
1	B	469	GLN
1	B	534	ASN
1	B	536	GLN
1	B	559	GLN
1	B	564	ASN
1	B	571	GLN
1	B	576	GLN
1	B	590	GLN
1	B	601	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
4	GOL	A	401	-	5,5,5	0.25	0	5,5,5	0.63	0
4	GOL	B	402	-	5,5,5	3.69	4 (80%)	5,5,5	1.97	2 (40%)
5	IPA	B	412	-	3,3,3	0.33	0	3,3,3	1.80	1 (33%)
5	IPA	A	411	-	3,3,3	0.24	0	3,3,3	1.69	1 (33%)

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
4	GOL	A	401	-	-	4/4/4/4	-
4	GOL	B	402	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	GOL	C3-C2	4.98	1.70	1.51
4	B	402	GOL	O2-C2	4.16	1.55	1.43
4	B	402	GOL	O3-C3	3.87	1.58	1.42
4	B	402	GOL	O1-C1	-2.73	1.31	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	GOL	O2-C2-C3	3.31	122.88	109.18
5	B	412	IPA	C3-C2-C1	-2.94	91.37	113.38
5	A	411	IPA	C3-C2-C1	-2.80	92.45	113.38
4	B	402	GOL	O2-C2-C1	2.45	119.33	109.18

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	GOL	O1-C1-C2-C3
4	B	402	GOL	O2-C2-C3-O3
4	B	402	GOL	O1-C1-C2-O2
4	A	401	GOL	O1-C1-C2-C3
4	A	401	GOL	C1-C2-C3-O3
4	A	401	GOL	O1-C1-C2-O2
4	A	401	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	GOL	6	0
5	A	411	IPA	2	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	180/188 (95%)	0.40	13 (7%) 21 23	21, 37, 57, 72	1 (0%)
1	B	180/188 (95%)	0.54	21 (11%) 9 9	21, 39, 64, 74	3 (1%)
All	All	360/376 (95%)	0.47	34 (9%) 14 14	21, 38, 61, 74	4 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	VAL	5.7
1	B	475	GLY	5.4
1	B	478	PRO	4.5
1	B	477	ALA	4.5
1	B	568	GLU	4.5
1	B	479	VAL	4.4
1	A	477	ALA	4.1
1	A	485	LEU	3.9
1	A	614	ASP	3.7
1	B	570	ALA	3.5
1	A	565	LEU	3.4
1	A	478	PRO	3.3
1	B	569	HIS	3.2
1	A	568	GLU	3.1
1	B	567	SER	3.1
1	B	613	LYS	3.0
1	B	480[A]	CYS	2.9
1	B	485	LEU	2.9
1	A	567	SER	2.9
1	A	480	CYS	2.8
1	B	482	GLN	2.7
1	A	475	GLY	2.6
1	A	570	ALA	2.6
1	B	443	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	433	GLN	2.4
1	B	517	ASP	2.4
1	A	433	GLN	2.3
1	A	564	ASN	2.3
1	B	483	PRO	2.2
1	B	495	GLU	2.2
1	B	591	LEU	2.2
1	B	534	ASN	2.2
1	B	486	ILE	2.1
1	B	494	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	NA	A	423	1/1	0.57	0.46	105,105,105,105	0
4	GOL	A	401	6/6	0.73	0.17	66,68,70,76	0
5	IPA	A	411	4/4	0.78	0.18	55,56,58,60	0
5	IPA	B	412	4/4	0.78	0.25	59,61,62,62	0
4	GOL	B	402	6/6	0.82	0.27	37,40,42,43	6
2	CL	A	422	1/1	0.99	0.07	34,34,34,34	0
2	CL	A	421	1/1	0.99	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.