



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:16 PM UTC

PDB ID : 3TFI / pdb_00003tfi
Title : DMSP-dependent demethylase from *P. ubique* - with substrate DMSP
Authors : Schuller, D.J.; Reisch, C.R.; Moran, M.A.; Whitman, W.B.; Lanzilotta, W.N.
Deposited on : 2011-08-15
Resolution : 1.60 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

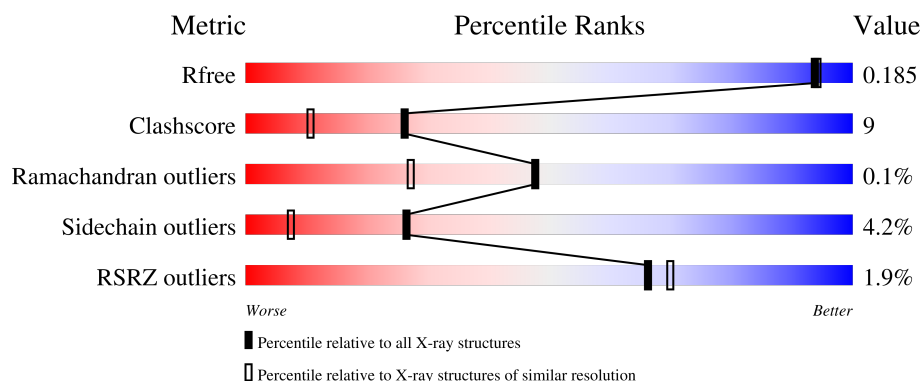
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	369	
1	B	369	

2 Entry composition [i](#)

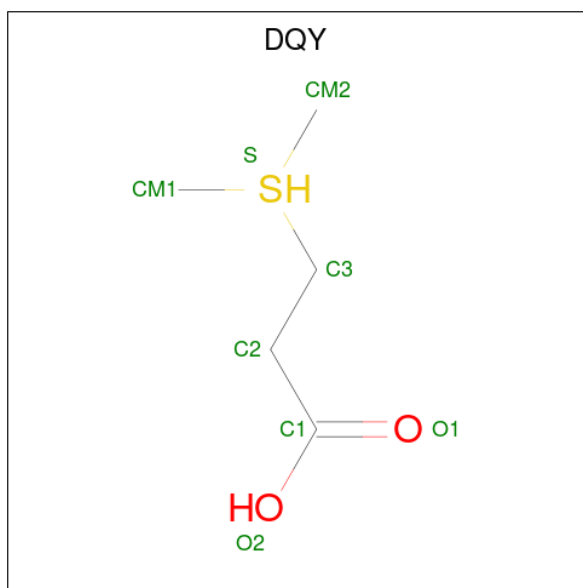
There are 5 unique types of molecules in this entry. The entry contains 6835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GcvT-like Aminomethyltransferase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	27	0
			3101	2001	509	578	13			
1	B	369	Total	C	N	O	S	0	14	0
			3027	1942	501	570	14			

- Molecule 2 is 3-(dimethyl-lambda 4 -sulfanyl)propanoic acid (CCD ID: DQY) (formula: C₅H₁₂O₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	5	2	1		
2	B	1	Total	C	O	S	0	0
			8	5	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

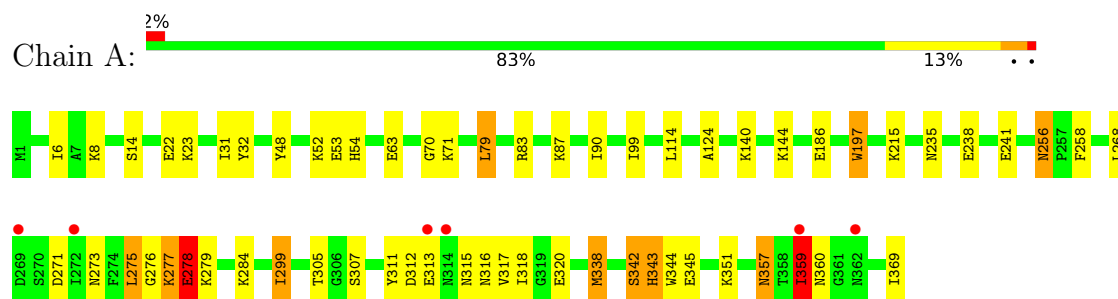
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	315	Total	O	0	0
			315	315		
5	B	362	Total	O	0	0
			362	362		

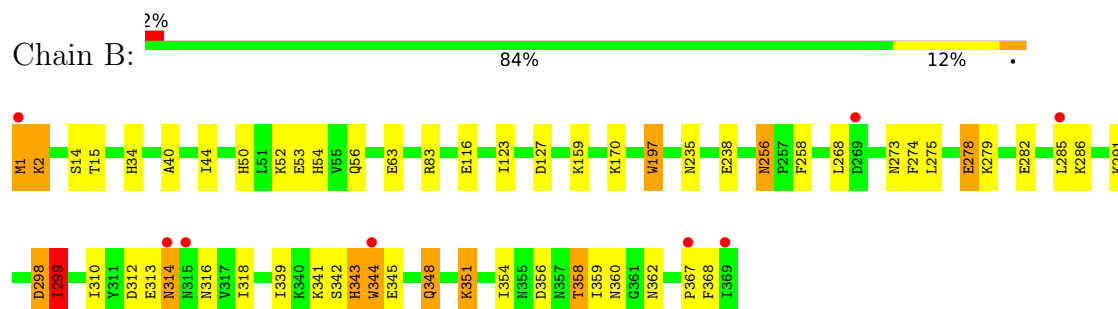
3 Residue-property plots

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: GcvT-like Aminomethyltransferase protein



• Molecule 1: GcvT-like Aminomethyltransferase protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.75Å 121.99Å 59.37Å 90.00° 100.17° 90.00°	Depositor
Resolution (Å)	29.20 – 1.60 29.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.20-1.60) 97.4 (29.20-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.43 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.130 , 0.184 0.135 , 0.185	Depositor DCC
R_{free} test set	2376 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.2	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	0.96	EDS
Total number of atoms	6835	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: NA, GOL, DQY

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	1.25	7/3244 (0.2%)	1.10	9/4357 (0.2%)
1	B	1.25	8/3127 (0.3%)	1.08	4/4205 (0.1%)
All	All	1.25	15/6371 (0.2%)	1.09	13/8562 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ILE	CG1-CD1	-7.27	1.23	1.51
1	A	83	ARG	CG-CD	-7.13	1.31	1.52
1	B	83	ARG	CG-CD	-6.78	1.32	1.52
1	A	279	LYS	N-CA	-6.19	1.38	1.46
1	B	15	THR	N-CA	-5.97	1.41	1.46
1	A	316	ASN	N-CA	-5.89	1.38	1.46
1	B	344	TRP	CA-C	-5.45	1.45	1.52
1	B	358	THR	CA-CB	5.38	1.61	1.53
1	A	70	GLY	N-CA	5.36	1.51	1.45
1	A	342	SER	N-CA	5.30	1.52	1.46
1	A	83	ARG	CA-C	5.14	1.59	1.52
1	A	338	MET	CB-CG	-5.06	1.37	1.52
1	B	345	GLU	CA-C	-5.05	1.46	1.52
1	B	275	LEU	N-CA	5.03	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	PHE	C-O	5.01	1.30	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	HIS	N-CA-C	8.48	122.39	112.72
1	B	343	HIS	N-CA-C	6.20	120.47	112.41
1	A	277	LYS	O-C-N	6.05	128.30	122.07
1	A	338	MET	CB-CG-SD	6.03	130.80	112.70
1	A	344	TRP	N-CA-C	5.91	118.50	111.71
1	B	344	TRP	CB-CA-C	-5.68	100.13	110.63
1	B	123	ILE	N-CA-C	5.58	117.62	108.97
1	A	278[A]	GLU	CA-C-N	5.53	128.71	120.31
1	A	278[A]	GLU	C-N-CA	5.53	128.71	120.31
1	A	278[B]	GLU	CA-C-N	5.53	128.71	120.31
1	A	278[B]	GLU	C-N-CA	5.53	128.71	120.31
1	B	2	LYS	N-CA-CB	5.42	119.65	110.49
1	A	359	ILE	CB-CA-C	5.12	118.38	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	LYS	Peptide
1	B	1[A]	MET	Peptide
1	B	1[B]	MET	Peptide

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	3101	0	3167	72	0
1	B	3027	0	3040	48	0
2	A	8	0	11	3	0
2	B	8	0	11	2	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	315	0	0	9	0
5	B	362	0	0	12	0
All	All	6835	0	6245	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (116) 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:B:367:PRO:HB2	5:B:678:HOH:O	1.27	1.32
1:B:273[B]:ASN:ND2	5:B:615:HOH:O	1.94	0.99
1:A:276:GLY:HA2	1:A:278[A]:GLU:OE1	1.63	0.98
1:A:48[A]:TYR:CE1	1:A:52[A]:LYS:HD2	1.97	0.98
1:A:99:ILE:HD11	1:A:275:LEU:O	1.62	0.97
1:A:299:ILE:HG23	1:A:359:ILE:CD1	1.97	0.94
1:A:14[A]:SER:OG	5:A:595:HOH:O	1.86	0.93
1:A:22:GLU:O	1:B:1[B]:MET:HE2	1.70	0.92
1:A:23:LYS:NZ	5:A:434:HOH:O	2.02	0.90
1:B:1[A]:MET:CE	5:B:469:HOH:O	2.18	0.89
1:B:1[A]:MET:HE1	5:B:469:HOH:O	1.71	0.89
1:A:48[A]:TYR:OH	5:A:474:HOH:O	1.90	0.89
1:A:140[B]:LYS:HE3	1:A:140[B]:LYS:HA	1.59	0.85
1:B:44:ILE:HD12	5:B:546:HOH:O	1.78	0.82
1:B:116[A]:GLU:HG2	5:B:567:HOH:O	1.81	0.80
1:A:99:ILE:C	1:A:99:ILE:HD12	2.06	0.80
1:A:305:THR:O	5:A:546:HOH:O	2.00	0.79
1:A:197:TRP:CG	2:A:370:DQY:HM2A	2.20	0.77
1:B:53[A]:GLU:HG3	5:B:510:HOH:O	1.85	0.77
1:A:369:ILE:HD11	5:A:476:HOH:O	1.85	0.76
1:B:235:ASN:HD22	1:B:238:GLU:H	1.34	0.75
1:A:53[A]:GLU:HG3	1:A:54:HIS:CD2	2.22	0.74
1:A:318:ILE:HD12	1:A:343:HIS:CG	2.22	0.73
1:A:235:ASN:HD22	1:A:238:GLU:H	1.41	0.68
1:A:307:SER:HB3	1:A:320:GLU:CG	2.23	0.68
1:B:63[B]:GLU:OE2	2:B:370:DQY:HM2	1.92	0.68
1:B:50:HIS:HD2	1:B:56:GLN:HE21	1.41	0.67
1:A:307:SER:HB3	1:A:320:GLU:HG3	1.76	0.67
1:B:299:ILE:HG12	1:B:359:ILE:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:HG23	1:A:359:ILE:HD13	1.78	0.66
1:A:345:GLU:H	1:A:345:GLU:CD	2.03	0.66
1:A:48[B]:TYR:CZ	1:A:52[B]:LYS:HD2	2.32	0.65
1:B:367:PRO:CB	5:B:678:HOH:O	2.05	0.65
1:B:50:HIS:CD2	1:B:56:GLN:HE21	2.15	0.64
1:B:14[B]:SER:OG	5:B:714:HOH:O	2.15	0.64
1:A:276:GLY:HA2	1:A:278[A]:GLU:CD	2.24	0.62
1:A:369:ILE:C	1:A:369:ILE:HD12	2.25	0.62
1:A:48[A]:TYR:CE1	1:A:52[A]:LYS:CD	2.79	0.60
1:A:299:ILE:CG2	1:A:359:ILE:HD13	2.31	0.59
1:B:285:LEU:HD12	1:B:286:LYS:N	2.17	0.58
1:A:48[A]:TYR:OH	1:A:241:GLU:OE1	2.18	0.58
1:B:312:ASP:CG	1:B:314:ASN:ND2	2.62	0.57
1:A:276:GLY:C	1:A:278[A]:GLU:HB2	2.29	0.57
1:B:318:ILE:HD12	1:B:343:HIS:CD2	2.40	0.57
1:B:285:LEU:HD12	1:B:286:LYS:HG2	1.86	0.57
1:B:278[A]:GLU:OE2	1:B:279:LYS:N	2.33	0.56
1:B:343:HIS:CD2	1:B:348:GLN:HE22	2.24	0.56
1:A:48[A]:TYR:CZ	1:A:52[A]:LYS:HD2	2.39	0.56
1:A:307:SER:HB3	1:A:320:GLU:CD	2.30	0.56
1:B:310:ILE:HD11	1:B:339:ILE:HD13	1.87	0.55
1:A:307:SER:OG	1:A:320:GLU:CD	2.49	0.55
1:A:342:SER:OG	1:A:343:HIS:HD2	1.88	0.55
1:B:354:ILE:HD12	1:B:359:ILE:HD12	1.88	0.55
1:A:99:ILE:CD1	1:A:275:LEU:O	2.48	0.55
1:A:307:SER:CB	1:A:320:GLU:CD	2.80	0.55
1:B:298[B]:ASP:OD1	1:B:360:ASN:O	2.25	0.54
1:A:197:TRP:CD1	2:A:370:DQY:HM2A	2.43	0.54
1:A:23:LYS:HG2	1:B:1[B]:MET:HE1	1.90	0.53
1:A:23:LYS:CG	1:B:1[B]:MET:HE1	2.38	0.53
1:B:313:GLU:HA	1:B:351:LYS:HD3	1.92	0.52
1:B:54:HIS:HD2	1:B:159:LYS:NZ	2.08	0.52
1:B:354:ILE:HD12	1:B:359:ILE:CD1	2.40	0.52
1:A:48[B]:TYR:CE2	1:A:52[B]:LYS:HD2	2.45	0.51
1:B:343:HIS:CD2	1:B:348:GLN:NE2	2.78	0.51
1:A:256:ASN:HD22	1:A:258:PHE:H	1.57	0.51
1:A:357:ASN:N	1:A:357:ASN:OD1	2.43	0.51
1:A:90:ILE:HD13	5:A:446:HOH:O	2.10	0.51
1:A:48[A]:TYR:HE1	1:A:52[A]:LYS:HD2	1.66	0.50
1:A:278[B]:GLU:OE2	5:A:381:HOH:O	2.19	0.50
1:A:53[A]:GLU:HG3	1:A:54:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HD11	1:A:31:ILE:HD11	1.94	0.50
1:B:40:ALA:HB2	1:B:44:ILE:HD11	1.93	0.50
1:A:140[B]:LYS:HE3	1:A:140[B]:LYS:CA	2.37	0.49
1:A:299:ILE:CG2	1:A:359:ILE:CD1	2.79	0.49
1:B:312:ASP:OD2	1:B:316:ASN:HB2	2.12	0.49
1:A:22:GLU:C	1:B:1[B]:MET:HE2	2.36	0.49
1:B:197:TRP:CG	2:B:370:DQY:HM2A	2.48	0.49
1:B:312:ASP:OD1	1:B:314:ASN:ND2	2.42	0.48
1:A:307:SER:CB	1:A:320:GLU:OE2	2.62	0.48
1:A:63[B]:GLU:OE2	2:A:370:DQY:HM2	2.13	0.48
1:A:186[B]:GLU:OE1	1:A:215[B]:LYS:HD3	2.13	0.48
1:A:8:LYS:NZ	5:A:603:HOH:O	2.47	0.48
1:A:312:ASP:OD1	1:A:315:ASN:N	2.46	0.47
1:A:318:ILE:HD12	1:A:343:HIS:ND1	2.30	0.47
1:A:71[B]:LYS:NZ	5:A:659:HOH:O	2.47	0.47
1:A:99:ILE:HD11	1:A:275:LEU:C	2.37	0.46
1:B:310:ILE:HD11	1:B:339:ILE:CD1	2.44	0.46
1:A:307:SER:HB3	1:A:320:GLU:OE2	2.16	0.46
1:B:299:ILE:HD12	1:B:299:ILE:C	2.40	0.45
1:A:79:LEU:HD22	1:A:275:LEU:HD13	1.99	0.45
1:B:285:LEU:CD1	1:B:286:LYS:HG2	2.46	0.45
1:A:369:ILE:HD12	1:A:369:ILE:O	2.17	0.44
1:A:268:LEU:HD12	1:A:284:LYS:HD2	1.99	0.44
1:B:44:ILE:HD13	5:B:378:HOH:O	2.18	0.44
1:A:311:TYR:CE1	1:A:317:VAL:HG22	2.52	0.44
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.91	0.44
1:B:368:PHE:N	5:B:678:HOH:O	2.50	0.43
1:B:52:LYS:NZ	5:B:625:HOH:O	2.38	0.43
1:A:48[A]:TYR:CE1	1:A:238:GLU:HB2	2.53	0.43
1:B:34:HIS:HE1	1:B:127:ASP:OD2	2.01	0.43
1:A:345:GLU:CD	1:A:345:GLU:N	2.73	0.43
1:A:53[A]:GLU:CG	1:A:54:HIS:CD2	2.99	0.42
1:A:186[B]:GLU:OE1	1:A:215[B]:LYS:HE2	2.20	0.42
1:B:341:LYS:HA	1:B:344:TRP:CE2	2.54	0.42
1:A:351:LYS:NZ	1:A:360[A]:ASN:HD21	2.18	0.42
1:B:291:LYS:HG3	1:B:344:TRP:CZ2	2.55	0.41
1:B:342:SER:OG	1:B:343:HIS:ND1	2.39	0.41
1:A:140[B]:LYS:HA	1:A:140[B]:LYS:CE	2.39	0.41
1:B:256:ASN:HD22	1:B:258:PHE:H	1.67	0.41
1:A:32:TYR:OH	1:A:124:ALA:HA	2.20	0.41
1:A:369:ILE:C	1:A:369:ILE:CD1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:O	1:B:285:LEU:HG	2.22	0.40
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.91	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	394/369 (107%)	384 (98%)	8 (2%)	2 (0%)	24	10
1	B	380/369 (103%)	370 (97%)	10 (3%)	0	100	100
All	All	774/738 (105%)	754 (97%)	18 (2%)	2 (0%)	48	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278[A]	GLU
1	A	278[B]	GLU

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	351/324 (108%)	333 (95%)	18 (5%)	21	5
1	B	338/324 (104%)	323 (96%)	15 (4%)	25	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	689/648 (106%)	656 (95%)	33 (5%)	26 6

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	87[A]	LYS
1	A	87[B]	LYS
1	A	114	LEU
1	A	144[A]	LYS
1	A	144[B]	LYS
1	A	197	TRP
1	A	256	ASN
1	A	271[A]	ASP
1	A	271[B]	ASP
1	A	273[A]	ASN
1	A	273[B]	ASN
1	A	275	LEU
1	A	299	ILE
1	A	313	GLU
1	A	338	MET
1	A	357	ASN
1	A	359	ILE
1	B	2	LYS
1	B	170	LYS
1	B	197	TRP
1	B	256	ASN
1	B	278[A]	GLU
1	B	278[B]	GLU
1	B	298[A]	ASP
1	B	298[B]	ASP
1	B	299	ILE
1	B	314	ASN
1	B	348	GLN
1	B	351	LYS
1	B	356	ASP
1	B	358	THR
1	B	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	33	ASN
1	A	65	GLN
1	A	104	ASN
1	A	139	HIS
1	A	156	GLN
1	A	200	GLN
1	A	211	GLN
1	A	235	ASN
1	A	256	ASN
1	A	289	GLN
1	A	314	ASN
1	A	315	ASN
1	A	316	ASN
1	A	329	HIS
1	A	343	HIS
1	A	362	ASN
1	B	33	ASN
1	B	34	HIS
1	B	50	HIS
1	B	54	HIS
1	B	102	ASN
1	B	117	ASN
1	B	156	GLN
1	B	211	GLN
1	B	228	ASN
1	B	235	ASN
1	B	256	ASN
1	B	314	ASN
1	B	316	ASN
1	B	348	GLN
1	B	353	GLN
1	B	360	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
2	DQY	A	370	-	7,7,7	3.67	3 (42%)	6,8,8	3.35	3 (50%)
3	GOL	B	371	-	5,5,5	0.53	0	5,5,5	0.79	0
3	GOL	A	371	-	5,5,5	0.69	0	5,5,5	0.79	0
2	DQY	B	370	-	7,7,7	4.34	3 (42%)	6,8,8	3.62	2 (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
2	DQY	A	370	-	-	0/5/5/5	-
3	GOL	B	371	-	-	4/4/4/4	-
3	GOL	A	371	-	-	2/4/4/4	-
2	DQY	B	370	-	-	2/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	DQY	CM1-S	-7.39	1.64	1.78
2	B	370	DQY	C3-S	-6.85	1.70	1.80
2	A	370	DQY	CM1-S	-5.68	1.67	1.78
2	A	370	DQY	CM2-S	-5.39	1.68	1.78
2	A	370	DQY	C3-S	-5.12	1.73	1.80
2	B	370	DQY	CM2-S	-4.94	1.69	1.78

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	370	DQY	CM2-S-C3	8.21	116.11	101.63
2	A	370	DQY	CM2-S-C3	6.66	113.37	101.63
2	A	370	DQY	O2-C1-C2	2.89	123.13	114.00
2	A	370	DQY	CM1-S-C3	2.37	105.80	101.63
2	B	370	DQY	CM1-S-C3	2.27	105.63	101.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	371	GOL	C1-C2-C3-O3
3	A	371	GOL	O2-C2-C3-O3
3	B	371	GOL	O1-C1-C2-O2
3	B	371	GOL	O1-C1-C2-C3
3	B	371	GOL	C1-C2-C3-O3
3	B	371	GOL	O2-C2-C3-O3
2	B	370	DQY	O1-C1-C2-C3
2	B	370	DQY	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	370	DQY	3	0
2	B	370	DQY	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	369/369 (100%)	0.05	6 (1%) 70 74	9, 23, 40, 56	27 (7%)
1	B	369/369 (100%)	-0.03	8 (2%) 62 66	9, 22, 43, 55	14 (3%)
All	All	738/738 (100%)	0.01	14 (1%) 66 70	9, 23, 42, 56	41 (5%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	ILE	5.0
1	B	285	LEU	3.6
1	B	344	TRP	3.1
1	A	313	GLU	3.0
1	B	314	ASN	2.9
1	A	314	ASN	2.7
1	A	269	ASP	2.7
1	B	315	ASN	2.3
1	A	272	ILE	2.2
1	B	367	PRO	2.2
1	B	269	ASP	2.1
1	A	359	ILE	2.1
1	A	362	ASN	2.1
1	B	1[A]	MET	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(Å ²)	Q<0.9
2	DQY	A	370	8/8	0.88	0.14	23,26,26,34	8
3	GOL	B	371	6/6	0.89	0.12	38,58,66,67	0
3	GOL	A	371	6/6	0.92	0.12	45,60,62,64	0
2	DQY	B	370	8/8	0.92	0.12	25,28,31,32	8
4	NA	B	372	1/1	0.99	0.03	20,20,20,20	0
4	NA	A	372	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.