



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:53 PM UTC

PDB ID : 3MFL / pdb_00003mfl
Title : Axial Ligand Swapping In Double Mutant Maintains Intradiol-cleavage Chemistry in Protocatechuate 3,4-Dioxygenase
Authors : Purpero, V.M.; Lipscomb, J.D.
Deposited on : 2010-04-02
Resolution : 1.78 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

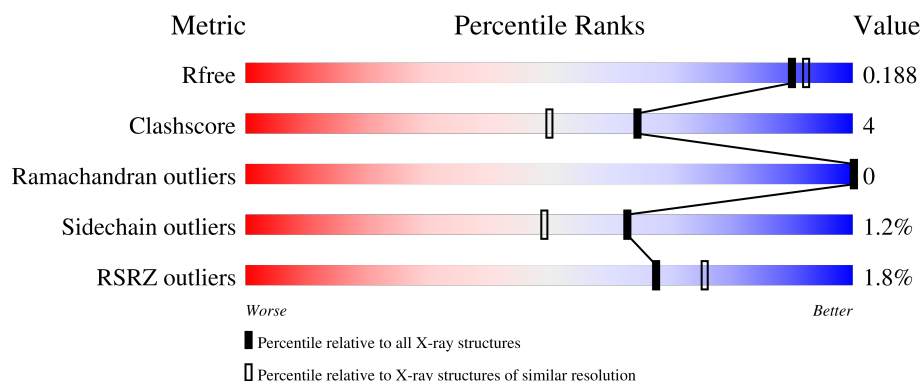
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	200	4% 92% 8%
1	B	200	96% .
1	C	200	4% 93% 6%
2	M	238	2% 94% 6%
2	N	238	% 93% 7%

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Mol	Chain	Length	Quality of chain
2	O	238	% 92% 8%

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
5	BME	B	204	-	-	X	-
8	DHY	M	539[B]	-	-	X	-
8	DHY	O	540[B]	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11806 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 Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	9	0
			1624	1033	279	309	3			
1	B	200	Total	C	N	O	S	0	4	0
			1599	1011	280	305	3			
1	C	200	Total	C	N	O	S	0	1	0
			1581	1000	277	301	3			

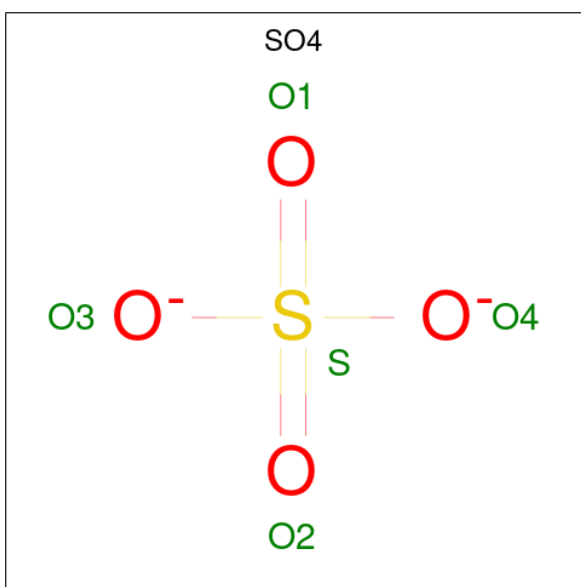
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	238	Total	C	N	O	S	0	6	0
			1915	1215	351	340	9			
2	N	238	Total	C	N	O	S	0	8	0
			1921	1220	348	344	9			
2	O	238	Total	C	N	O	S	0	9	0
			1933	1228	353	343	9			

There are 6 discrepancies between the modelled and reference sequences:

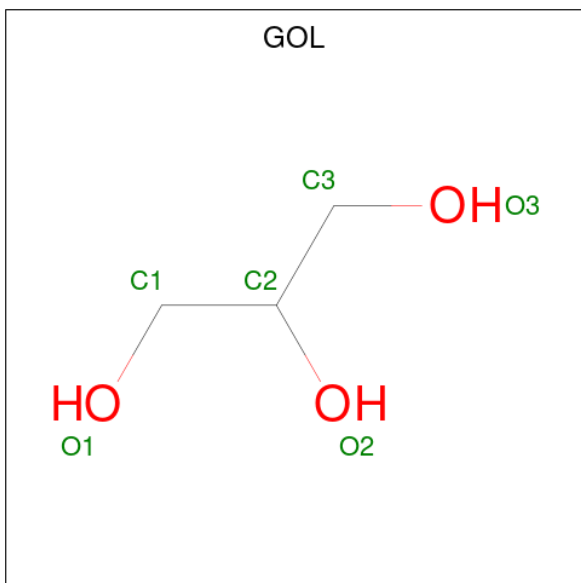
Chain	Residue	Modelled	Actual	Comment	Reference
M	447	HIS	TYR	engineered mutation	UNP P00437
M	462	TYR	HIS	engineered mutation	UNP P00437
N	447	HIS	TYR	engineered mutation	UNP P00437
N	462	TYR	HIS	engineered mutation	UNP P00437
O	447	HIS	TYR	engineered mutation	UNP P00437
O	462	TYR	HIS	engineered mutation	UNP P00437

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



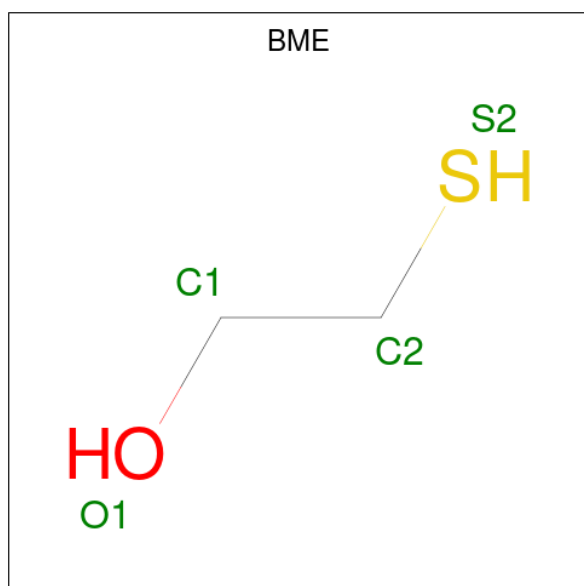
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	1
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 12 6 6	0	1
4	N	1	Total C O 12 6 6	0	1
4	C	1	Total C O 6 3 3	0	0
4	O	1	Total C O 12 6 6	0	1

- Molecule 5 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



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

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

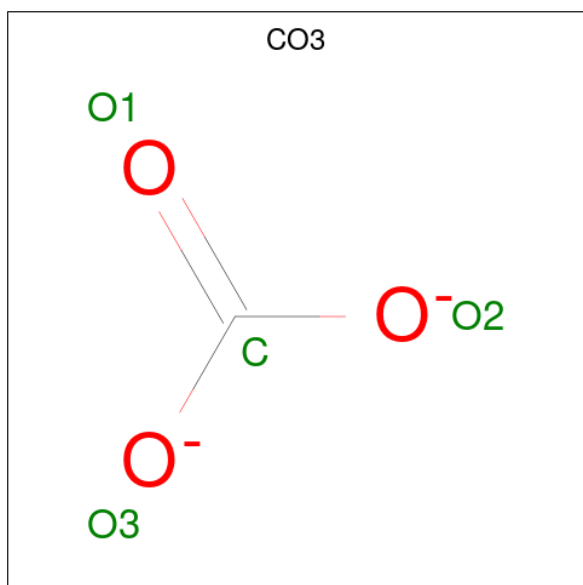
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Fe 1 1	0	0

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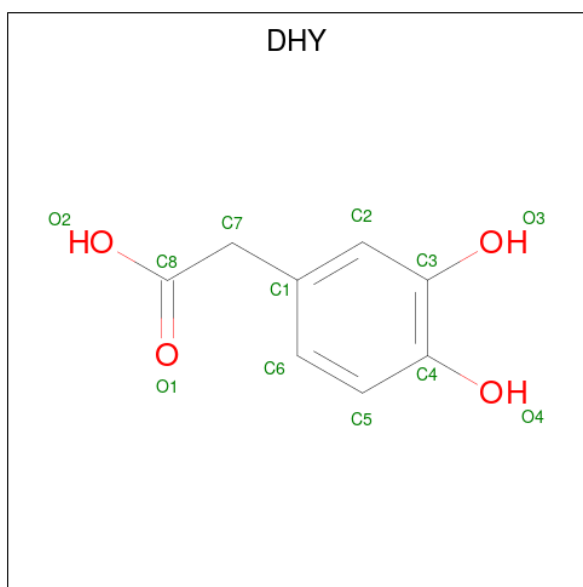
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	1	Total	Fe	0	0
			1	1		
6	O	1	Total	Fe	0	0
			1	1		

- Molecule 7 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is 2-(3,4-DIHYDROXYPHENYL)ACETIC ACID (CCD ID: DHY) (formula: C₈H₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	1
			24	16	8		
8	N	1	Total	C	O	0	1
			24	16	8		
8	O	1	Total	C	O	0	1
			24	16	8		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	O	1	Total	Cl	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	149	Total	O	0	5
			154	154		
10	M	211	Total	O	0	1
			212	212		
10	B	163	Total	O	0	1
			164	164		
10	N	209	Total	O	0	1
			210	210		
10	C	126	Total	O	0	2
			128	128		

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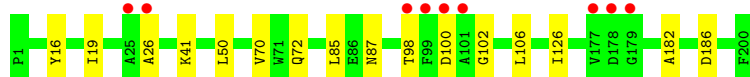
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	O	190	Total 193	O 193	0	3

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.

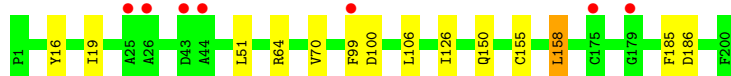
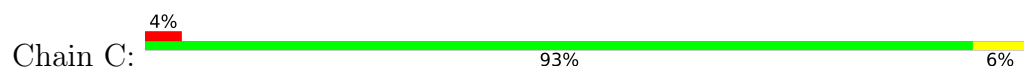
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



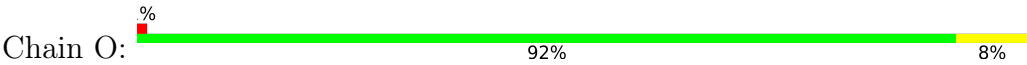
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.32Å 140.77Å 168.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.87 – 1.78 23.87 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.87-1.78) 99.8 (23.87-1.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 1.78Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.185 0.160 , 0.188	Depositor DCC
R_{free} test set	7292 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.2	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	11806	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: DHY, CO3, FE, CL, BME, GOL, SO4

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	0.73	0/1693	0.77	0/2305
1	B	0.73	0/1651	0.80	0/2247
1	C	0.67	0/1624	0.76	0/2211
2	M	0.73	0/1990	0.83	0/2706
2	N	0.72	0/2002	0.83	0/2725
2	O	0.69	0/2017	0.82	0/2744
All	All	0.71	0/10977	0.80	0/14938

There are no bond length outliers.

There are no bond angle outliers.

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	1624	0	1572	16	0
1	B	1599	0	1537	9	0
1	C	1581	0	1516	12	0
2	M	1915	0	1886	14	0
2	N	1921	0	1890	13	0
2	O	1933	0	1910	22	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	N	5	0	0	0	0
4	A	18	0	24	4	0
4	B	12	0	16	0	0
4	C	6	0	8	3	0
4	N	12	0	16	0	0
4	O	12	0	16	1	0
5	A	4	0	6	0	0
5	B	8	0	12	4	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
7	M	4	0	0	0	0
8	M	24	0	10	8	0
8	N	24	0	10	6	0
8	O	24	0	10	8	0
9	O	1	0	0	0	0
10	A	154	0	0	0	0
10	B	164	0	0	0	0
10	C	128	0	0	1	0
10	M	212	0	0	0	0
10	N	210	0	0	0	0
10	O	193	0	0	1	0
All	All	11806	0	10439	82	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 4.

All (82) 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)
5:B:204:BME:H12	2:N:470:ILE:HD12	1.26	1.11
2:O:414[B]:ARG:HG2	2:O:414[B]:ARG:HH21	1.09	1.09
2:O:414[B]:ARG:HH21	2:O:414[B]:ARG:CG	1.80	0.92
2:O:414[B]:ARG:HG2	2:O:414[B]:ARG:NH2	1.91	0.85
2:O:447[B]:HIS:CE1	8:O:540[B]:DHY:C4	2.68	0.76
1:C:186:ASP:H	4:C:202:GOL:H32	1.51	0.75
2:O:447[B]:HIS:HE1	8:O:540[B]:DHY:C4	2.01	0.73
2:M:447[B]:HIS:CE1	8:M:539[B]:DHY:C4	2.73	0.72
1:B:70:VAL:HG11	1:B:106:LEU:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:447[B]:HIS:HE1	8:M:539[B]:DHY:C4	2.02	0.71
5:B:204:BME:H12	2:N:470:ILE:CD1	2.15	0.68
1:A:16:TYR:CE2	8:M:539[B]:DHY:H2	2.30	0.67
2:O:414[B]:ARG:CG	2:O:414[B]:ARG:NH2	2.45	0.66
2:N:447[B]:HIS:CE1	8:N:539[B]:DHY:C4	2.81	0.64
1:A:41:LYS:HE3	4:A:203:GOL:H2	1.80	0.63
1:C:186:ASP:H	4:C:202:GOL:C3	2.11	0.62
1:A:19[B]:ILE:CD1	1:A:26:ALA:HB1	2.31	0.61
2:N:447[B]:HIS:HE1	8:N:539[B]:DHY:C4	2.14	0.61
2:M:447[B]:HIS:HE1	8:M:539[B]:DHY:C5	2.15	0.60
1:C:16:TYR:CE2	8:O:540[A]:DHY:H2	2.38	0.59
1:B:129:SER:OG	5:B:204:BME:H11	2.03	0.57
2:O:414[B]:ARG:CZ	2:O:414[B]:ARG:HB2	2.34	0.57
2:O:447[B]:HIS:CE1	8:O:540[B]:DHY:C3	2.89	0.56
1:A:19[B]:ILE:HD11	2:M:410:HIS:HB2	1.88	0.55
1:C:64:ARG:NH2	1:C:100:ASP:O	2.40	0.55
1:A:85:LEU:O	4:A:203:GOL:H12	2.05	0.55
2:O:414[B]:ARG:NH2	2:O:414[B]:ARG:CB	2.70	0.55
2:O:447[B]:HIS:HE1	8:O:540[B]:DHY:C3	2.20	0.55
2:N:478:LEU:C	2:N:478:LEU:HD23	2.33	0.54
1:B:16:TYR:CE2	8:N:539[B]:DHY:H2	2.44	0.53
1:B:128:ILE:C	5:B:204:BME:H21	2.33	0.52
2:M:478:LEU:HD23	2:M:478:LEU:C	2.34	0.52
1:A:16:TYR:CE2	8:M:539[A]:DHY:H2	2.45	0.52
1:A:70:VAL:HG11	1:A:106:LEU:HD11	1.94	0.50
1:C:185:PHE:HA	4:C:202:GOL:H31	1.91	0.50
2:O:449:TRP:CE3	8:O:540[B]:DHY:H6	2.47	0.50
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.42	0.49
1:A:19[B]:ILE:HD13	1:A:26:ALA:CB	2.44	0.48
2:M:352:SER:HA	2:M:430:LEU:HD11	1.94	0.48
2:N:447[B]:HIS:CE1	8:N:539[B]:DHY:C3	2.97	0.48
2:O:400:TRP:HA	2:O:425:GLY:O	2.13	0.48
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.96	0.47
1:A:87:ASN:O	4:A:203:GOL:H32	2.14	0.47
2:N:400:TRP:HA	2:N:425:GLY:O	2.15	0.47
1:C:70:VAL:HG11	1:C:106:LEU:HD11	1.95	0.47
2:O:334[B]:GLN:OE1	10:O:574:HOH:O	2.21	0.47
2:N:352:SER:HA	2:N:430:LEU:HD11	1.95	0.47
2:M:449:TRP:CB	8:M:539[B]:DHY:H6	2.45	0.47
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.46	0.46
1:A:19[B]:ILE:HD13	1:A:26:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:HB3	1:A:126[B]:ILE:HG23	1.98	0.45
1:C:64:ARG:HD3	1:C:99:PHE:O	2.17	0.45
2:M:400:TRP:HA	2:M:425:GLY:O	2.17	0.45
2:O:457:ARG:HD3	8:O:540[B]:DHY:H5	1.98	0.45
1:B:16:TYR:CE2	8:N:539[A]:DHY:H2	2.53	0.44
2:M:326:THR:HG22	2:M:330:ARG:HD2	1.99	0.44
2:N:326[A]:THR:HG22	2:N:330:ARG:HD2	1.99	0.44
2:O:478:LEU:C	2:O:478:LEU:HD23	2.43	0.44
2:O:414[B]:ARG:CZ	2:O:414[B]:ARG:CB	2.93	0.43
2:N:429[A]:CYS:SG	2:N:437:TYR:HB2	2.58	0.43
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.99	0.43
2:O:399:MET:HA	2:O:462:TYR:O	2.18	0.43
1:A:186:ASP:H	4:A:202[B]:GOL:H31	1.83	0.43
2:N:399:MET:HA	2:N:462:TYR:O	2.20	0.42
1:A:98:THR:O	1:A:102:GLY:HA2	2.20	0.42
2:M:304:ASP:HB2	2:M:343:ILE:HB	2.00	0.42
2:O:326[A]:THR:HG22	2:O:330:ARG:HD2	2.01	0.42
2:M:447[B]:HIS:CE1	8:M:539[B]:DHY:C3	3.03	0.42
1:A:19[B]:ILE:HD11	2:M:410:HIS:CB	2.49	0.42
1:B:190:GLN:HG3	2:N:333:ARG:HG2	2.02	0.42
2:M:399:MET:HA	2:M:462:TYR:O	2.20	0.41
2:O:449:TRP:HB2	8:O:540[A]:DHY:H6	2.01	0.41
1:B:51:LEU:HD11	1:B:126:ILE:HD12	2.01	0.41
2:M:447[B]:HIS:CE1	8:M:539[B]:DHY:C5	3.00	0.40
2:N:447[B]:HIS:HE1	8:N:539[B]:DHY:C3	2.33	0.40
1:C:51:LEU:HD11	1:C:126:ILE:HD12	2.03	0.40
1:C:19:ILE:HD11	2:O:408:TYR:HB3	2.04	0.40
2:O:524:ASP:HB2	4:O:1[A]:GOL:H2	2.03	0.40
1:A:50:LEU:O	1:A:182:ALA:HA	2.22	0.40
1:C:150:GLN:HG3	10:C:286:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/200 (104%)	203 (98%)	4 (2%)	0	100	100
1	B	202/200 (101%)	199 (98%)	3 (2%)	0	100	100
1	C	199/200 (100%)	195 (98%)	4 (2%)	0	100	100
2	M	242/238 (102%)	237 (98%)	5 (2%)	0	100	100
2	N	244/238 (102%)	239 (98%)	5 (2%)	0	100	100
2	O	245/238 (103%)	240 (98%)	5 (2%)	0	100	100
All	All	1339/1314 (102%)	1313 (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	172/163 (106%)	171 (99%)	1 (1%)	78	70
1	B	167/163 (102%)	167 (100%)	0	100	100
1	C	164/163 (101%)	163 (99%)	1 (1%)	78	70
2	M	208/202 (103%)	206 (99%)	2 (1%)	68	55
2	N	210/202 (104%)	206 (98%)	4 (2%)	50	32
2	O	211/202 (104%)	205 (97%)	6 (3%)	38	17
All	All	1132/1095 (103%)	1118 (99%)	14 (1%)	63	49

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
2	M	395	THR
2	M	430	LEU
2	N	395	THR

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Mol	Chain	Res	Type
2	N	414	ARG
2	N	478	LEU
2	N	534	HIS
1	C	158	LEU
2	O	303[A]	GLN
2	O	303[B]	GLN
2	O	390	LYS
2	O	395	THR
2	O	478	LEU
2	O	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	334	GLN
1	B	54	GLN
2	N	303	GLN
2	N	530	GLN
1	C	59	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	BME	A	204	-	3,3,3	0.42	0	2,2,2	0.55	0
4	GOL	N	1[B]	-	5,5,5	0.48	0	5,5,5	0.35	0
8	DHY	M	539[B]	6	12,12,12	1.56	1 (8%)	16,16,16	0.80	0
5	BME	B	204	-	3,3,3	0.69	0	2,2,2	1.36	0
3	SO4	B	201	-	4,4,4	0.22	0	6,6,6	0.15	0
4	GOL	B	202[B]	-	5,5,5	0.40	0	5,5,5	0.36	0
4	GOL	A	203	-	5,5,5	0.33	0	5,5,5	0.45	0
3	SO4	C	201	-	4,4,4	0.23	0	6,6,6	0.22	0
8	DHY	N	539[B]	6	12,12,12	1.51	1 (8%)	16,16,16	1.03	0
4	GOL	N	1[A]	-	5,5,5	0.50	0	5,5,5	0.43	0
8	DHY	M	539[A]	6	12,12,12	1.58	1 (8%)	16,16,16	0.83	0
4	GOL	O	1[B]	-	5,5,5	0.36	0	5,5,5	0.36	0
4	GOL	B	202[A]	-	5,5,5	0.33	0	5,5,5	0.74	0
7	CO3	M	1	-	3,3,3	0.85	0	2,3,3	0.29	0
4	GOL	A	202[B]	-	5,5,5	0.31	0	5,5,5	0.46	0
8	DHY	N	539[A]	6	12,12,12	1.48	1 (8%)	16,16,16	0.82	0
8	DHY	O	540[B]	6	12,12,12	1.50	1 (8%)	16,16,16	0.89	0
3	SO4	N	4	-	4,4,4	0.26	0	6,6,6	0.13	0
3	SO4	A	201	-	4,4,4	0.31	0	6,6,6	0.28	0
4	GOL	O	1[A]	-	5,5,5	0.40	0	5,5,5	0.27	0
4	GOL	C	202	-	5,5,5	0.33	0	5,5,5	0.34	0
4	GOL	A	202[A]	-	5,5,5	0.31	0	5,5,5	0.91	0
8	DHY	O	540[A]	6	12,12,12	1.58	1 (8%)	16,16,16	1.51	2 (12%)
5	BME	B	203	-	3,3,3	0.31	0	2,2,2	0.52	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	BME	A	204	-	-	0/1/1/1	-
4	GOL	N	1[B]	-	-	4/4/4/4	-
8	DHY	M	539[B]	6	-	0/4/4/4	0/1/1/1
5	BME	B	204	-	-	0/1/1/1	-
4	GOL	B	202[B]	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	203	-	-	1/4/4/4	-
8	DHY	N	539[B]	6	-	2/4/4/4	0/1/1/1
4	GOL	N	1[A]	-	-	4/4/4/4	-
8	DHY	M	539[A]	6	-	0/4/4/4	0/1/1/1
4	GOL	O	1[B]	-	-	4/4/4/4	-
4	GOL	B	202[A]	-	-	0/4/4/4	-
4	GOL	A	202[B]	-	-	2/4/4/4	-
8	DHY	O	540[B]	6	-	0/4/4/4	0/1/1/1
8	DHY	N	539[A]	6	-	0/4/4/4	0/1/1/1
4	GOL	O	1[A]	-	-	4/4/4/4	-
4	GOL	C	202	-	-	2/4/4/4	-
4	GOL	A	202[A]	-	-	2/4/4/4	-
8	DHY	O	540[A]	6	-	2/4/4/4	0/1/1/1
5	BME	B	203	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	539[B]	DHY	C4-C3	4.97	1.48	1.40
8	M	539[A]	DHY	C4-C3	4.86	1.48	1.40
8	O	540[B]	DHY	C4-C3	4.82	1.48	1.40
8	N	539[A]	DHY	C4-C3	4.70	1.48	1.40
8	N	539[B]	DHY	C4-C3	4.62	1.47	1.40
8	O	540[A]	DHY	C4-C3	4.61	1.47	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	540[A]	DHY	C7-C1-C2	-3.45	115.15	120.38
8	O	540[A]	DHY	C7-C1-C6	3.22	125.62	120.89

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202[B]	GOL	C1-C2-C3-O3
4	N	1[A]	GOL	O1-C1-C2-C3
4	N	1[A]	GOL	C1-C2-C3-O3
4	N	1[B]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	O	1[A]	GOL	O1-C1-C2-C3
4	O	1[A]	GOL	C1-C2-C3-O3
4	O	1[B]	GOL	C1-C2-C3-O3
8	N	539[B]	DHY	C6-C1-C7-C8
4	A	202[B]	GOL	O2-C2-C3-O3
4	N	1[A]	GOL	O1-C1-C2-O2
4	N	1[A]	GOL	O2-C2-C3-O3
4	N	1[B]	GOL	O2-C2-C3-O3
4	C	202	GOL	O2-C2-C3-O3
4	O	1[A]	GOL	O1-C1-C2-O2
4	O	1[A]	GOL	O2-C2-C3-O3
8	N	539[B]	DHY	C2-C1-C7-C8
4	A	202[A]	GOL	O1-C1-C2-C3
4	B	202[B]	GOL	O1-C1-C2-C3
4	N	1[B]	GOL	C1-C2-C3-O3
4	C	202	GOL	C1-C2-C3-O3
4	O	1[B]	GOL	O1-C1-C2-C3
4	N	1[B]	GOL	O1-C1-C2-O2
8	O	540[A]	DHY	C6-C1-C7-C8
8	O	540[A]	DHY	C2-C1-C7-C8
4	B	202[B]	GOL	O1-C1-C2-O2
4	O	1[B]	GOL	O2-C2-C3-O3
4	A	202[A]	GOL	O1-C1-C2-O2
4	A	203	GOL	O2-C2-C3-O3
4	O	1[B]	GOL	O1-C1-C2-O2
4	B	202[B]	GOL	O2-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	539[B]	DHY	7	0
5	B	204	BME	4	0
4	A	203	GOL	3	0
8	N	539[B]	DHY	5	0
8	M	539[A]	DHY	1	0
4	A	202[B]	GOL	1	0
8	N	539[A]	DHY	1	0
8	O	540[B]	DHY	6	0
4	O	1[A]	GOL	1	0
4	C	202	GOL	3	0
8	O	540[A]	DHY	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	200/200 (100%)	-0.21	9 (4%) 38 44	9, 18, 31, 45	12 (6%)
1	B	200/200 (100%)	-0.35	0 100 100	11, 18, 28, 31	7 (3%)
1	C	200/200 (100%)	0.18	7 (3%) 47 53	13, 24, 39, 51	7 (3%)
2	M	238/238 (100%)	-0.38	4 (1%) 69 77	10, 17, 27, 41	7 (2%)
2	N	238/238 (100%)	-0.49	2 (0%) 82 87	9, 16, 25, 39	11 (4%)
2	O	238/238 (100%)	-0.21	2 (0%) 82 87	10, 19, 29, 42	10 (4%)
All	All	1314/1314 (100%)	-0.25	24 (1%) 67 75	9, 18, 30, 51	54 (4%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	538	CYS	4.0
1	A	99	PHE	3.6
2	N	538	CYS	3.5
1	A	98	THR	3.2
2	M	538	CYS	3.1
1	C	25	ALA	3.0
2	O	537	ASN	2.8
1	C	179	GLY	2.8
1	A	25	ALA	2.6
2	M	302	ALA	2.5
1	C	99	PHE	2.4
2	M	305	ASN	2.4
1	C	43	ASP	2.4
1	A	26	ALA	2.3
1	C	26	ALA	2.3
1	A	178	ASP	2.3
2	N	537	ASN	2.2
1	C	175	CYS	2.2
1	A	179	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASP	2.1
2	M	301	PRO	2.1
1	A	101	ALA	2.1
1	A	177	VAL	2.0
1	C	44	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
4	GOL	N	1[A]	6/6	0.68	0.19	36,38,38,39	6
4	GOL	N	1[B]	6/6	0.68	0.19	36,38,38,38	6
5	BME	A	204	4/4	0.71	0.21	37,39,39,42	4
4	GOL	O	1[A]	6/6	0.74	0.20	30,33,33,34	6
4	GOL	O	1[B]	6/6	0.74	0.20	37,38,38,39	6
3	SO4	N	4	5/5	0.74	0.12	53,53,53,54	5
4	GOL	B	202[B]	6/6	0.78	0.15	32,33,35,36	6
4	GOL	B	202[A]	6/6	0.78	0.15	28,30,32,34	6
4	GOL	A	203	6/6	0.79	0.15	43,49,49,53	0
4	GOL	C	202	6/6	0.82	0.13	33,35,38,41	0
8	DHY	M	539[A]	12/12	0.82	0.16	22,23,29,32	12
8	DHY	M	539[B]	12/12	0.82	0.16	17,18,18,18	12
7	CO3	M	1	4/4	0.83	0.12	58,58,58,58	0
5	BME	B	203	4/4	0.84	0.15	35,40,41,46	4
8	DHY	O	540[A]	12/12	0.84	0.14	20,22,26,27	12
8	DHY	O	540[B]	12/12	0.84	0.14	15,17,17,18	12
5	BME	B	204	4/4	0.85	0.16	17,23,27,35	4
3	SO4	C	201	5/5	0.86	0.12	49,49,49,50	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	DHY	N	539[B]	12/12	0.87	0.10	22,24,28,29	12
3	SO4	B	201	5/5	0.87	0.12	48,48,48,49	5
8	DHY	N	539[A]	12/12	0.87	0.10	21,23,25,26	12
9	CL	O	539	1/1	0.89	0.12	66,66,66,66	0
3	SO4	A	201	5/5	0.91	0.12	38,39,40,41	5
4	GOL	A	202[B]	6/6	0.93	0.08	30,32,34,35	6
4	GOL	A	202[A]	6/6	0.93	0.08	16,19,22,23	6
6	FE	N	600	1/1	0.97	0.06	24,24,24,24	1
6	FE	O	600	1/1	0.97	0.06	24,24,24,24	1
6	FE	M	600	1/1	0.98	0.08	25,25,25,25	1

6.5 Other polymers [i](#)

There are no such residues in this entry.