



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 09:33 AM EDT

PDB ID : 3T63
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 : 2011-07-28
Resolution : 1.54 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

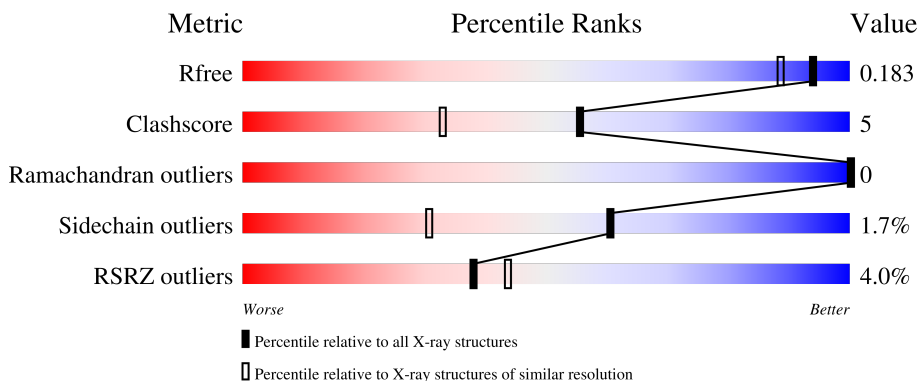
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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% 90% 10%
1	B	200	 6% 90% 10%
1	C	200	 8% 94% 6%
2	M	238	 2% 93% 7%
2	N	238	 3% 95% 5%

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Mol	Chain	Length	Quality of chain
2	O	238	<p>3% 93% 7%</p>

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	BME	M	1	-	-	X	-
3	BME	M	542[A]	-	-	X	-
3	BME	M	543	-	-	X	-
3	BME	N	540[A]	-	-	X	-
3	BME	O	540	-	-	X	-
4	GOL	C	201	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12175 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
			Total	C	N	O	S			
1	A	200	Total 1600	C 1011	N 280	O 306	S 3	0	3	0
1	B	200	Total 1666	C 1049	N 295	O 319	S 3	0	11	0
1	C	200	Total 1587	C 1003	N 279	O 302	S 3	3	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	238	Total 1915	C 1214	N 348	O 345	S 8	1	6	0
2	N	238	Total 1885	C 1194	N 343	O 340	S 8	0	1	0
2	O	238	Total 1888	C 1197	N 343	O 340	S 8	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	M	1	Total	C	O	S	0	0
			4	2	1	1		
3	M	1	Total	C	O	S	0	0
			4	2	1	1		
3	M	1	Total	C	O	S	0	0
			4	2	1	1		
3	M	1	Total	C	O	S	0	1
			8	4	2	2		
3	M	1	Total	C	O	S	0	0
			4	2	1	1		
3	N	1	Total	C	O	S	0	0
			4	2	1	1		
3	N	1	Total	C	O	S	0	0
			4	2	1	1		
3	N	1	Total	C	O	S	0	1
			8	4	2	2		
3	O	1	Total	C	O	S	0	1
			8	4	2	2		
3	O	1	Total	C	O	S	0	0
			4	2	1	1		
3	O	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

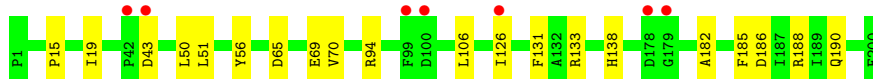
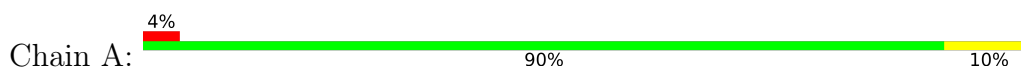
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	229	Total O 231 231	0	2
7	B	217	Total O 217 217	0	0
7	C	204	Total O 205 205	0	1
7	M	298	Total O 299 299	0	1
7	N	290	Total O 292 292	0	2
7	O	274	Total O 277 277	0	3

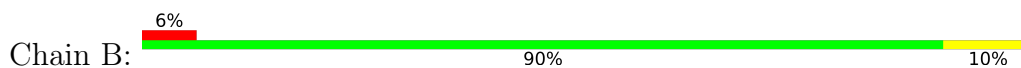
3 Residue-property plots [i](#)

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.

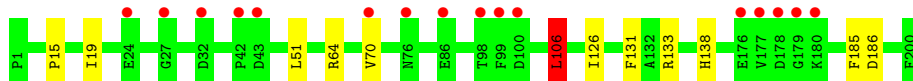
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



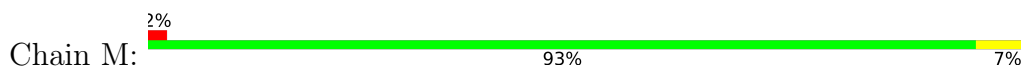
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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



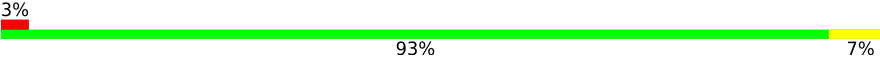
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



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



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

Chain O:  3% 93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.12Å 140.62Å 167.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 1.54 29.09 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.09-1.54) 99.0 (29.09-1.54)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 1.54Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.155 , 0.178 0.160 , 0.183	Depositor DCC
R_{free} test set	10986 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12175	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: GOL, FE, SO4, BME

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	0.56	0/1640	0.66	0/2233
1	B	0.51	0/1710	0.66	0/2327
1	C	0.51	0/1630	0.64	1/2219 (0.0%)
2	M	0.53	0/1978	0.71	1/2691 (0.0%)
2	N	0.53	0/1940	0.67	0/2640
2	O	0.53	0/1946	0.70	1/2648 (0.0%)
All	All	0.53	0/10844	0.68	3/14758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	LEU	CA-CB-CG	5.55	128.07	115.30
2	M	416	LEU	CA-CB-CG	5.37	127.65	115.30
2	O	416	LEU	CA-CB-CG	5.11	127.04	115.30

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	1600	0	1528	18	0
1	B	1666	0	1588	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1587	0	1522	20	0
2	M	1915	0	1875	15	0
2	N	1885	0	1841	11	0
2	O	1888	0	1848	11	0
3	A	4	0	6	3	0
3	M	24	0	32	17	0
3	N	16	0	20	8	0
3	O	16	0	20	14	0
4	A	12	0	16	5	0
4	B	6	0	8	0	0
4	C	6	0	8	5	0
4	M	6	0	8	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	M	5	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
7	A	231	0	0	0	0
7	B	217	0	0	5	0
7	C	205	0	0	2	0
7	M	299	0	0	5	0
7	N	292	0	0	6	0
7	O	277	0	0	3	0
All	All	12175	0	10320	107	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 5.

All (107) 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)
3:M:542[B]:BME:H21	7:M:1488:HOH:O	1.25	1.34
3:O:1[B]:BME:S2	3:O:539:BME:O1	1.92	1.27
1:C:133:ARG:HG3	3:O:540:BME:H11	1.35	1.04
3:M:1:BME:C1	7:M:1559:HOH:O	2.03	1.04
1:B:184:ARG:NH1	7:B:1526:HOH:O	1.93	1.01
1:A:65:ASP:OD2	1:A:133:ARG:HD3	1.64	0.98
1:B:133:ARG:HD2	3:N:540[A]:BME:H11	1.46	0.97
3:N:540[B]:BME:H21	7:N:1536:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:543:BME:H21	2:O:453:PRO:HB3	1.49	0.94
3:N:540[B]:BME:C2	7:N:1536:HOH:O	2.19	0.87
1:C:133:ARG:CG	3:O:540:BME:H11	2.08	0.84
1:B:133:ARG:CD	3:N:540[A]:BME:H11	2.09	0.82
2:M:339:ILE:O	3:M:543:BME:H22	1.83	0.76
3:O:1[B]:BME:S2	3:O:540:BME:H22	2.25	0.76
1:B:64[B]:ARG:NE	1:B:99:PHE:O	2.17	0.76
1:B:64[B]:ARG:O	1:B:99:PHE:HD2	1.68	0.76
1:C:133:ARG:HD2	3:O:540:BME:H12	1.68	0.76
2:O:369:ASN:H	2:O:422:ASN:HD22	1.32	0.75
2:M:369:ASN:H	2:M:422:ASN:HD22	1.36	0.72
2:N:369:ASN:H	2:N:422:ASN:HD22	1.38	0.71
1:C:133:ARG:CD	3:O:540:BME:H12	2.20	0.70
2:O:324:TYR:OH	3:O:540:BME:S2	2.49	0.70
1:C:133:ARG:HG3	3:O:540:BME:C1	2.18	0.69
1:A:186:ASP:H	4:A:202[B]:GOL:H12	1.58	0.69
3:M:1:BME:H11	7:M:1559:HOH:O	1.82	0.69
1:C:64:ARG:HD2	7:C:1465:HOH:O	1.95	0.67
1:B:70:VAL:HG11	1:B:106:LEU:HD11	1.76	0.66
1:C:133:ARG:HD2	3:O:540:BME:C1	2.24	0.66
1:C:186:ASP:H	4:C:201:GOL:C3	2.10	0.64
3:M:543:BME:H12	7:M:547:HOH:O	1.98	0.64
1:B:19[B]:ILE:HD12	1:B:26:ALA:HB1	1.80	0.63
1:C:133:ARG:CD	3:O:540:BME:C1	2.77	0.62
1:B:98[B]:THR:CG2	1:B:103:GLU:H	2.13	0.62
1:A:185:PHE:HA	4:A:202[A]:GOL:H11	1.82	0.61
1:A:186:ASP:H	4:A:202[B]:GOL:C1	2.13	0.61
1:B:19[B]:ILE:HD13	2:N:410:HIS:HD2	1.65	0.61
1:A:133:ARG:HE	3:M:542[A]:BME:H11	1.66	0.61
1:A:15:PRO:HB3	1:A:133:ARG:HD2	1.82	0.60
2:O:369:ASN:H	2:O:422:ASN:ND2	2.00	0.60
1:C:186:ASP:H	4:C:201:GOL:H32	1.66	0.60
1:C:133:ARG:HG2	2:O:326:THR:HG21	1.83	0.60
3:M:543:BME:C2	2:O:453:PRO:HB3	2.27	0.59
1:C:19:ILE:O	2:O:426[B]:VAL:HG11	2.02	0.59
1:B:64[B]:ARG:O	1:B:99:PHE:CD2	2.53	0.57
1:B:98[B]:THR:HG22	1:B:103:GLU:H	1.69	0.57
1:B:98[B]:THR:HG21	7:B:849:HOH:O	2.04	0.57
4:C:201:GOL:O3	7:C:1492:HOH:O	2.17	0.57
1:B:51:LEU:HD11	1:B:126[A]:ILE:CD1	2.34	0.56
1:B:18[A]:HIS:CE1	7:B:511:HOH:O	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64[A]:ARG:NH1	1:B:100:ASP:O	2.35	0.56
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.88	0.55
1:B:19[B]:ILE:HD12	1:B:26:ALA:CB	2.36	0.55
2:M:324:TYR:OH	3:M:542[A]:BME:S2	2.64	0.54
2:M:339:ILE:O	3:M:543:BME:C2	2.53	0.54
1:B:133:ARG:HG2	2:N:326[A]:THR:HG21	1.89	0.54
2:M:324:TYR:HH	3:M:542[A]:BME:HS2	1.56	0.53
2:N:329:ALA:HB3	7:N:891:HOH:O	2.07	0.53
1:C:185:PHE:HA	4:C:201:GOL:H31	1.92	0.52
1:C:133:ARG:CG	3:O:540:BME:C1	2.83	0.52
2:M:369:ASN:H	2:M:422:ASN:ND2	2.06	0.51
1:C:186:ASP:H	4:C:201:GOL:H31	1.76	0.50
1:B:24:GLU:OE2	7:B:970:HOH:O	2.19	0.50
1:B:18[A]:HIS:HE1	7:B:511:HOH:O	1.92	0.49
2:N:369:ASN:H	2:N:422:ASN:ND2	2.08	0.49
2:M:329:ALA:HB3	7:M:1441:HOH:O	2.12	0.49
2:M:478:LEU:HD23	2:M:478:LEU:C	2.33	0.48
2:M:340:PRO:HA	3:M:543:BME:H22	1.96	0.48
1:A:65:ASP:OD2	1:A:133:ARG:CD	2.51	0.48
1:B:19[B]:ILE:HD11	2:N:410:HIS:HB2	1.95	0.48
1:C:15:PRO:HD3	3:O:540:BME:S2	2.53	0.48
2:N:478:LEU:C	2:N:478:LEU:HD23	2.35	0.47
1:A:51:LEU:HD11	1:A:126[B]:ILE:CD1	2.44	0.47
2:M:457:ARG:NH1	3:M:1:BME:S2	2.80	0.47
4:A:202[A]:GOL:O3	4:A:202[A]:GOL:O1	2.04	0.46
3:O:1[A]:BME:C1	7:O:1561:HOH:O	2.59	0.46
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.49	0.46
2:M:339:ILE:C	3:M:543:BME:H22	2.36	0.46
1:A:56:TYR:HB3	3:A:201:BME:H11	1.96	0.46
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.46	0.46
1:B:19[B]:ILE:HD13	2:N:410:HIS:CD2	2.49	0.45
1:B:133:ARG:HG3	3:N:540[A]:BME:S2	2.57	0.45
1:B:19[B]:ILE:CD1	2:N:410:HIS:CD2	3.00	0.44
2:N:524:ASP:HB3	7:N:1263:HOH:O	2.18	0.44
1:B:15:PRO:HD3	3:N:540[B]:BME:H21	2.00	0.44
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.53	0.44
2:O:329:ALA:HB3	7:O:1159:HOH:O	2.18	0.44
1:A:15:PRO:HD3	3:M:542[A]:BME:S2	2.59	0.43
1:A:70:VAL:HG11	1:A:106:LEU:HD11	2.01	0.43
1:B:133:ARG:HD2	3:N:540[A]:BME:C1	2.34	0.42
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64[B]:ARG:HH21	1:B:100:ASP:HA	1.84	0.42
2:M:457:ARG:HG3	3:M:1:BME:S2	2.59	0.42
1:A:69:GLU:HG2	1:A:94:ARG:HG2	2.01	0.42
1:A:188:ARG:HG2	3:A:201:BME:H12	2.01	0.42
1:C:131:PHE:CD2	2:O:475:ILE:HD12	2.55	0.41
2:M:304:ASP:HB2	2:M:343:ILE:HB	2.02	0.41
1:A:50:LEU:O	1:A:182:ALA:HA	2.21	0.41
1:B:51:LEU:HD11	1:B:126[A]:ILE:HD12	2.01	0.41
3:N:1:BME:C1	7:N:1560:HOH:O	2.67	0.41
2:M:341:GLN:HG3	3:M:543:BME:S2	2.60	0.41
2:O:449:TRP:CZ3	3:O:540:BME:H21	2.55	0.41
1:A:190:GLN:O	3:A:201:BME:S2	2.71	0.41
2:O:531:ARG:HG2	7:O:1302:HOH:O	2.20	0.40
2:N:531:ARG:HG2	7:N:1281:HOH:O	2.21	0.40
1:A:185:PHE:HA	4:A:202[B]:GOL:H12	2.03	0.40
1:B:69:GLU:HG2	1:B:94:ARG:HG2	2.02	0.40
1:A:19:ILE:O	2:M:426:VAL:HG21	2.22	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	201/200 (100%)	197 (98%)	4 (2%)	0	100	100
1	B	209/200 (104%)	205 (98%)	4 (2%)	0	100	100
1	C	200/200 (100%)	197 (98%)	3 (2%)	0	100	100
2	M	242/238 (102%)	239 (99%)	3 (1%)	0	100	100
2	N	237/238 (100%)	232 (98%)	5 (2%)	0	100	100
2	O	238/238 (100%)	234 (98%)	4 (2%)	0	100	100
All	All	1327/1314 (101%)	1304 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	166/163 (102%)	164 (99%)	2 (1%)	71	47
1	B	174/163 (107%)	172 (99%)	2 (1%)	73	51
1	C	165/163 (101%)	164 (99%)	1 (1%)	86	72
2	M	207/201 (103%)	202 (98%)	5 (2%)	49	18
2	N	202/201 (100%)	199 (98%)	3 (2%)	65	36
2	O	203/201 (101%)	196 (97%)	7 (3%)	37	9
All	All	1117/1092 (102%)	1097 (98%)	20 (2%)	60	29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43[A]	ASP
1	A	43[B]	ASP
1	B	100	ASP
1	B	192	GLU
1	C	106	LEU
2	M	395	THR
2	M	414	ARG
2	M	416	LEU
2	M	473	LYS
2	M	534	HIS
2	N	395	THR
2	N	473	LYS
2	N	534	HIS
2	O	372	LEU
2	O	390	LYS
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	473	LYS

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Mol	Chain	Res	Type
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	422	ASN
2	N	303	GLN
2	N	422	ASN
2	N	537	ASN
2	O	422	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 3 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	$\# Z > 2$
3	BME	M	542[A]	-	3,3,3	0.27	0	1,2,2	0.81	0
4	GOL	C	201	-	5,5,5	0.39	0	5,5,5	0.30	0
3	BME	M	539	-	3,3,3	0.29	0	1,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	O	1[B]	-	3,3,3	0.29	0	1,2,2	0.57	0
5	SO4	M	7	-	4,4,4	0.13	0	6,6,6	0.05	0
3	BME	M	540	-	3,3,3	0.38	0	1,2,2	0.32	0
4	GOL	A	202[B]	-	5,5,5	0.29	0	5,5,5	0.33	0
3	BME	M	542[B]	-	3,3,3	0.34	0	1,2,2	0.33	0
3	BME	A	201	-	3,3,3	0.45	0	1,2,2	0.51	0
4	GOL	B	201	-	5,5,5	0.31	0	5,5,5	0.35	0
3	BME	N	1	6	3,3,3	0.31	0	1,2,2	1.04	0
5	SO4	C	202	-	4,4,4	0.14	0	6,6,6	0.10	0
3	BME	N	540[A]	-	3,3,3	0.37	0	1,2,2	0.61	0
3	BME	M	1	6	3,3,3	0.23	0	1,2,2	1.71	0
3	BME	O	539	-	3,3,3	0.36	0	1,2,2	0.50	0
5	SO4	B	202	-	4,4,4	0.19	0	6,6,6	0.22	0
3	BME	O	540	-	3,3,3	0.25	0	1,2,2	0.13	0
3	BME	N	540[B]	-	3,3,3	0.40	0	1,2,2	0.09	0
3	BME	M	543	-	3,3,3	0.20	0	1,2,2	1.52	0
3	BME	N	539	-	3,3,3	0.35	0	1,2,2	0.49	0
4	GOL	M	541	-	5,5,5	0.55	0	5,5,5	0.58	0
3	BME	O	1[A]	6	3,3,3	0.26	0	1,2,2	0.98	0
5	SO4	A	203	-	4,4,4	0.20	0	6,6,6	0.22	0
4	GOL	A	202[A]	-	5,5,5	0.44	0	5,5,5	0.47	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	M	542[A]	-	-	1/1/1/1	-
4	GOL	C	201	-	-	2/4/4/4	-
3	BME	M	539	-	-	1/1/1/1	-
3	BME	O	1[B]	-	-	1/1/1/1	-
3	BME	M	540	-	-	1/1/1/1	-
4	GOL	A	202[B]	-	-	2/4/4/4	-
3	BME	M	542[B]	-	-	0/1/1/1	-
3	BME	A	201	-	-	1/1/1/1	-
4	GOL	B	201	-	-	4/4/4/4	-
3	BME	N	1	6	-	1/1/1/1	-
3	BME	N	540[A]	-	-	0/1/1/1	-
3	BME	M	1	6	-	1/1/1/1	-
3	BME	O	539	-	-	0/1/1/1	-
3	BME	O	540	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	N	540[B]	-	-	1/1/1/1	-
3	BME	M	543	-	-	0/1/1/1	-
3	BME	N	539	-	-	1/1/1/1	-
4	GOL	M	541	-	-	4/4/4/4	-
3	BME	O	1[A]	6	-	1/1/1/1	-
4	GOL	A	202[A]	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	BME	O1-C1-C2-S2
3	M	539	BME	O1-C1-C2-S2
3	M	540	BME	O1-C1-C2-S2
3	N	539	BME	O1-C1-C2-S2
3	O	1[B]	BME	O1-C1-C2-S2
3	O	540	BME	O1-C1-C2-S2
4	A	202[B]	GOL	O1-C1-C2-C3
4	B	201	GOL	C1-C2-C3-O3
4	C	201	GOL	C1-C2-C3-O3
4	M	541	GOL	O1-C1-C2-C3
4	A	202[A]	GOL	C1-C2-C3-O3
4	B	201	GOL	O1-C1-C2-C3
4	M	541	GOL	C1-C2-C3-O3
4	A	202[B]	GOL	O1-C1-C2-O2
4	C	201	GOL	O2-C2-C3-O3
4	M	541	GOL	O1-C1-C2-O2
3	M	1	BME	O1-C1-C2-S2
3	N	1	BME	O1-C1-C2-S2
3	O	1[A]	BME	O1-C1-C2-S2
4	B	201	GOL	O1-C1-C2-O2
4	B	201	GOL	O2-C2-C3-O3
4	M	541	GOL	O2-C2-C3-O3
4	A	202[A]	GOL	O2-C2-C3-O3
3	M	542[A]	BME	O1-C1-C2-S2
3	N	540[B]	BME	O1-C1-C2-S2

There are no ring outliers.

15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	542[A]	BME	4	0
4	C	201	GOL	5	0
3	O	1[B]	BME	2	0
4	A	202[B]	GOL	3	0
3	M	542[B]	BME	1	0
3	A	201	BME	3	0
3	N	1	BME	1	0
3	N	540[A]	BME	4	0
3	M	1	BME	4	0
3	O	539	BME	1	0
3	O	540	BME	12	0
3	N	540[B]	BME	3	0
3	M	543	BME	8	0
3	O	1[A]	BME	1	0
4	A	202[A]	GOL	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	200/200 (100%)	0.04	7 (3%) 44 50	13, 17, 29, 40	0
1	B	200/200 (100%)	0.04	11 (5%) 25 28	13, 17, 29, 35	2 (1%)
1	C	200/200 (100%)	0.32	16 (8%) 12 14	13, 21, 33, 43	1 (0%)
2	M	238/238 (100%)	-0.18	5 (2%) 63 69	13, 16, 24, 33	1 (0%)
2	N	238/238 (100%)	-0.16	6 (2%) 57 63	13, 16, 24, 33	0
2	O	238/238 (100%)	-0.05	8 (3%) 45 51	13, 17, 26, 34	1 (0%)
All	All	1314/1314 (100%)	-0.01	53 (4%) 38 44	13, 17, 29, 43	5 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	PHE	6.7
1	C	178	ASP	5.4
1	C	177	VAL	5.2
1	A	178	ASP	5.2
2	O	301	PRO	5.0
1	C	43	ASP	4.7
1	C	99	PHE	4.5
2	N	538	CYS	4.4
2	M	538	CYS	4.3
1	C	179	GLY	4.1
1	B	100	ASP	4.0
2	O	538	CYS	3.9
1	A	99	PHE	3.6
2	O	305	ASN	3.5
1	C	100	ASP	3.4
1	B	25	ALA	3.4
1	B	43	ASP	3.4
2	M	411	LYS	3.2
1	B	98[A]	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	180	LYS	3.2
1	B	27	GLY	3.0
1	C	42	PRO	3.0
2	O	411	LYS	2.9
2	M	414	ARG	2.8
1	C	176	GLU	2.7
2	O	303	GLN	2.7
1	B	24	GLU	2.7
1	A	42	PRO	2.7
1	B	101	ALA	2.7
1	B	26	ALA	2.6
2	N	537	ASN	2.6
2	O	353	HIS	2.6
2	N	303	GLN	2.6
2	N	414	ARG	2.6
2	O	414	ARG	2.6
2	O	537	ASN	2.5
2	N	411	LYS	2.5
1	C	70	VAL	2.5
1	A	179	GLY	2.5
2	M	305	ASN	2.4
1	C	86	GLU	2.4
1	C	32	ASP	2.4
2	N	305	ASN	2.4
1	A	43[A]	ASP	2.3
1	C	24	GLU	2.3
1	A	100	ASP	2.3
1	C	98	THR	2.3
2	M	370	GLY	2.1
1	B	192	GLU	2.1
1	C	27	GLY	2.1
1	B	126[A]	ILE	2.1
1	A	126[A]	ILE	2.0
1	C	76	ASN	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 monosaccharides 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	M	541	6/6	0.64	0.25	31,38,39,39	0
3	BME	M	540	4/4	0.72	0.23	39,41,41,43	4
3	BME	O	540	4/4	0.76	0.19	26,29,31,36	4
4	GOL	B	201	6/6	0.79	0.22	37,41,42,43	0
3	BME	M	539	4/4	0.79	0.22	37,37,38,39	4
4	GOL	C	201	6/6	0.80	0.12	34,35,37,39	0
3	BME	M	542[A]	4/4	0.81	0.16	20,23,26,27	4
3	BME	M	542[B]	4/4	0.81	0.16	33,36,36,37	4
3	BME	N	540[A]	4/4	0.81	0.22	20,24,25,27	4
3	BME	N	540[B]	4/4	0.81	0.22	51,51,52,52	4
3	BME	M	1	4/4	0.84	0.24	27,28,28,28	4
3	BME	A	201	4/4	0.85	0.27	37,39,39,40	0
4	GOL	A	202[B]	6/6	0.87	0.16	20,20,20,23	6
4	GOL	A	202[A]	6/6	0.87	0.16	24,27,29,31	6
3	BME	O	1[A]	4/4	0.88	0.14	34,34,34,35	4
3	BME	O	1[B]	4/4	0.88	0.14	37,38,39,41	4
3	BME	O	539	4/4	0.88	0.20	25,27,29,29	4
5	SO4	M	7	5/5	0.89	0.18	41,41,42,42	5
3	BME	M	543	4/4	0.90	0.20	26,26,28,28	4
3	BME	N	539	4/4	0.90	0.13	45,46,47,47	0
5	SO4	B	202	5/5	0.91	0.19	39,42,42,42	5
3	BME	N	1	4/4	0.91	0.19	30,30,30,30	4
5	SO4	C	202	5/5	0.95	0.15	36,38,39,39	5
5	SO4	A	203	5/5	0.95	0.12	30,33,34,35	5
6	FE	M	600	1/1	0.95	0.07	30,30,30,30	1
6	FE	N	600	1/1	0.96	0.05	28,28,28,28	1
6	FE	O	600	1/1	0.99	0.05	29,29,29,29	1

6.5 Other polymers [i](#)

There are no such residues in this entry.