wwPDB X-ray Structure Validation Summary Report (i)

Sep 30, 2021 – 11:39 AM EDT

PDB ID	:	3MI5
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	:	2010-04-09
Resolution	:	1.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

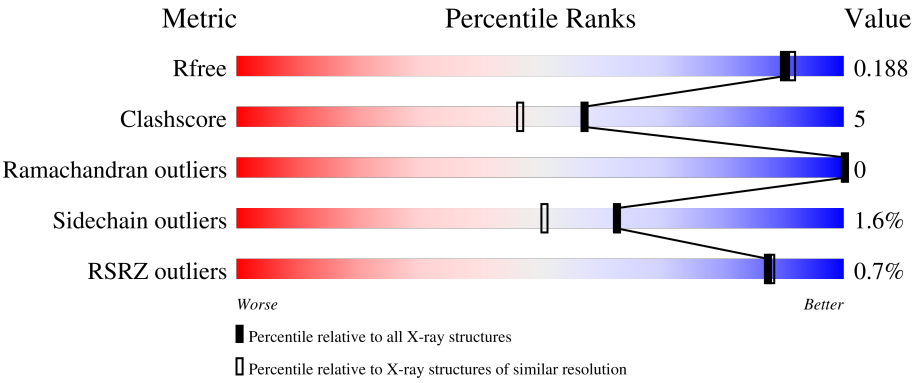
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	92% 8%
1	B	200	2% 90% 10%
1	C	200	94% 6%
1	D	200	93% 7%
1	E	200	2% 94% 6%

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Mol	Chain	Length	Quality of chain
1	F	200	94% 6%
2	M	238	90% 10%
2	N	238	93% 7%
2	O	238	92% 8%
2	P	238	92% 7%
2	Q	238	92% 8%
2	R	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
4	BME	B	202	-	-	X	-
4	BME	D	202	-	-	X	-
4	BME	F	207	-	-	X	-
4	BME	O	542	-	-	X	-
5	GOL	B	203	-	-	X	-
5	GOL	M	14[A]	-	-	X	-
5	GOL	M	16	-	-	X	-
5	GOL	Q	540	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 24211 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
			1629	1031	284	311	3			
1	B	200	Total	C	N	O	S	0	4	0
			1596	1010	278	305	3			
1	C	200	Total	C	N	O	S	0	9	0
			1632	1032	282	315	3			
1	D	200	Total	C	N	O	S	0	6	0
			1606	1016	277	310	3			
1	E	200	Total	C	N	O	S	0	7	0
			1615	1022	281	309	3			
1	F	200	Total	C	N	O	S	2	8	0
			1630	1030	283	314	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
			1921	1218	353	342	8			
2	N	238	Total	C	N	O	S	0	7	0
			1924	1220	353	343	8			
2	O	238	Total	C	N	O	S	0	5	0
			1913	1213	350	342	8			
2	P	238	Total	C	N	O	S	0	7	0
			1922	1221	349	344	8			
2	Q	238	Total	C	N	O	S	0	11	0
			1946	1238	356	344	8			
2	R	238	Total	C	N	O	S	0	7	0
			1927	1224	352	343	8			

There are 12 discrepancies between the modelled and reference sequences:

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

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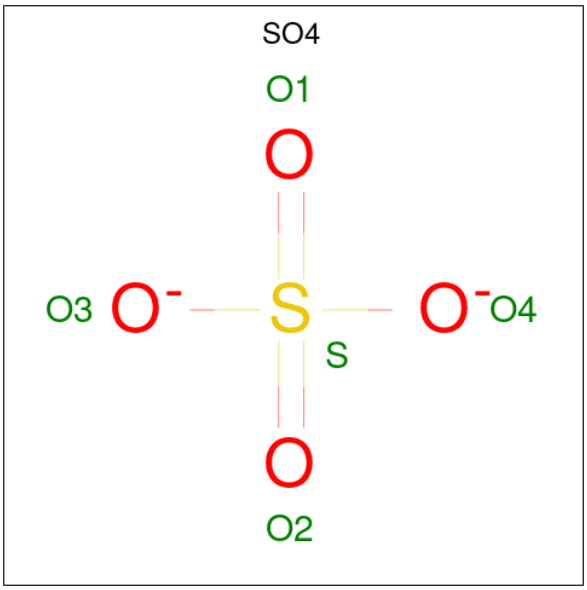
Chain	Residue	Modelled	Actual	Comment	Reference
M	462	TYR	HIS	engineered mutation	UNP P00437
N	447	HIS	TYR	engineered mutation	UNP P00437
N	462	TYR	HIS	engineered mutation	UNP P00437
O	447	HIS	TYR	engineered mutation	UNP P00437
O	462	TYR	HIS	engineered mutation	UNP P00437
P	447	HIS	TYR	engineered mutation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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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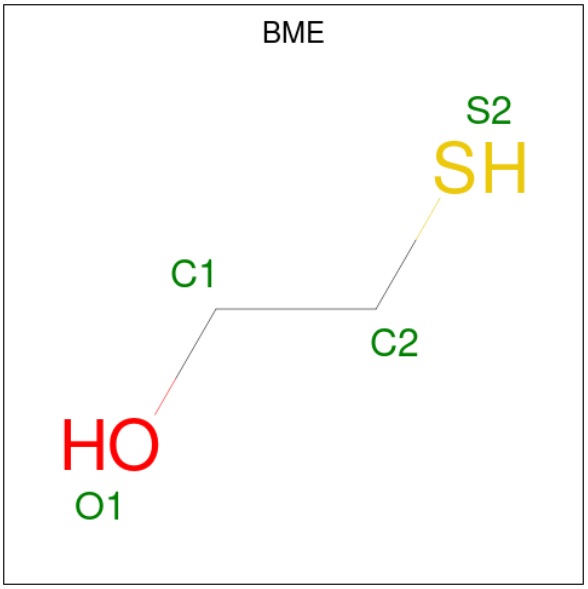
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	Q	1	Total O S 5 4 1	0	0
3	Q	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

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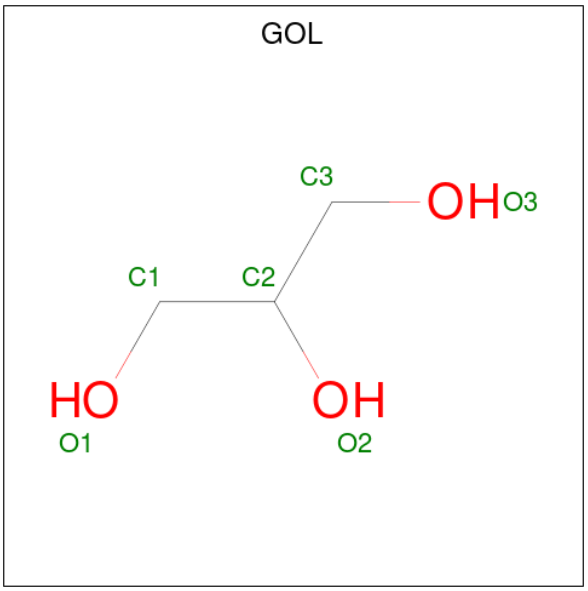
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	N	1	Total	C	O	S	0	0
			4	2	1	1		
4	N	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	O	1	Total	C	O	S	0	0
			4	2	1	1		
4	O	1	Total	C	O	S	0	0
			4	2	1	1		
4	O	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	P	1	Total	C	O	S	0	0
			4	2	1	1		
4	P	1	Total	C	O	S	0	1
			8	4	2	2		
4	P	1	Total	C	O	S	0	0
			4	2	1	1		
4	P	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	1
			8	4	2	2		
4	F	1	Total	C	O	S	0	0
			4	2	1	1		
4	F	1	Total	C	O	S	0	0
			4	2	1	1		
4	R	1	Total	C	O	S	0	0
			4	2	1	1		
4	R	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 12	C 6	O 6	0	1
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	O	1	Total 6	C 3	O 3	0	0
5	O	1	Total 12	C 6	O 6	0	1
5	O	1	Total 6	C 3	O 3	0	0
5	O	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 12	C 6	O 6	0	1
5	D	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	P	1	Total 12	C 6	O 6	0	1
5	P	1	Total 6	C 3	O 3	0	0
5	P	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 12	C 6	O 6	0	1
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	Q	1	Total 12	C 6	O 6	0	1
5	Q	1	Total 6	C 3	O 3	0	0

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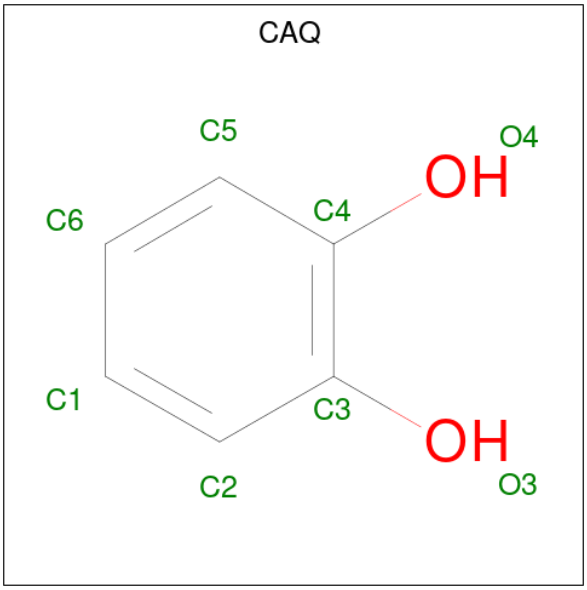
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 12 6 6	0	1
5	R	1	Total C O 12 6 6	0	1
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 12 6 6	0	1

- Molecule 6 is CATECHOL (three-letter code: CAQ) (formula: $C_6H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 6 2	0	0
6	M	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	N	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 8 6 2	0	0
6	O	1	Total C O 8 6 2	0	0
6	D	1	Total C O 8 6 2	0	0
6	P	1	Total C O 8 6 2	0	0
6	E	1	Total C O 8 6 2	0	0
6	Q	1	Total C O 8 6 2	0	0
6	F	1	Total C O 8 6 2	0	0
6	R	1	Total C O 8 6 2	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total Fe 1 1	0	0
7	N	1	Total Fe 1 1	0	0
7	O	1	Total Fe 1 1	0	0
7	P	1	Total Fe 1 1	0	0
7	Q	1	Total Fe 1 1	0	0
7	R	1	Total Fe 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Cl 1 1	0	0
8	N	1	Total Cl 1 1	0	0
8	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Q	1	Total Cl 1 1	0	0
8	R	1	Total Cl 1 1	0	0

- Molecule 9 is water.

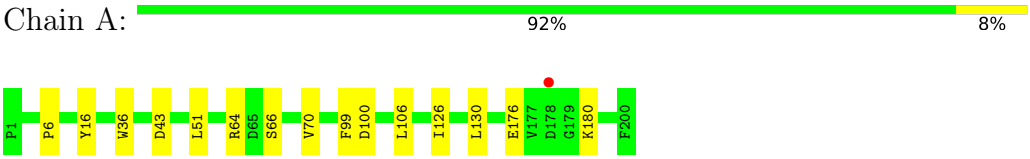
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	164	Total O 166 166	0	2
9	M	228	Total O 230 230	0	2
9	B	154	Total O 156 156	0	2
9	N	208	Total O 211 211	0	3
9	C	168	Total O 169 169	0	1
9	O	217	Total O 218 218	0	1
9	D	163	Total O 166 166	0	3
9	P	226	Total O 229 229	0	3
9	E	143	Total O 145 145	0	2
9	Q	211	Total O 214 214	0	3
9	F	181	Total O 182 182	0	1
9	R	237	Total O 239 239	0	2

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.

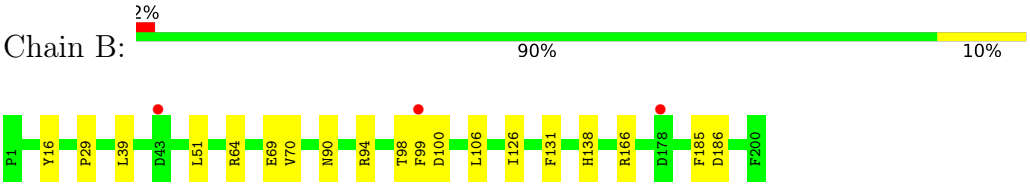
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A:



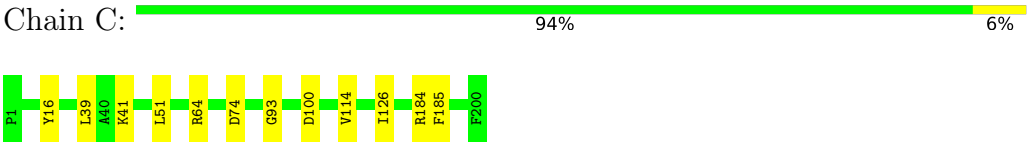
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain B:



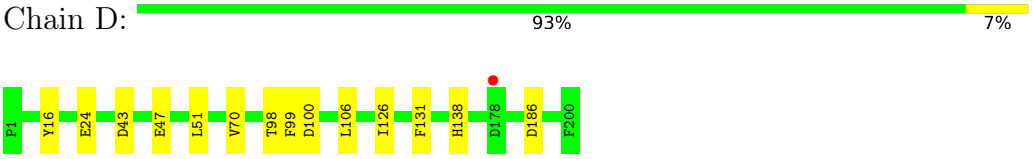
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain C:



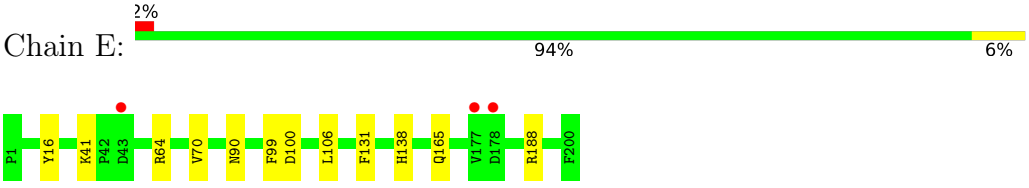
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain D:



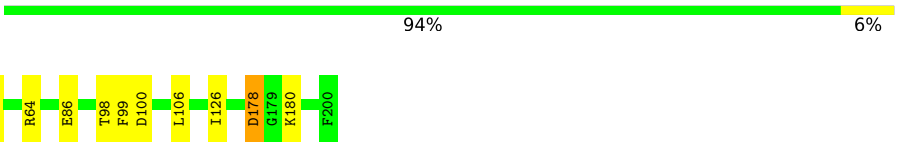
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain E:



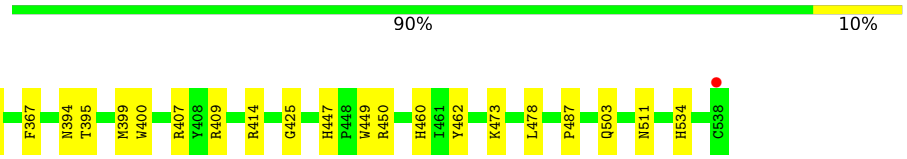
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain F:



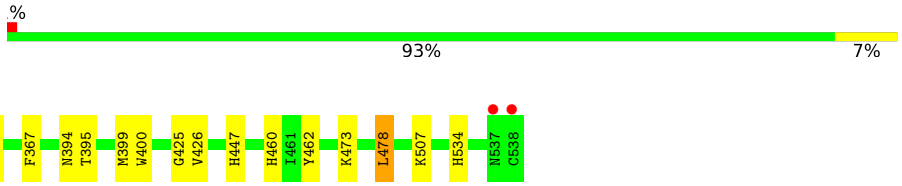
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain M:



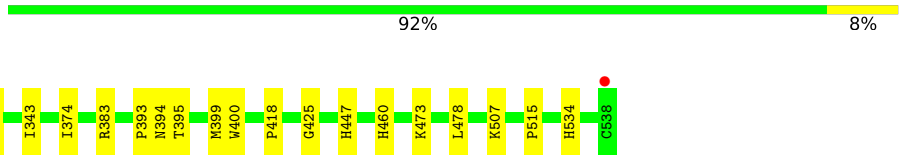
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain N:



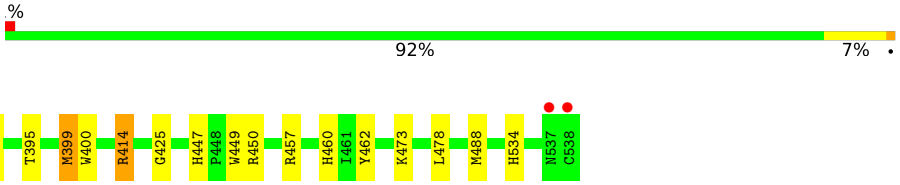
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain O:



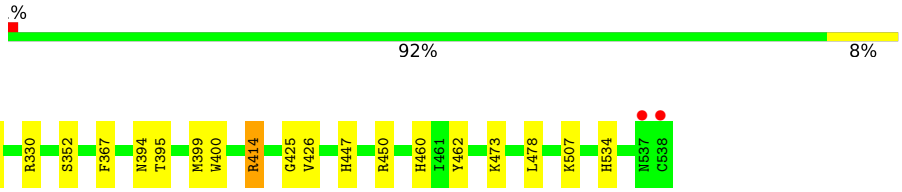
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain P:



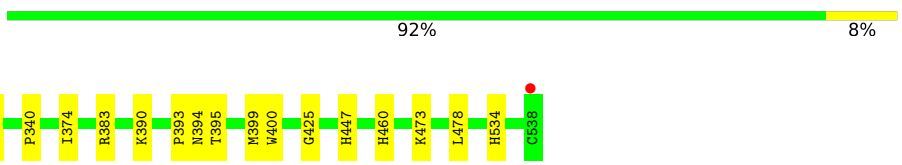
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain Q:



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

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.54Å 168.00Å 128.34Å 90.00° 132.40° 90.00°	Depositor
Resolution (Å)	30.62 – 1.78 29.97 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.62-1.78) 99.0 (29.97-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 1.78Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.151 , 0.185 0.155 , 0.188	Depositor DCC
R_{free} test set	14311 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	24211	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CAQ, SO4, FE, CL, BME, 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	0.66	0/1694	0.64	0/2304
1	B	0.62	0/1648	0.63	0/2243
1	C	0.63	0/1693	0.65	1/2304 (0.0%)
1	D	0.68	0/1664	0.65	0/2265
1	E	0.65	0/1676	0.64	0/2280
1	F	0.95	2/1685 (0.1%)	0.67	0/2293
2	M	0.66	0/1993	0.70	0/2711
2	N	0.65	0/2002	0.67	0/2724
2	O	0.64	0/1982	0.69	0/2696
2	P	0.66	0/1997	0.72	1/2717 (0.0%)
2	Q	0.64	0/2037	0.67	0/2769
2	R	0.68	0/2002	0.70	1/2724 (0.0%)
All	All	0.68	2/22073 (0.0%)	0.67	3/30030 (0.0%)

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	F	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	178[A]	ASP	CG-OD1	19.81	1.71	1.25
1	F	178[B]	ASP	CG-OD1	19.81	1.71	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	311	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	P	457	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	74	ASP	CB-CG-OD1	5.19	122.97	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	178[A]	ASP	Sidechain
1	F	178[B]	ASP	Sidechain

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	1629	0	1573	9	0
1	B	1596	0	1535	21	0
1	C	1632	0	1566	9	0
1	D	1606	0	1541	13	0
1	E	1615	0	1558	12	0
1	F	1630	0	1561	12	0
2	M	1921	0	1888	27	0
2	N	1924	0	1892	12	0
2	O	1913	0	1875	22	0
2	P	1922	0	1891	18	0
2	Q	1946	0	1932	28	0
2	R	1927	0	1896	15	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	10	0	0	0	0
3	R	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	2	0
4	B	8	0	12	7	0
4	C	4	0	6	0	0
4	D	8	0	12	7	0
4	E	12	0	18	3	0
4	F	8	0	12	8	0
4	M	24	0	36	5	0
4	N	8	0	12	1	0
4	O	12	0	18	7	0
4	P	20	0	30	1	0
4	R	8	0	12	3	0
5	A	42	0	55	3	0
5	B	24	0	32	10	0
5	C	30	0	39	2	0
5	D	30	0	40	2	0
5	E	30	0	40	7	0
5	F	24	0	32	0	0
5	M	36	0	48	18	0
5	N	18	0	24	1	0
5	O	30	0	40	1	0
5	P	24	0	32	4	0
5	Q	24	0	32	12	0
5	R	30	0	40	2	0
6	A	8	0	5	0	0
6	B	8	0	4	0	0
6	C	8	0	6	0	0
6	D	8	0	5	0	0
6	E	8	0	4	0	0
6	F	8	0	5	0	0
6	M	8	0	4	3	0
6	N	8	0	4	1	0
6	O	8	0	4	2	0
6	P	8	0	4	2	0
6	Q	8	0	4	2	0
6	R	8	0	4	2	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
8	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
9	A	166	0	0	2	0
9	B	156	0	0	0	0
9	C	169	0	0	1	0
9	D	166	0	0	6	0
9	E	145	0	0	3	0
9	F	182	0	0	4	0
9	M	230	0	0	7	0
9	N	211	0	0	1	0
9	O	218	0	0	0	0
9	P	229	0	0	0	0
9	Q	214	0	0	2	0
9	R	239	0	0	1	0
All	All	24211	0	21389	210	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.

The worst 5 of 210 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)
2:M:450[A]:ARG:NH1	5:M:14[A]:GOL:H32	1.26	1.40
2:M:450[A]:ARG:NH1	5:M:14[A]:GOL:C3	1.96	1.28
2:Q:450[A]:ARG:NH1	5:Q:540:GOL:H32	1.47	1.25
5:D:203:GOL:O1	9:D:1227:HOH:O	1.58	1.20
1:F:86[A]:GLU:OE2	9:F:1738:HOH:O	1.60	1.19

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	207/200 (104%)	202 (98%)	5 (2%)	0	100	100
1	B	202/200 (101%)	199 (98%)	3 (2%)	0	100	100
1	C	207/200 (104%)	204 (99%)	3 (1%)	0	100	100
1	D	204/200 (102%)	200 (98%)	4 (2%)	0	100	100
1	E	205/200 (102%)	202 (98%)	3 (2%)	0	100	100
1	F	206/200 (103%)	202 (98%)	4 (2%)	0	100	100
2	M	242/238 (102%)	236 (98%)	6 (2%)	0	100	100
2	N	243/238 (102%)	238 (98%)	5 (2%)	0	100	100
2	O	241/238 (101%)	236 (98%)	5 (2%)	0	100	100
2	P	243/238 (102%)	237 (98%)	6 (2%)	0	100	100
2	Q	247/238 (104%)	241 (98%)	6 (2%)	0	100	100
2	R	243/238 (102%)	239 (98%)	4 (2%)	0	100	100
All	All	2690/2628 (102%)	2636 (98%)	54 (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	172/163 (106%)	168 (98%)	4 (2%)	50	34
1	B	167/163 (102%)	167 (100%)	0	100	100
1	C	172/163 (106%)	172 (100%)	0	100	100
1	D	169/163 (104%)	166 (98%)	3 (2%)	59	45
1	E	170/163 (104%)	170 (100%)	0	100	100
1	F	171/163 (105%)	168 (98%)	3 (2%)	59	45
2	M	208/202 (103%)	203 (98%)	5 (2%)	49	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	209/202 (104%)	205 (98%)	4 (2%)	57	43
2	O	207/202 (102%)	203 (98%)	4 (2%)	57	43
2	P	209/202 (104%)	204 (98%)	5 (2%)	49	33
2	Q	213/202 (105%)	208 (98%)	5 (2%)	50	34
2	R	209/202 (104%)	204 (98%)	5 (2%)	49	33
All	All	2276/2190 (104%)	2238 (98%)	38 (2%)	62	48

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	473	LYS
2	R	399	MET
2	Q	534	HIS
1	F	180	LYS
2	R	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	N	530	GLN
1	E	87	ASN
1	E	90	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 121 ligands modelled in this entry, 11 are monoatomic - leaving 110 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	BME	E	208[A]	-	3,3,3	0.34	0	1,2,2	0.47	0
5	GOL	E	205	-	5,5,5	0.44	0	5,5,5	0.68	0
5	GOL	O	29[B]	-	5,5,5	0.38	0	5,5,5	0.37	0
5	GOL	O	1	-	5,5,5	0.54	0	5,5,5	0.53	0
5	GOL	B	207	-	5,5,5	0.39	0	5,5,5	0.90	0
5	GOL	R	15[B]	-	5,5,5	0.59	0	5,5,5	0.40	0
5	GOL	D	205	-	5,5,5	0.34	0	5,5,5	0.29	0
5	GOL	P	17[B]	-	5,5,5	0.38	0	5,5,5	0.28	0
5	GOL	A	204[B]	-	5,5,5	0.36	0	5,5,5	0.32	0
3	SO4	O	12	-	4,4,4	0.14	0	6,6,6	0.11	0
5	GOL	E	203[A]	-	5,5,5	0.38	0	5,5,5	0.75	0
5	GOL	C	204	-	5,5,5	0.37	0	5,5,5	0.59	0
5	GOL	B	203	-	5,5,5	0.23	0	5,5,5	0.71	0
5	GOL	F	203	-	5,5,5	0.42	0	5,5,5	0.28	0
4	BME	P	543	-	3,3,3	0.30	0	1,2,2	0.24	0
6	CAQ	F	206	-	8,8,8	1.95	1 (12%)	10,10,10	0.82	0
4	BME	R	21	-	3,3,3	0.41	0	1,2,2	0.38	0
5	GOL	N	1[B]	-	5,5,5	0.43	0	5,5,5	0.27	0
4	BME	O	9	-	3,3,3	0.43	0	1,2,2	0.23	0
5	GOL	Q	1	-	5,5,5	0.64	0	5,5,5	0.41	0
3	SO4	Q	10	-	4,4,4	0.12	0	6,6,6	0.22	0
4	BME	B	202	-	3,3,3	0.66	0	1,2,2	0.46	0
6	CAQ	O	4	7	8,8,8	1.85	1 (12%)	10,10,10	0.69	0
4	BME	N	18	-	3,3,3	0.52	0	1,2,2	0.27	0
4	BME	P	541	-	3,3,3	0.56	0	1,2,2	0.08	0
5	GOL	D	203	-	5,5,5	0.45	0	5,5,5	0.43	0
6	CAQ	N	3	7	8,8,8	1.75	1 (12%)	10,10,10	0.88	0
5	GOL	M	16	-	5,5,5	0.42	0	5,5,5	0.45	0
6	CAQ	M	539	7	8,8,8	1.74	1 (12%)	10,10,10	0.83	0
6	CAQ	C	206	-	8,8,8	2.05	1 (12%)	10,10,10	0.64	0
5	GOL	R	23	-	5,5,5	0.31	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	C	202[A]	-	5,5,5	1.05	0	5,5,5	1.50	1 (20%)
4	BME	M	1[A]	-	3,3,3	0.41	0	1,2,2	0.49	0
4	BME	D	207	-	3,3,3	0.34	0	1,2,2	0.50	0
3	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.21	0
4	BME	P	539[A]	-	3,3,3	0.49	0	1,2,2	0.80	0
4	BME	M	28	-	3,3,3	0.31	0	1,2,2	0.51	0
5	GOL	M	12	-	5,5,5	0.47	0	5,5,5	0.37	0
5	GOL	B	205[A]	-	5,5,5	0.27	0	5,5,5	0.40	0
5	GOL	A	203[A]	-	5,5,5	0.36	0	5,5,5	0.38	0
6	CAQ	Q	6	7	8,8,8	1.63	1 (12%)	10,10,10	0.83	0
4	BME	R	540	-	3,3,3	0.25	0	1,2,2	0.17	0
5	GOL	E	202	-	5,5,5	0.42	0	5,5,5	0.57	0
5	GOL	O	17	-	5,5,5	0.37	0	5,5,5	0.61	0
4	BME	O	540	-	3,3,3	0.41	0	1,2,2	0.66	0
4	BME	B	204	-	3,3,3	0.43	0	1,2,2	0.24	0
5	GOL	Q	15[A]	-	5,5,5	0.34	0	5,5,5	0.30	0
4	BME	E	208[B]	-	3,3,3	0.35	0	1,2,2	0.20	0
5	GOL	M	10[A]	-	5,5,5	0.36	0	5,5,5	0.14	0
4	BME	F	205	-	3,3,3	0.37	0	1,2,2	0.67	0
3	SO4	R	3	-	4,4,4	0.11	0	6,6,6	0.24	0
3	SO4	E	201	-	4,4,4	0.15	0	6,6,6	0.12	0
5	GOL	B	205[B]	-	5,5,5	0.41	0	5,5,5	0.54	0
5	GOL	A	205	-	5,5,5	0.46	0	5,5,5	0.57	0
5	GOL	E	203[B]	-	5,5,5	0.81	0	5,5,5	0.86	0
6	CAQ	P	542	7	8,8,8	1.75	1 (12%)	10,10,10	0.76	0
5	GOL	R	13[A]	-	5,5,5	0.33	0	5,5,5	0.51	0
5	GOL	M	14[A]	-	5,5,5	0.39	0	5,5,5	0.37	0
5	GOL	E	206	-	5,5,5	0.27	0	5,5,5	0.70	0
5	GOL	D	204[A]	-	5,5,5	0.33	0	5,5,5	0.41	0
4	BME	M	30[A]	-	3,3,3	0.36	0	1,2,2	0.20	0
6	CAQ	D	208	-	8,8,8	1.93	1 (12%)	10,10,10	0.73	0
6	CAQ	E	207	-	8,8,8	2.02	1 (12%)	10,10,10	0.55	0
4	BME	M	540	-	3,3,3	0.31	0	1,2,2	1.14	0
4	BME	N	8	-	3,3,3	0.30	0	1,2,2	0.22	0
5	GOL	F	202	-	5,5,5	0.32	0	5,5,5	0.55	0
5	GOL	C	202[B]	-	5,5,5	0.34	0	5,5,5	0.82	0
4	BME	M	1[B]	-	3,3,3	1.06	0	1,2,2	0.74	0
5	GOL	A	208	-	5,5,5	1.24	1 (20%)	5,5,5	1.17	0
5	GOL	P	540	-	5,5,5	0.42	0	5,5,5	0.74	0
5	GOL	M	14[B]	-	5,5,5	0.42	0	5,5,5	0.30	0
5	GOL	D	204[B]	-	5,5,5	0.36	0	5,5,5	0.31	0
5	GOL	P	17[A]	-	5,5,5	0.36	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BME	M	30[B]	-	3,3,3	0.37	0	1,2,2	0.70	0
6	CAQ	B	206	-	8,8,8	2.03	1 (12%)	10,10,10	0.57	0
5	GOL	A	204[A]	-	5,5,5	0.39	0	5,5,5	0.26	0
3	SO4	D	201	-	4,4,4	0.17	0	6,6,6	0.23	0
3	SO4	N	11	-	4,4,4	0.13	0	6,6,6	0.23	0
4	BME	P	539[B]	-	3,3,3	0.25	0	1,2,2	1.62	0
5	GOL	A	206	-	5,5,5	0.27	0	5,5,5	0.47	0
3	SO4	F	201	-	4,4,4	0.14	0	6,6,6	0.13	0
5	GOL	A	203[B]	-	5,5,5	0.29	0	5,5,5	0.75	0
4	BME	A	202	-	3,3,3	0.61	0	1,2,2	0.26	0
5	GOL	N	1[A]	-	5,5,5	0.43	0	5,5,5	0.31	0
5	GOL	C	203	-	5,5,5	0.50	0	5,5,5	0.93	0
5	GOL	C	207	-	5,5,5	1.56	1 (20%)	5,5,5	0.85	0
6	CAQ	R	1	7	8,8,8	1.85	1 (12%)	10,10,10	0.74	0
5	GOL	Q	540	-	5,5,5	0.55	0	5,5,5	0.90	0
4	BME	P	5	-	3,3,3	0.37	0	1,2,2	0.17	0
5	GOL	Q	15[B]	-	5,5,5	0.41	0	5,5,5	0.24	0
5	GOL	M	10[B]	-	5,5,5	0.29	0	5,5,5	0.58	0
3	SO4	P	2	-	4,4,4	0.13	0	6,6,6	0.15	0
5	GOL	P	1	-	5,5,5	0.45	0	5,5,5	0.59	0
5	GOL	F	204[A]	-	5,5,5	0.27	0	5,5,5	0.39	0
5	GOL	O	539	-	5,5,5	0.43	0	5,5,5	0.22	0
3	SO4	A	201	-	4,4,4	0.17	0	6,6,6	0.21	0
4	BME	O	542	-	3,3,3	0.28	0	1,2,2	2.02	1 (100%)
5	GOL	O	29[A]	-	5,5,5	0.39	0	5,5,5	0.27	0
5	GOL	R	15[A]	-	5,5,5	0.48	0	5,5,5	0.37	0
5	GOL	R	13[B]	-	5,5,5	0.37	0	5,5,5	0.23	0
6	CAQ	A	207	-	8,8,8	2.11	1 (12%)	10,10,10	0.58	0
3	SO4	Q	539	-	4,4,4	0.12	0	6,6,6	0.13	0
5	GOL	N	26	-	5,5,5	0.46	0	5,5,5	0.61	0
4	BME	F	207	-	3,3,3	0.49	0	1,2,2	0.07	0
4	BME	E	204	-	3,3,3	0.57	0	1,2,2	0.31	0
5	GOL	D	206	-	5,5,5	0.46	0	5,5,5	0.74	0
5	GOL	F	204[B]	-	5,5,5	0.35	0	5,5,5	0.28	0
4	BME	C	205	-	3,3,3	0.22	0	1,2,2	1.20	0
4	BME	D	202	-	3,3,3	0.68	0	1,2,2	0.29	0
3	SO4	B	201	-	4,4,4	0.15	0	6,6,6	0.17	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
4	BME	E	208[A]	-	-	1/1/1/1	-
5	GOL	E	205	-	-	2/4/4/4	-
5	GOL	O	29[B]	-	-	2/4/4/4	-
5	GOL	O	1	-	-	2/4/4/4	-
5	GOL	B	207	-	-	2/4/4/4	-
5	GOL	R	15[B]	-	-	4/4/4/4	-
5	GOL	D	205	-	-	0/4/4/4	-
5	GOL	P	17[B]	-	-	4/4/4/4	-
5	GOL	A	204[B]	-	-	2/4/4/4	-
5	GOL	E	203[A]	-	-	2/4/4/4	-
5	GOL	C	204	-	-	4/4/4/4	-
5	GOL	B	203	-	-	3/4/4/4	-
5	GOL	F	203	-	-	0/4/4/4	-
4	BME	P	543	-	-	1/1/1/1	-
6	CAQ	F	206	-	-	-	0/1/1/1
4	BME	R	21	-	-	0/1/1/1	-
5	GOL	N	1[B]	-	-	2/4/4/4	-
4	BME	O	9	-	-	1/1/1/1	-
5	GOL	Q	1	-	-	0/4/4/4	-
4	BME	B	202	-	-	0/1/1/1	-
6	CAQ	O	4	7	-	-	0/1/1/1
4	BME	N	18	-	-	1/1/1/1	-
4	BME	P	541	-	-	1/1/1/1	-
5	GOL	D	203	-	-	0/4/4/4	-
6	CAQ	N	3	7	-	-	0/1/1/1
5	GOL	M	16	-	-	2/4/4/4	-
6	CAQ	M	539	7	-	-	0/1/1/1
6	CAQ	C	206	-	-	-	0/1/1/1
5	GOL	R	23	-	-	2/4/4/4	-
5	GOL	C	202[A]	-	-	1/4/4/4	-
4	BME	M	1[A]	-	-	1/1/1/1	-
4	BME	D	207	-	-	0/1/1/1	-
4	BME	P	539[A]	-	-	1/1/1/1	-
4	BME	M	28	-	-	1/1/1/1	-
5	GOL	M	12	-	-	1/4/4/4	-
5	GOL	B	205[A]	-	-	2/4/4/4	-
5	GOL	A	203[A]	-	-	4/4/4/4	-
6	CAQ	Q	6	7	-	-	0/1/1/1
4	BME	R	540	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	202	-	-	3/4/4/4	-
5	GOL	O	17	-	-	2/4/4/4	-
4	BME	O	540	-	-	0/1/1/1	-
4	BME	B	204	-	-	1/1/1/1	-
5	GOL	Q	15[A]	-	-	2/4/4/4	-
4	BME	E	208[B]	-	-	0/1/1/1	-
5	GOL	M	10[A]	-	-	2/4/4/4	-
4	BME	F	205	-	-	0/1/1/1	-
5	GOL	B	205[B]	-	-	4/4/4/4	-
5	GOL	A	205	-	-	2/4/4/4	-
5	GOL	E	203[B]	-	-	4/4/4/4	-
6	CAQ	P	542	7	-	-	0/1/1/1
5	GOL	R	13[A]	-	-	2/4/4/4	-
5	GOL	M	14[A]	-	-	4/4/4/4	-
5	GOL	E	206	-	-	3/4/4/4	-
5	GOL	D	204[A]	-	-	3/4/4/4	-
4	BME	M	30[A]	-	-	1/1/1/1	-
6	CAQ	D	208	-	-	-	0/1/1/1
6	CAQ	E	207	-	-	-	0/1/1/1
4	BME	M	540	-	-	0/1/1/1	-
4	BME	N	8	-	-	0/1/1/1	-
5	GOL	F	202	-	-	4/4/4/4	-
5	GOL	C	202[B]	-	-	2/4/4/4	-
4	BME	M	1[B]	-	-	0/1/1/1	-
5	GOL	A	208	-	-	2/4/4/4	-
5	GOL	P	540	-	-	1/4/4/4	-
5	GOL	M	14[B]	-	-	2/4/4/4	-
5	GOL	D	204[B]	-	-	0/4/4/4	-
5	GOL	P	17[A]	-	-	1/4/4/4	-
4	BME	M	30[B]	-	-	0/1/1/1	-
6	CAQ	B	206	-	-	-	0/1/1/1
5	GOL	A	204[A]	-	-	0/4/4/4	-
4	BME	P	539[B]	-	-	1/1/1/1	-
5	GOL	A	206	-	-	2/4/4/4	-
5	GOL	A	203[B]	-	-	4/4/4/4	-
4	BME	A	202	-	-	1/1/1/1	-
5	GOL	N	1[A]	-	-	4/4/4/4	-
5	GOL	C	203	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	207	-	-	2/4/4/4	-
6	CAQ	R	1	7	-	-	0/1/1/1
5	GOL	Q	540	-	-	4/4/4/4	-
4	BME	P	5	-	-	1/1/1/1	-
5	GOL	Q	15[B]	-	-	2/4/4/4	-
5	GOL	M	10[B]	-	-	3/4/4/4	-
5	GOL	P	1	-	-	2/4/4/4	-
5	GOL	F	204[A]	-	-	4/4/4/4	-
5	GOL	O	539	-	-	4/4/4/4	-
4	BME	O	542	-	-	1/1/1/1	-
5	GOL	O	29[A]	-	-	4/4/4/4	-
5	GOL	R	15[A]	-	-	4/4/4/4	-
5	GOL	R	13[B]	-	-	1/4/4/4	-
6	CAQ	A	207	-	-	-	0/1/1/1
5	GOL	N	26	-	-	2/4/4/4	-
4	BME	F	207	-	-	1/1/1/1	-
4	BME	E	204	-	-	1/1/1/1	-
5	GOL	D	206	-	-	0/4/4/4	-
5	GOL	F	204[B]	-	-	0/4/4/4	-
4	BME	C	205	-	-	0/1/1/1	-
4	BME	D	202	-	-	1/1/1/1	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	207	CAQ	C4-C3	5.65	1.49	1.40
6	B	206	CAQ	C4-C3	5.63	1.49	1.40
6	E	207	CAQ	C4-C3	5.56	1.49	1.40
6	C	206	CAQ	C4-C3	5.53	1.49	1.40
6	F	206	CAQ	C4-C3	5.27	1.48	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	202[A]	GOL	O1-C1-C2	-2.72	97.16	110.20
4	O	542	BME	O1-C1-C2	-2.02	102.88	110.83

There are no chirality outliers.

5 of 145 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	28	BME	O1-C1-C2-S2
4	M	1[A]	BME	O1-C1-C2-S2
4	N	18	BME	O1-C1-C2-S2
4	D	202	BME	O1-C1-C2-S2
4	P	5	BME	O1-C1-C2-S2

There are no ring outliers.

47 monomers are involved in 117 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	205	GOL	3	0
5	O	1	GOL	1	0
5	B	207	GOL	2	0
5	P	17[B]	GOL	1	0
5	E	203[A]	GOL	1	0
5	C	204	GOL	1	0
5	B	203	GOL	4	0
5	Q	1	GOL	1	0
4	B	202	BME	7	0
6	O	4	CAQ	2	0
5	D	203	GOL	1	0
6	N	3	CAQ	1	0
5	M	16	GOL	4	0
6	M	539	CAQ	3	0
5	C	202[A]	GOL	1	0
4	M	1[A]	BME	2	0
4	D	207	BME	1	0
4	M	28	BME	1	0
5	B	205[A]	GOL	2	0
6	Q	6	CAQ	2	0
4	R	540	BME	3	0
5	Q	15[A]	GOL	2	0
5	M	10[A]	GOL	2	0
5	B	205[B]	GOL	2	0
6	P	542	CAQ	2	0
5	M	14[A]	GOL	7	0
5	E	206	GOL	3	0
4	M	540	BME	1	0
4	N	8	BME	1	0
4	M	1[B]	BME	1	0
5	M	14[B]	GOL	3	0
5	D	204[B]	GOL	1	0
5	P	17[A]	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	204[A]	GOL	1	0
4	P	539[B]	BME	1	0
5	A	206	GOL	2	0
4	A	202	BME	2	0
5	N	1[A]	GOL	1	0
6	R	1	CAQ	2	0
5	Q	540	GOL	8	0
5	Q	15[B]	GOL	1	0
5	M	10[B]	GOL	2	0
4	O	542	BME	7	0
5	R	13[B]	GOL	2	0
4	F	207	BME	8	0
4	E	204	BME	3	0
4	D	202	BME	6	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, 95^{th} 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%)	-0.35	1 (0%) 91 91	13, 18, 30, 40	4 (2%)
1	B	200/200 (100%)	-0.18	3 (1%) 73 73	14, 24, 37, 50	2 (1%)
1	C	200/200 (100%)	-0.41	0 100 100	13, 18, 28, 33	1 (0%)
1	D	200/200 (100%)	-0.39	1 (0%) 91 91	13, 19, 31, 45	0
1	E	200/200 (100%)	-0.18	3 (1%) 73 73	14, 24, 37, 49	3 (1%)
1	F	200/200 (100%)	-0.44	0 100 100	13, 18, 28, 32	1 (0%)
2	M	238/238 (100%)	-0.45	1 (0%) 92 92	13, 17, 25, 40	2 (0%)
2	N	238/238 (100%)	-0.37	3 (1%) 77 77	14, 19, 29, 44	2 (0%)
2	O	238/238 (100%)	-0.46	1 (0%) 92 92	14, 17, 26, 39	1 (0%)
2	P	238/238 (100%)	-0.45	2 (0%) 86 86	14, 17, 26, 40	0
2	Q	238/238 (100%)	-0.41	3 (1%) 77 77	14, 19, 29, 42	1 (0%)
2	R	238/238 (100%)	-0.45	1 (0%) 92 92	14, 17, 25, 36	4 (1%)
All	All	2628/2628 (100%)	-0.38	19 (0%) 87 88	13, 18, 30, 50	21 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	538	CYS	5.2
2	R	538	CYS	4.0
2	M	538	CYS	3.9
2	Q	538	CYS	3.7
2	O	538	CYS	3.5

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	BME	O	542	4/4	0.35	0.35	34,35,37,38	4
5	GOL	M	10[A]	6/6	0.60	0.23	42,43,44,44	6
5	GOL	M	10[B]	6/6	0.60	0.23	28,31,31,33	6
4	BME	M	30[B]	4/4	0.69	0.29	45,45,46,48	4
4	BME	M	30[A]	4/4	0.69	0.29	38,39,40,42	4
4	BME	F	205	4/4	0.71	0.15	57,57,57,58	0
5	GOL	R	23	6/6	0.73	0.17	52,53,54,54	0
4	BME	E	204	4/4	0.75	0.24	38,43,44,48	4
4	BME	C	205	4/4	0.76	0.20	44,45,45,48	0
5	GOL	E	203[A]	6/6	0.79	0.21	50,52,52,52	6
5	GOL	E	203[B]	6/6	0.79	0.21	50,52,52,52	6
5	GOL	Q	540	6/6	0.79	0.16	33,34,35,36	6
5	GOL	B	203	6/6	0.79	0.19	44,47,48,48	0
5	GOL	Q	1	6/6	0.81	0.19	37,43,45,46	0
4	BME	P	539[A]	4/4	0.82	0.20	42,44,45,47	4
4	BME	P	539[B]	4/4	0.82	0.20	28,32,33,34	4
5	GOL	Q	15[A]	6/6	0.83	0.19	30,31,32,33	6
5	GOL	Q	15[B]	6/6	0.83	0.19	47,48,48,49	6
5	GOL	O	539	6/6	0.83	0.15	47,49,50,50	0
4	BME	B	204	4/4	0.83	0.12	41,43,44,48	4
4	BME	O	9	4/4	0.83	0.14	56,57,57,59	0
5	GOL	M	12	6/6	0.84	0.18	39,44,44,48	0
5	GOL	M	14[A]	6/6	0.84	0.24	19,19,19,20	6
5	GOL	D	203	6/6	0.84	0.19	27,27,30,30	6
5	GOL	P	17[A]	6/6	0.84	0.16	36,37,37,38	6
5	GOL	P	17[B]	6/6	0.84	0.16	41,42,43,43	6
5	GOL	F	202	6/6	0.84	0.15	46,51,53,53	0
5	GOL	M	14[B]	6/6	0.84	0.24	20,21,21,23	6
5	GOL	O	1	6/6	0.86	0.18	30,36,38,40	0
5	GOL	E	205	6/6	0.86	0.19	47,49,49,49	0
4	BME	A	202	4/4	0.86	0.16	68,68,68,70	0
5	GOL	A	205	6/6	0.86	0.18	31,34,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BME	M	1[A]	4/4	0.87	0.16	32,35,35,37	4
4	BME	R	21	4/4	0.87	0.14	63,63,63,63	0
5	GOL	E	202	6/6	0.87	0.15	40,42,43,48	0
4	BME	M	1[B]	4/4	0.87	0.16	45,46,46,47	4
3	SO4	O	12	5/5	0.87	0.14	58,59,59,59	5
5	GOL	D	206	6/6	0.87	0.17	38,44,47,48	0
3	SO4	Q	539	5/5	0.88	0.13	63,63,63,64	5
5	GOL	O	17	6/6	0.88	0.15	30,39,41,44	0
5	GOL	E	206	6/6	0.88	0.14	42,47,48,49	0
5	GOL	O	29[A]	6/6	0.89	0.14	39,41,41,41	6
5	GOL	O	29[B]	6/6	0.89	0.14	36,37,38,38	6
3	SO4	P	2	5/5	0.89	0.19	55,55,56,56	5
5	GOL	M	16	6/6	0.89	0.13	36,44,45,46	0
4	BME	N	18	4/4	0.89	0.15	52,52,52,56	0
5	GOL	D	204[A]	6/6	0.89	0.15	20,23,24,26	6
5	GOL	D	204[B]	6/6	0.89	0.15	34,36,37,38	6
5	GOL	C	202[A]	6/6	0.89	0.19	33,34,35,35	6
5	GOL	C	202[B]	6/6	0.89	0.19	30,30,31,32	6
4	BME	N	8	4/4	0.89	0.09	52,52,52,54	0
5	GOL	F	204[A]	6/6	0.89	0.13	29,32,32,33	6
5	GOL	F	204[B]	6/6	0.89	0.13	28,35,36,38	6
5	GOL	P	1	6/6	0.89	0.17	38,42,43,46	0
5	GOL	A	206	6/6	0.90	0.15	44,46,48,51	0
5	GOL	N	1[A]	6/6	0.90	0.16	24,29,29,30	6
5	GOL	R	15[A]	6/6	0.90	0.20	32,34,35,37	6
5	GOL	R	15[B]	6/6	0.90	0.20	21,27,28,32	6
5	GOL	N	1[B]	6/6	0.90	0.16	40,41,41,41	6
5	GOL	R	13[A]	6/6	0.90	0.14	30,32,33,33	6
5	GOL	R	13[B]	6/6	0.90	0.14	35,37,37,38	6
6	CAQ	M	539	8/8	0.90	0.15	20,21,22,22	8
6	CAQ	N	3	8/8	0.90	0.16	23,25,26,28	8
6	CAQ	C	206	8/8	0.90	0.10	32,33,33,34	0
6	CAQ	P	542	8/8	0.90	0.16	19,22,23,23	8
4	BME	D	202	4/4	0.91	0.14	68,68,69,69	0
4	BME	O	540	4/4	0.91	0.10	32,35,35,37	4
5	GOL	P	540	6/6	0.91	0.14	28,38,40,43	0
3	SO4	N	11	5/5	0.91	0.24	50,50,51,51	5
4	BME	P	541	4/4	0.91	0.07	49,51,52,53	0
5	GOL	C	203	6/6	0.91	0.15	29,37,39,39	0
5	GOL	F	203	6/6	0.92	0.17	28,34,36,39	0
4	BME	P	5	4/4	0.92	0.15	61,62,63,63	0
6	CAQ	D	208	8/8	0.92	0.13	29,32,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BME	M	28	4/4	0.92	0.12	39,39,39,41	4
8	CL	R	539	1/1	0.92	0.20	54,54,54,54	0
4	BME	M	540	4/4	0.93	0.14	41,42,43,43	0
5	GOL	B	207	6/6	0.93	0.13	31,32,33,37	0
3	SO4	Q	10	5/5	0.93	0.21	51,51,51,52	5
6	CAQ	R	1	8/8	0.93	0.11	21,22,22,23	8
8	CL	M	2	1/1	0.93	0.09	59,59,59,59	0
3	SO4	R	3	5/5	0.93	0.17	50,52,52,53	5
6	CAQ	A	207	8/8	0.94	0.12	28,32,33,35	0
5	GOL	D	205	6/6	0.94	0.08	36,40,41,41	0
6	CAQ	B	206	8/8	0.94	0.10	36,37,38,39	0
5	GOL	N	26	6/6	0.94	0.12	44,47,49,50	0
5	GOL	A	203[A]	6/6	0.94	0.12	29,31,31,32	6
6	CAQ	O	4	8/8	0.94	0.10	21,22,22,23	8
5	GOL	A	203[B]	6/6	0.94	0.12	15,20,22,23	6
4	BME	E	208[A]	4/4	0.94	0.09	36,37,37,38	4
6	CAQ	Q	6	8/8	0.94	0.16	22,23,24,25	8
5	GOL	B	205[A]	6/6	0.94	0.12	28,28,30,32	6
5	GOL	B	205[B]	6/6	0.94	0.12	34,35,36,36	6
8	CL	Q	541	1/1	0.94	0.05	46,46,46,46	0
4	BME	E	208[B]	4/4	0.94	0.09	33,35,35,38	4
3	SO4	A	201	5/5	0.95	0.13	39,41,42,42	5
3	SO4	C	201	5/5	0.95	0.17	49,50,51,51	5
5	GOL	C	204	6/6	0.95	0.08	37,42,43,45	0
6	CAQ	E	207	8/8	0.95	0.10	37,38,39,40	0
4	BME	B	202	4/4	0.95	0.08	46,47,47,50	0
6	CAQ	F	206	8/8	0.95	0.13	32,33,33,33	0
3	SO4	B	201	5/5	0.95	0.13	49,50,51,51	5
3	SO4	F	201	5/5	0.95	0.15	47,48,48,49	5
8	CL	N	539	1/1	0.95	0.09	45,45,45,45	0
8	CL	O	541	1/1	0.95	0.07	47,47,47,47	0
3	SO4	D	201	5/5	0.95	0.12	44,45,46,47	5
5	GOL	A	208	6/6	0.95	0.14	20,20,20,20	0
3	SO4	E	201	5/5	0.96	0.14	52,52,53,54	5
5	GOL	A	204[A]	6/6	0.96	0.15	33,34,35,35	6
5	GOL	A	204[B]	6/6	0.96	0.15	26,27,29,30	6
4	BME	D	207	4/4	0.96	0.16	47,48,48,50	0
4	BME	P	543	4/4	0.97	0.20	20,20,20,20	0
4	BME	F	207	4/4	0.97	0.23	20,20,20,20	0
7	FE	M	600	1/1	0.98	0.04	20,20,20,20	1
4	BME	R	540	4/4	0.98	0.24	20,20,20,20	0
5	GOL	C	207	6/6	0.98	0.08	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	FE	N	600	1/1	0.99	0.04	21,21,21,21	1
7	FE	O	600	1/1	0.99	0.04	21,21,21,21	1
7	FE	P	600	1/1	0.99	0.05	21,21,21,21	1
7	FE	Q	600	1/1	0.99	0.06	21,21,21,21	1
7	FE	R	600	1/1	0.99	0.07	22,22,22,22	1

6.5 Other polymers (i)

There are no such residues in this entry.