



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:22 AM GMT

PDB ID : 3LKT  
Title : Tyrosine 447 of Protocatechuate 3,4-Dioxygenase Controls Efficient Progress Through Catalysis  
Authors : Lipscomb, J.D.; Purpero, V.M.  
Deposited on : 2010-01-27  
Resolution : 1.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

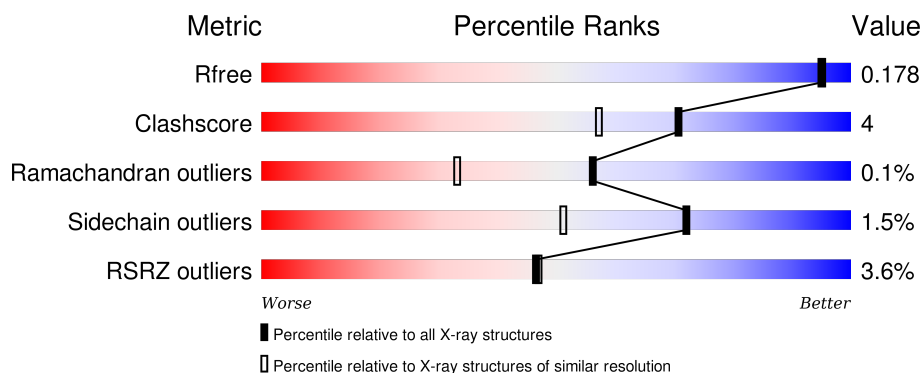
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
1	B	200	<div> <div>8%</div> <div>94%</div> <div>7%</div> </div>
1	C	200	<div> <div>5%</div> <div>91%</div> <div>9%</div> </div>
1	D	200	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>
1	E	200	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	200	
2	M	238	
2	N	238	
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

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	A	202	-	-	-	X
4	BME	C	203	-	-	-	X
4	BME	M	21[A]	-	-	-	X
4	BME	M	21[B]	-	-	-	X
4	BME	M	21[C]	-	-	X	X
4	BME	M	29	-	-	-	X
4	BME	M	36	-	-	-	X
4	BME	N	18	-	-	X	X
4	BME	N	32[A]	-	-	-	X
4	BME	N	32[B]	-	-	-	X
4	BME	N	44	-	-	-	X
4	BME	O	33	-	-	X	X
4	BME	O	42	-	-	-	X
4	BME	O	45	-	-	-	X
4	BME	P	22[A]	-	-	X	X
4	BME	P	22[B]	-	-	-	X
4	BME	P	40	-	-	-	X
4	BME	Q	19	-	-	X	X
4	BME	Q	24	-	-	-	X
4	BME	Q	34[A]	-	-	-	X
4	BME	Q	34[B]	-	-	-	X
4	BME	R	20	-	-	X	X
4	BME	R	28	-	-	-	X
4	BME	R	43	-	-	-	X
5	TRS	A	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TRS	B	202	-	-	-	X
5	TRS	D	202	-	-	-	X
5	TRS	E	202	-	-	-	X
5	TRS	F	202	-	-	-	X
7	CL	M	7	-	-	-	X
8	GOL	M	16	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23995 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	0	0
			1575	996	277	299	3			
1	B	200	Total	C	N	O	S	0	2	0
			1591	1005	282	301	3			
1	C	200	Total	C	N	O	S	0	10	0
			1640	1037	287	313	3			
1	D	200	Total	C	N	O	S	0	1	0
			1586	1002	281	300	3			
1	E	200	Total	C	N	O	S	0	2	0
			1591	1004	280	304	3			
1	F	200	Total	C	N	O	S	0	11	0
			1646	1041	287	315	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	3	0
			1893	1199	347	339	8			
2	N	238	Total	C	N	O	S	0	2	0
			1889	1197	346	338	8			
2	O	238	Total	C	N	O	S	0	1	0
			1885	1193	346	338	8			
2	P	238	Total	C	N	O	S	0	2	0
			1890	1196	347	339	8			
2	Q	238	Total	C	N	O	S	0	3	0
			1904	1203	352	341	8			
2	R	238	Total	C	N	O	S	0	2	0
			1892	1198	347	339	8			

There are 6 discrepancies between the modelled and reference sequences:

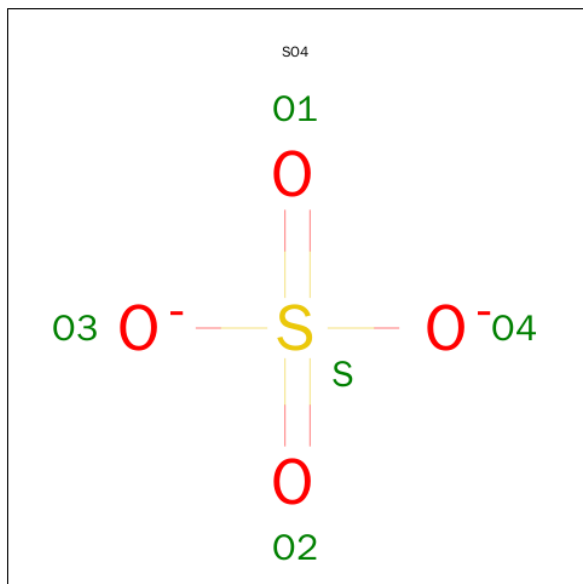
Chain	Residue	Modelled	Actual	Comment	Reference
M	447	HIS	TYR	ENGINEERED	UNP P00437

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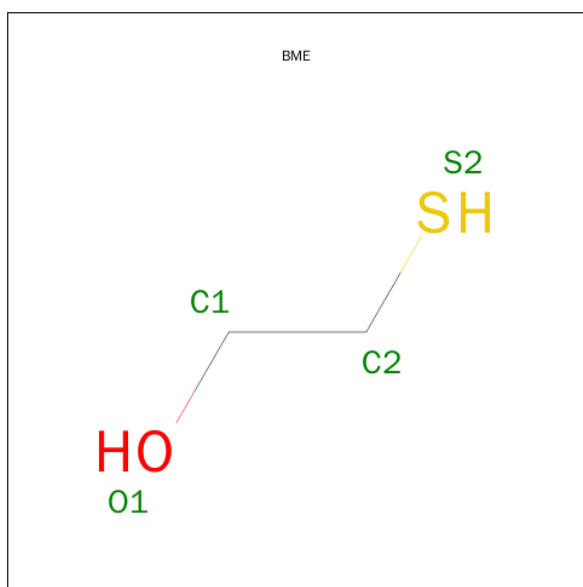
Chain	Residue	Modelled	Actual	Comment	Reference
N	447	HIS	TYR	ENGINEERED	UNP P00437
O	447	HIS	TYR	ENGINEERED	UNP P00437
P	447	HIS	TYR	ENGINEERED	UNP P00437
Q	447	HIS	TYR	ENGINEERED	UNP P00437
R	447	HIS	TYR	ENGINEERED	UNP P00437

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	M	1	Total	C	O	S	0	1
			12	6	3	3		
4	M	1	Total	C	O	S	0	0
			4	2	1	1		
4	M	1	Total	C	O	S	0	0
			4	2	1	1		
4	M	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	1
			8	4	2	2		
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	O	1	Total	C	O	S	0	0
			4	2	1	1		

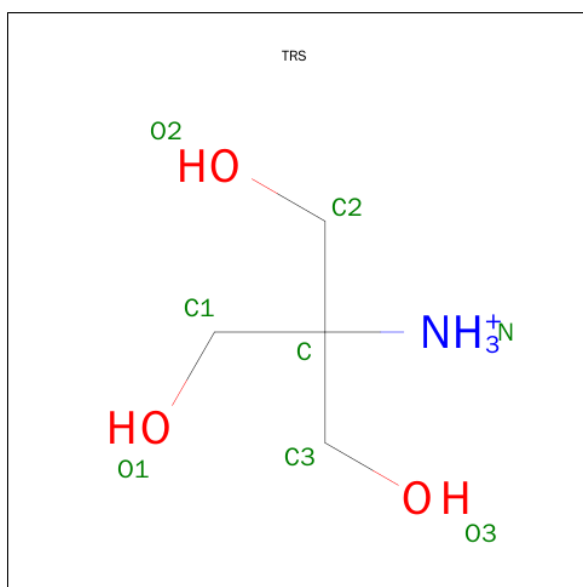
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	O	1	Total 4	C 2	O 1	S 1	0	0
4	O	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 8	C 4	O 2	S 2	0	1
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0
4	Q	1	Total 4	C 2	O 1	S 1	0	0
4	Q	1	Total 4	C 2	O 1	S 1	0	0
4	Q	1	Total 8	C 4	O 2	S 2	0	1
4	Q	1	Total 4	C 2	O 1	S 1	0	0
4	R	1	Total 4	C 2	O 1	S 1	0	0
4	R	1	Total 4	C 2	O 1	S 1	0	0
4	R	1	Total 4	C 2	O 1	S 1	0	0
4	R	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	D	1	Total	C	N	O	0	0
			8	4	1	3		
5	E	1	Total	C	N	O	0	0
			8	4	1	3		
5	F	1	Total	C	N	O	0	0
			8	4	1	3		

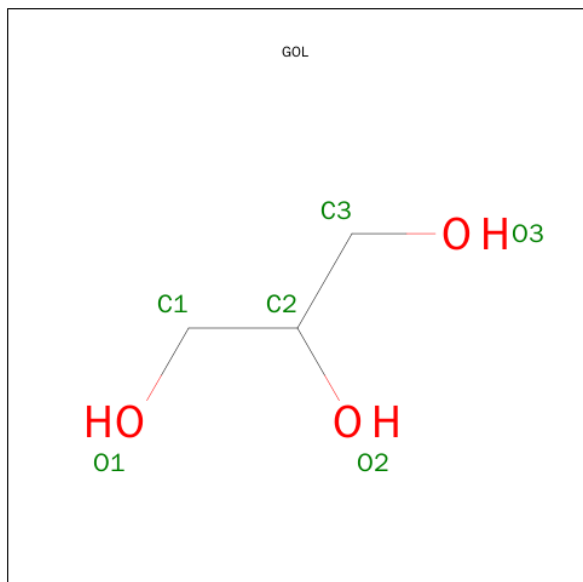
- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	1	Total Cl 1 1	0	0
7	Q	1	Total Cl 1 1	0	0
7	N	1	Total Cl 1 1	0	0
7	O	1	Total Cl 1 1	0	0
7	R	1	Total Cl 1 1	0	0
7	M	4	Total Cl 4 4	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	213	Total O 214 214	0	1
9	M	288	Total O 289 289	0	1

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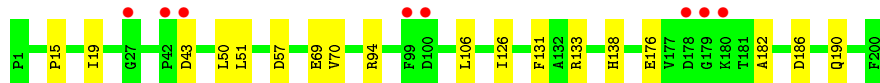
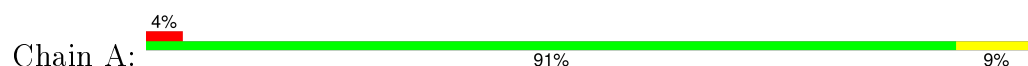
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	190	Total 190	O 190	0	0
9	N	264	Total 265	O 265	0	1
9	C	202	Total 203	O 203	0	1
9	O	257	Total 257	O 257	0	0
9	D	191	Total 192	O 192	0	1
9	P	270	Total 271	O 271	0	1
9	E	173	Total 174	O 174	0	1
9	Q	250	Total 251	O 251	0	1
9	F	201	Total 201	O 201	0	0
9	R	260	Total 261	O 261	0	1

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

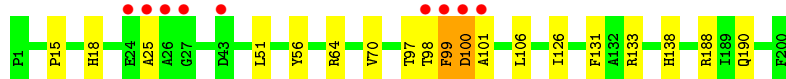
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



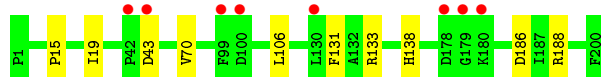
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



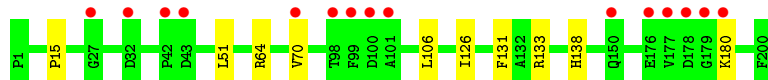
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



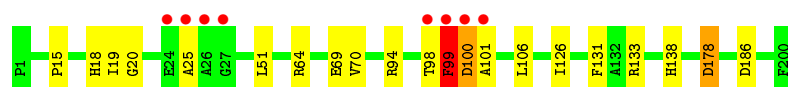
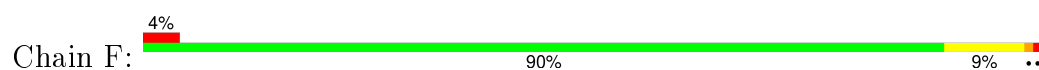
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



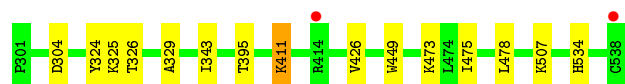
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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



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



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



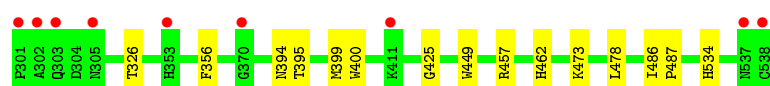
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.31Å 168.04Å 128.16Å 90.00° 132.30° 90.00°	Depositor
Resolution (Å)	29.57 – 1.65 29.30 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.57-1.65) 98.2 (29.30-1.65)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.148 , 0.173 0.153 , 0.178	Depositor DCC
$R_{free}$ test set	17677 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.3	EDS
Estimated twinning fraction	0.480 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 351443 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL, BME, SO4, TRS, FE

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	0.61	0/1615	0.65	0/2199
1	B	0.55	0/1634	0.62	0/2224
1	C	0.56	0/1690	0.72	0/2301
1	D	0.59	0/1626	0.65	0/2213
1	E	0.55	0/1631	0.62	0/2221
1	F	0.59	0/1699	0.72	1/2313 (0.0%)
2	M	0.57	0/1958	0.68	0/2664
2	N	0.57	0/1951	0.68	0/2655
2	O	0.57	0/1944	0.67	0/2645
2	P	0.56	0/1952	0.68	0/2656
2	Q	0.57	0/1963	0.67	0/2670
2	R	0.56	0/1951	0.67	0/2655
All	All	0.57	0/21614	0.67	1/29416 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	178	ASP	CB-CG-OD1	5.54	123.28	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1575	0	1510	18	0
1	B	1591	0	1528	15	0
1	C	1640	0	1574	38	0
1	D	1586	0	1522	13	0
1	E	1591	0	1518	11	0
1	F	1646	0	1580	32	0
2	M	1893	0	1856	12	0
2	N	1889	0	1852	5	0
2	O	1885	0	1843	10	0
2	P	1890	0	1849	10	0
2	Q	1904	0	1860	11	0
2	R	1892	0	1851	14	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
4	A	4	0	6	2	0
4	C	4	0	6	3	0
4	M	24	0	34	11	0
4	N	20	0	26	14	0
4	O	24	0	34	10	0
4	P	36	0	52	11	0
4	Q	20	0	26	13	0
4	R	16	0	22	13	0
5	A	8	0	12	1	0
5	B	8	0	12	1	0
5	D	8	0	12	4	0
5	E	8	0	12	0	0
5	F	8	0	12	1	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
7	M	4	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	6	0	8	0	0
8	M	6	0	8	1	0
9	A	214	0	0	0	0
9	B	190	0	0	1	0
9	C	203	0	0	3	0
9	D	192	0	0	0	0
9	E	174	0	0	1	0
9	F	201	0	0	2	0
9	M	289	0	0	2	0
9	N	265	0	0	4	0
9	O	257	0	0	3	0
9	P	271	0	0	5	0
9	Q	251	0	0	2	0
9	R	261	0	0	5	0
All	All	23995	0	20625	185	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 (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99[B]:PHE:HD2	1:C:99[B]:PHE:N	1.25	1.23
1:F:99[A]:PHE:HD1	1:F:99[A]:PHE:N	1.46	1.12
1:C:99[B]:PHE:CD2	1:C:99[B]:PHE:N	2.02	1.10
4:Q:34[B]:BME:H22	9:Q:623:HOH:O	1.55	1.03
1:C:133:ARG:CD	4:O:33:BME:H12	1.93	0.97
1:C:133:ARG:HG3	4:O:33:BME:C1	1.94	0.97
1:B:133:ARG:HD2	4:N:18:BME:H12	1.50	0.94
1:B:133:ARG:CD	4:N:18:BME:H12	1.97	0.94
4:O:45:BME:S2	9:O:2610:HOH:O	2.25	0.92
1:F:133:ARG:HG3	4:R:20:BME:H11	1.52	0.91
1:D:133:ARG:HG3	4:P:22[A]:BME:H12	1.51	0.91
1:C:133:ARG:CG	4:O:33:BME:H12	2.04	0.88
1:C:133:ARG:HG3	4:O:33:BME:H12	1.55	0.87
1:F:99[A]:PHE:N	1:F:99[A]:PHE:CD1	2.19	0.87
1:C:98[B]:THR:HB	1:C:99[B]:PHE:CE2	2.12	0.84
4:R:43:BME:S2	9:R:2611:HOH:O	2.23	0.84
1:F:133:ARG:CD	4:R:20:BME:H11	2.09	0.82
1:E:133:ARG:HG3	4:Q:19:BME:H11	1.62	0.81
2:M:324:TYR:HE1	4:M:21[C]:BME:H22	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99[B]:PHE:CE1	2:O:411:LYS:HD2	2.15	0.81
1:B:133:ARG:HG3	4:N:18:BME:C1	2.11	0.81
1:C:133:ARG:HG3	4:O:33:BME:H11	1.61	0.80
4:M:21[C]:BME:H12	9:M:2291:HOH:O	1.79	0.80
1:F:133:ARG:CG	4:R:20:BME:H11	2.10	0.80
1:C:133:ARG:HD2	4:O:33:BME:H12	1.61	0.80
1:C:18:HIS:CE1	9:C:2667:HOH:O	2.35	0.79
4:P:40:BME:H22	9:P:21:HOH:O	1.83	0.78
1:D:186:ASP:H	5:D:202:TRS:H22	1.49	0.78
1:F:99[A]:PHE:CE2	2:R:411:LYS:HD2	2.20	0.77
1:E:133:ARG:CD	4:Q:19:BME:H11	2.14	0.77
1:B:99:PHE:HE2	9:B:2671:HOH:O	1.68	0.77
4:N:32[A]:BME:H22	9:N:2285:HOH:O	1.85	0.76
2:Q:462:HIS:CE1	4:Q:34[B]:BME:H21	2.21	0.75
1:B:133:ARG:HG3	4:N:18:BME:H11	1.66	0.75
1:A:133:ARG:HG3	4:M:21[B]:BME:H11	1.68	0.74
1:F:19:ILE:HG22	2:R:426[A]:VAL:HG22	1.67	0.74
4:P:23:BME:S2	9:P:2294:HOH:O	2.45	0.72
1:C:100[A]:ASP:N	1:C:100[A]:ASP:OD1	2.21	0.72
1:C:99[B]:PHE:HD2	1:C:99[B]:PHE:H	0.76	0.71
1:F:18:HIS:CE1	9:F:2668:HOH:O	2.43	0.71
1:A:133:ARG:HG3	4:M:21[C]:BME:H21	1.72	0.71
1:E:133:ARG:CG	4:Q:19:BME:H11	2.20	0.70
1:D:186:ASP:H	5:D:202:TRS:C2	2.04	0.70
2:O:374:ILE:HD12	2:R:374:ILE:HD12	1.72	0.70
1:D:133:ARG:HD2	4:P:22[A]:BME:O1	1.94	0.68
2:N:462:HIS:CE1	4:N:32[A]:BME:H21	2.27	0.68
1:B:186:ASP:HB2	5:B:202:TRS:H21	1.76	0.68
2:P:455:ASP:OD1	4:P:40:BME:H21	1.93	0.68
4:N:44:BME:S2	9:N:2609:HOH:O	2.52	0.67
1:E:64:ARG:HD2	9:E:2251:HOH:O	1.94	0.67
1:C:25:ALA:HB1	1:C:98[B]:THR:HG21	1.77	0.67
1:B:133:ARG:CG	4:N:18:BME:H12	2.24	0.67
1:E:133:ARG:HG2	2:Q:326[A]:THR:HG21	1.77	0.66
1:B:133:ARG:HG2	2:N:326[A]:THR:HG21	1.78	0.65
1:C:133:ARG:CG	4:O:33:BME:C1	2.69	0.64
1:B:133:ARG:HG3	4:N:18:BME:H12	1.79	0.64
2:P:407:ARG:HH12	4:P:35:BME:H12	1.61	0.64
1:C:64[B]:ARG:O	1:C:97[B]:THR:O	2.17	0.63
1:F:51:LEU:HD11	1:F:126:ILE:CD1	2.28	0.63
1:F:133:ARG:HD2	4:R:20:BME:C1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PRO:HD2	4:N:32[B]:BME:H11	1.81	0.63
1:C:64[A]:ARG:HB3	1:C:99[A]:PHE:HA	1.80	0.62
1:C:56:TYR:HB3	4:C:203:BME:H11	1.79	0.62
1:A:15:PRO:HD2	4:M:29:BME:H11	1.80	0.62
1:C:98[B]:THR:HB	1:C:99[B]:PHE:CD2	2.36	0.61
1:D:188:ARG:HH12	5:D:202:TRS:H32	1.65	0.60
1:F:133:ARG:HD2	4:R:20:BME:H11	1.83	0.59
1:F:15:PRO:HD2	4:R:28:BME:H11	1.83	0.59
4:R:20:BME:H22	9:R:2289:HOH:O	2.03	0.59
1:D:15:PRO:HD2	4:P:31:BME:H11	1.84	0.58
1:D:133:ARG:HG3	4:P:22[A]:BME:C1	2.30	0.58
1:F:70:VAL:HG11	1:F:106:LEU:HD11	1.85	0.57
1:C:70:VAL:HG11	1:C:106:LEU:HD11	1.85	0.57
1:F:99[A]:PHE:CZ	2:R:411:LYS:HD2	2.40	0.57
1:A:133:ARG:HG2	2:M:326:THR:HG21	1.87	0.56
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.35	0.56
1:C:99[B]:PHE:CZ	2:O:411:LYS:HD2	2.40	0.56
1:E:133:ARG:HD2	4:Q:19:BME:H11	1.88	0.56
1:C:98[B]:THR:O	1:C:99[B]:PHE:C	2.44	0.56
1:C:98[B]:THR:C	1:C:99[B]:PHE:HD2	2.04	0.55
1:F:64[B]:ARG:HH21	1:F:99[B]:PHE:HB3	1.71	0.55
1:F:18:HIS:CG	9:F:2295:HOH:O	2.59	0.55
4:Q:19:BME:H22	9:Q:2452:HOH:O	2.06	0.55
1:F:19:ILE:CG2	2:R:426[A]:VAL:HG22	2.37	0.54
1:C:18:HIS:CG	9:C:2296:HOH:O	2.60	0.54
1:F:133:ARG:CD	4:R:20:BME:C1	2.82	0.53
1:D:133:ARG:HG2	2:P:326[A]:THR:HG21	1.90	0.53
4:P:22[B]:BME:H12	9:P:2286:HOH:O	2.09	0.53
1:E:15:PRO:HD2	4:Q:34[A]:BME:H11	1.89	0.53
2:P:324:TYR:HE1	4:P:22[A]:BME:H11	1.73	0.53
2:M:324:TYR:CE1	4:M:21[C]:BME:H22	2.34	0.52
1:C:133:ARG:HG2	2:O:326[A]:THR:HG21	1.90	0.52
1:C:98[B]:THR:HB	1:C:99[B]:PHE:HE2	1.67	0.52
1:F:133:ARG:HG2	2:R:326[A]:THR:HG21	1.91	0.52
4:N:32[A]:BME:C2	9:N:2285:HOH:O	2.49	0.51
2:M:507:LYS:HG2	8:M:16:GOL:H32	1.92	0.51
4:M:36:BME:H21	2:N:453:PRO:O	2.11	0.51
2:R:329:ALA:HB3	9:R:1779:HOH:O	2.10	0.51
1:E:133:ARG:HD2	4:Q:19:BME:C1	2.40	0.51
2:M:478:LEU:C	2:M:478:LEU:HD23	2.31	0.51
2:Q:356:PHE:CD2	4:Q:46:BME:H11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.47	0.50
2:M:329:ALA:HB3	9:M:2298:HOH:O	2.11	0.50
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.41	0.50
2:Q:449:TRP:CE3	4:Q:19:BME:H21	2.47	0.50
1:F:64[B]:ARG:HE	1:F:99[B]:PHE:C	2.15	0.50
1:C:18:HIS:HE1	9:C:2667:HOH:O	1.86	0.50
2:P:478:LEU:HD23	2:P:478:LEU:C	2.32	0.50
1:C:188:ARG:HG2	4:C:203:BME:H12	1.95	0.49
1:A:190:GLN:O	4:A:202:BME:S2	2.70	0.49
1:F:64[B]:ARG:NH2	1:F:99[B]:PHE:HB3	2.26	0.49
1:F:98[A]:THR:O	1:F:101[A]:ALA:C	2.51	0.49
2:P:329:ALA:HB3	9:P:2588:HOH:O	2.13	0.48
2:R:449:TRP:CZ3	4:R:20:BME:H21	2.49	0.48
1:C:99[B]:PHE:CE1	2:O:411:LYS:CD	2.91	0.48
2:O:326[A]:THR:HG22	2:O:330:ARG:HD2	1.95	0.48
2:O:322:PRO:HD2	4:O:42:BME:H22	1.95	0.47
1:F:186:ASP:HB2	5:F:202:TRS:H31	1.95	0.47
2:R:449:TRP:CE3	4:R:20:BME:H21	2.48	0.47
1:A:133:ARG:HD2	4:M:21[C]:BME:O1	2.14	0.47
2:R:478:LEU:HD23	2:R:478:LEU:C	2.35	0.47
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.49	0.47
2:M:449:TRP:CZ3	4:M:21[B]:BME:H21	2.50	0.46
1:A:133:ARG:HD2	4:M:21[B]:BME:H12	1.97	0.46
2:O:478:LEU:C	2:O:478:LEU:HD23	2.35	0.46
1:F:51:LEU:HD11	1:F:126:ILE:HD12	1.96	0.46
1:A:57:ASP:O	4:A:202:BME:H11	2.16	0.46
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.50	0.46
1:F:99[B]:PHE:O	1:F:100[B]:ASP:C	2.55	0.45
2:R:531:ARG:HG2	9:R:2266:HOH:O	2.14	0.45
2:M:325:LYS:O	7:M:7:CL:CL	2.72	0.45
1:C:64[B]:ARG:O	1:C:97[B]:THR:C	2.55	0.45
4:N:18:BME:H22	9:N:2277:HOH:O	2.16	0.45
1:F:20:GLY:HA2	2:R:426[A]:VAL:HG13	1.98	0.45
2:Q:449:TRP:CZ3	4:Q:19:BME:H21	2.50	0.45
1:C:15:PRO:HD2	4:O:30:BME:H11	1.98	0.45
1:C:98[B]:THR:O	1:C:101[B]:ALA:N	2.50	0.45
1:A:19:ILE:O	2:M:426[B]:VAL:HG21	2.16	0.45
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.52	0.45
1:F:98[B]:THR:O	1:F:99[B]:PHE:C	2.56	0.45
4:R:26:BME:H12	9:R:1839:HOH:O	2.17	0.44
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:PHE:CE2	1:F:138:HIS:HB3	2.53	0.44
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.53	0.44
1:F:25:ALA:HB1	1:F:98[B]:THR:HG21	1.99	0.43
2:Q:399:MET:HA	2:Q:462:HIS:O	2.19	0.43
1:D:70:VAL:HG11	1:D:106:LEU:HD11	2.00	0.43
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.49	0.43
1:F:64[B]:ARG:HH21	1:F:99[B]:PHE:C	2.22	0.43
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.39	0.43
2:O:329:ALA:HB3	9:O:1951:HOH:O	2.19	0.43
1:F:69:GLU:HG2	1:F:94:ARG:HG2	2.01	0.42
1:F:99[A]:PHE:H	1:F:99[A]:PHE:HD1	0.61	0.42
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.01	0.42
1:C:99[A]:PHE:O	1:C:100[A]:ASP:C	2.58	0.42
4:P:40:BME:C2	9:P:21:HOH:O	2.52	0.42
2:M:411:LYS:HE3	2:M:411:LYS:HB3	1.52	0.42
2:R:326[A]:THR:HG22	2:R:326[A]:THR:O	2.19	0.42
1:C:190:GLN:O	4:C:203:BME:S2	2.78	0.42
2:M:304:ASP:HB2	2:M:343:ILE:HB	2.00	0.42
1:D:131:PHE:CD2	2:P:475:ILE:HD12	2.54	0.42
2:P:304:ASP:HB2	2:P:343:ILE:HB	2.01	0.42
1:C:100[A]:ASP:HB2	1:C:101[A]:ALA:H	1.73	0.41
2:R:457:ARG:HG3	4:R:28:BME:S2	2.60	0.41
1:C:51:LEU:HD11	1:C:126:ILE:HD12	2.02	0.41
1:B:69:GLU:HG2	1:B:94:ARG:HG2	2.02	0.41
2:N:486:ILE:HB	2:N:487:PRO:HD3	2.03	0.41
2:N:457:ARG:HG3	4:N:32[B]:BME:S2	2.61	0.41
1:A:70:VAL:HG11	1:A:106:LEU:HD11	2.02	0.41
2:Q:457:ARG:HG3	4:Q:34[A]:BME:S2	2.60	0.41
2:Q:394[B]:ASN:ND2	2:Q:394[B]:ASN:O	2.54	0.41
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.56	0.41
1:B:70:VAL:HG11	1:B:106:LEU:HD11	2.03	0.41
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.21	0.41
1:B:133:ARG:CG	4:N:18:BME:C1	2.84	0.41
1:E:70:VAL:HG11	1:E:106:LEU:HD11	2.02	0.41
1:A:50:LEU:O	1:A:182:ALA:HA	2.21	0.40
1:D:19:ILE:O	2:P:426:VAL:HG21	2.20	0.40
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.50	0.40
1:D:186:ASP:HB2	5:D:202:TRS:H22	2.03	0.40
2:O:531:ARG:HG2	9:O:2256:HOH:O	2.20	0.40
1:A:69:GLU:HG2	1:A:94:ARG:HG2	2.04	0.40
1:A:133:ARG:HG3	4:M:21[C]:BME:S2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:399:MET:HA	2:P:462:HIS:O	2.21	0.40
1:A:186:ASP:H	5:A:203:TRS:HN1	1.68	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	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	200/200 (100%)	197 (98%)	3 (2%)	0	100	100
1	C	208/200 (104%)	202 (97%)	6 (3%)	0	100	100
1	D	199/200 (100%)	196 (98%)	3 (2%)	0	100	100
1	E	200/200 (100%)	196 (98%)	4 (2%)	0	100	100
1	F	209/200 (104%)	200 (96%)	5 (2%)	4 (2%)	10	0
2	M	239/238 (100%)	235 (98%)	4 (2%)	0	100	100
2	N	238/238 (100%)	234 (98%)	4 (2%)	0	100	100
2	O	237/238 (100%)	232 (98%)	5 (2%)	0	100	100
2	P	238/238 (100%)	232 (98%)	6 (2%)	0	100	100
2	Q	239/238 (100%)	235 (98%)	4 (2%)	0	100	100
2	R	238/238 (100%)	231 (97%)	7 (3%)	0	100	100
All	All	2643/2628 (101%)	2583 (98%)	56 (2%)	4 (0%)	56	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	100[A]	ASP
1	F	100[B]	ASP

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Mol	Chain	Res	Type
1	F	99[A]	PHE
1	F	99[B]	PHE

### 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	163/163 (100%)	161 (99%)	2 (1%)	78	60
1	B	165/163 (101%)	164 (99%)	1 (1%)	90	81
1	C	171/163 (105%)	167 (98%)	4 (2%)	58	30
1	D	164/163 (101%)	163 (99%)	1 (1%)	90	81
1	E	165/163 (101%)	164 (99%)	1 (1%)	90	81
1	F	172/163 (106%)	169 (98%)	3 (2%)	68	45
2	M	205/202 (102%)	201 (98%)	4 (2%)	63	38
2	N	204/202 (101%)	200 (98%)	4 (2%)	63	38
2	O	203/202 (100%)	199 (98%)	4 (2%)	63	38
2	P	204/202 (101%)	200 (98%)	4 (2%)	63	38
2	Q	205/202 (102%)	202 (98%)	3 (2%)	72	51
2	R	204/202 (101%)	199 (98%)	5 (2%)	55	26
All	All	2225/2190 (102%)	2189 (98%)	36 (2%)	72	48

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	176	GLU
2	M	395	THR
2	M	411	LYS
2	M	473	LYS
2	M	534	HIS
1	B	174	ARG
2	N	395	THR

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Mol	Chain	Res	Type
2	N	438	SER
2	N	473	LYS
2	N	534	HIS
1	C	99[A]	PHE
1	C	99[B]	PHE
1	C	100[A]	ASP
1	C	100[B]	ASP
2	O	395	THR
2	O	399	MET
2	O	473	LYS
2	O	534	HIS
1	D	43	ASP
2	P	395	THR
2	P	399	MET
2	P	473	LYS
2	P	534	HIS
1	E	180	LYS
2	Q	395	THR
2	Q	473	LYS
2	Q	534	HIS
1	F	99[A]	PHE
1	F	99[B]	PHE
1	F	178	ASP
2	R	390	LYS
2	R	395	THR
2	R	399	MET
2	R	473	LYS
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	530	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 65 ligands modelled in this entry, 15 are monoatomic - leaving 50 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	SO4	A	201	-	4,4,4	0.33	0	6,6,6	0.13	0
4	BME	A	202	-	3,3,3	0.42	0	2,2,2	0.53	0
5	TRS	A	203	-	7,7,7	1.16	1 (14%)	9,9,9	0.87	0
3	SO4	B	201	-	4,4,4	0.18	0	6,6,6	0.11	0
5	TRS	B	202	-	7,7,7	0.92	1 (14%)	9,9,9	1.03	0
3	SO4	C	201	-	4,4,4	0.26	0	6,6,6	0.11	0
8	GOL	C	202	-	5,5,5	0.30	0	5,5,5	0.27	0
4	BME	C	203	-	3,3,3	0.38	0	2,2,2	0.72	0
3	SO4	D	201	-	4,4,4	0.29	0	6,6,6	0.24	0
5	TRS	D	202	-	7,7,7	0.99	1 (14%)	9,9,9	0.68	0
3	SO4	E	201	-	4,4,4	0.21	0	6,6,6	0.12	0
5	TRS	E	202	-	7,7,7	0.97	1 (14%)	9,9,9	0.86	0
3	SO4	F	201	-	4,4,4	0.23	0	6,6,6	0.12	0
5	TRS	F	202	-	7,7,7	0.88	1 (14%)	9,9,9	1.15	1 (11%)
8	GOL	M	16	-	5,5,5	0.63	0	5,5,5	0.42	0
4	BME	M	21[A]	-	3,3,3	0.33	0	2,2,2	0.27	0
4	BME	M	21[B]	-	3,3,3	0.66	0	2,2,2	0.59	0
4	BME	M	21[C]	-	3,3,3	0.26	0	2,2,2	0.80	0
4	BME	M	29	6	3,3,3	0.75	0	2,2,2	2.01	1 (50%)
4	BME	M	36	-	3,3,3	0.49	0	2,2,2	0.43	0
4	BME	M	47	-	3,3,3	0.30	0	2,2,2	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BME	N	18	-	3,3,3	0.28	0	2,2,2	0.46	0
4	BME	N	32[A]	6	3,3,3	0.30	0	2,2,2	1.58	1 (50%)
4	BME	N	32[B]	6	3,3,3	0.88	0	2,2,2	2.39	1 (50%)
4	BME	N	37	-	3,3,3	0.40	0	2,2,2	0.37	0
4	BME	N	44	-	3,3,3	0.36	0	2,2,2	0.58	0
4	BME	O	27	-	3,3,3	0.40	0	2,2,2	0.22	0
4	BME	O	30	6	3,3,3	0.71	0	2,2,2	1.69	1 (50%)
4	BME	O	33	-	3,3,3	0.25	0	2,2,2	0.68	0
4	BME	O	42	-	3,3,3	0.39	0	2,2,2	0.24	0
4	BME	O	45	-	3,3,3	0.40	0	2,2,2	0.63	0
4	BME	O	49	-	3,3,3	0.29	0	2,2,2	0.69	0
4	BME	P	22[A]	-	3,3,3	0.33	0	2,2,2	0.35	0
4	BME	P	22[B]	-	3,3,3	0.50	0	2,2,2	0.27	0
4	BME	P	23	-	3,3,3	0.31	0	2,2,2	0.97	0
4	BME	P	25	-	3,3,3	0.31	0	2,2,2	0.81	0
4	BME	P	31	6	3,3,3	0.76	0	2,2,2	1.83	1 (50%)
4	BME	P	35	-	3,3,3	0.29	0	2,2,2	0.73	0
4	BME	P	40	-	3,3,3	0.33	0	2,2,2	0.50	0
4	BME	P	41	-	3,3,3	0.32	0	2,2,2	0.69	0
4	BME	P	48	-	3,3,3	0.33	0	2,2,2	0.70	0
4	BME	Q	19	-	3,3,3	0.31	0	2,2,2	0.19	0
4	BME	Q	24	-	3,3,3	0.35	0	2,2,2	0.49	0
4	BME	Q	34[A]	6	3,3,3	0.56	0	2,2,2	1.83	1 (50%)
4	BME	Q	34[B]	6	3,3,3	0.40	0	2,2,2	1.42	0
4	BME	Q	46	-	3,3,3	0.43	0	2,2,2	0.46	0
4	BME	R	20	-	3,3,3	0.28	0	2,2,2	0.35	0
4	BME	R	26	-	3,3,3	0.40	0	2,2,2	0.22	0
4	BME	R	28	6	3,3,3	0.22	0	2,2,2	1.65	1 (50%)
4	BME	R	43	-	3,3,3	0.26	0	2,2,2	0.77	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
3	SO4	A	201	-	-	0/0/0/0	0/0/0/0
4	BME	A	202	-	-	0/1/1/1	0/0/0/0
5	TRS	A	203	-	-	0/9/9/9	0/0/0/0
3	SO4	B	201	-	-	0/0/0/0	0/0/0/0
5	TRS	B	202	-	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	201	-	-	0/0/0/0	0/0/0/0
8	GOL	C	202	-	-	0/4/4/4	0/0/0/0
4	BME	C	203	-	-	0/1/1/1	0/0/0/0
3	SO4	D	201	-	-	0/0/0/0	0/0/0/0
5	TRS	D	202	-	-	0/9/9/9	0/0/0/0
3	SO4	E	201	-	-	0/0/0/0	0/0/0/0
5	TRS	E	202	-	-	0/9/9/9	0/0/0/0
3	SO4	F	201	-	-	0/0/0/0	0/0/0/0
5	TRS	F	202	-	-	0/9/9/9	0/0/0/0
8	GOL	M	16	-	-	0/4/4/4	0/0/0/0
4	BME	M	21[A]	-	-	0/1/1/1	0/0/0/0
4	BME	M	21[B]	-	-	0/1/1/1	0/0/0/0
4	BME	M	21[C]	-	-	0/1/1/1	0/0/0/0
4	BME	M	29	6	-	0/1/1/1	0/0/0/0
4	BME	M	36	-	-	0/1/1/1	0/0/0/0
4	BME	M	47	-	-	0/1/1/1	0/0/0/0
4	BME	N	18	-	-	0/1/1/1	0/0/0/0
4	BME	N	32[A]	6	-	0/1/1/1	0/0/0/0
4	BME	N	32[B]	6	-	0/1/1/1	0/0/0/0
4	BME	N	37	-	-	0/1/1/1	0/0/0/0
4	BME	N	44	-	-	0/1/1/1	0/0/0/0
4	BME	O	27	-	-	0/1/1/1	0/0/0/0
4	BME	O	30	6	-	0/1/1/1	0/0/0/0
4	BME	O	33	-	-	0/1/1/1	0/0/0/0
4	BME	O	42	-	-	0/1/1/1	0/0/0/0
4	BME	O	45	-	-	0/1/1/1	0/0/0/0
4	BME	O	49	-	-	0/1/1/1	0/0/0/0
4	BME	P	22[A]	-	-	0/1/1/1	0/0/0/0
4	BME	P	22[B]	-	-	0/1/1/1	0/0/0/0
4	BME	P	23	-	-	0/1/1/1	0/0/0/0
4	BME	P	25	-	-	0/1/1/1	0/0/0/0
4	BME	P	31	6	-	0/1/1/1	0/0/0/0
4	BME	P	35	-	-	0/1/1/1	0/0/0/0
4	BME	P	40	-	-	0/1/1/1	0/0/0/0
4	BME	P	41	-	-	0/1/1/1	0/0/0/0
4	BME	P	48	-	-	0/1/1/1	0/0/0/0
4	BME	Q	19	-	-	0/1/1/1	0/0/0/0
4	BME	Q	24	-	-	0/1/1/1	0/0/0/0
4	BME	Q	34[A]	6	-	0/1/1/1	0/0/0/0
4	BME	Q	34[B]	6	-	0/1/1/1	0/0/0/0
4	BME	Q	46	-	-	0/1/1/1	0/0/0/0
4	BME	R	20	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	R	26	-	-	0/1/1/1	0/0/0/0
4	BME	R	28	6	-	0/1/1/1	0/0/0/0
4	BME	R	43	-	-	0/1/1/1	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	203	TRS	C-N	-3.02	1.46	1.50
5	E	202	TRS	C-N	-2.47	1.47	1.50
5	D	202	TRS	C-N	-2.39	1.47	1.50
5	B	202	TRS	C-N	-2.35	1.47	1.50
5	F	202	TRS	C-N	-2.24	1.47	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	32[B]	BME	C1-C2-S2	-3.37	94.22	112.58
4	M	29	BME	C1-C2-S2	-2.82	97.21	112.58
4	P	31	BME	C1-C2-S2	-2.58	98.50	112.58
4	Q	34[A]	BME	C1-C2-S2	-2.35	99.78	112.58
4	N	32[A]	BME	C1-C2-S2	-2.22	100.47	112.58
4	R	28	BME	C1-C2-S2	-2.22	100.49	112.58
4	O	30	BME	C1-C2-S2	-2.22	100.49	112.58
5	F	202	TRS	C1-C-N	2.09	111.89	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	BME	2	0
5	A	203	TRS	1	0
5	B	202	TRS	1	0
4	C	203	BME	3	0
5	D	202	TRS	4	0
5	F	202	TRS	1	0
8	M	16	GOL	1	0
4	M	21[B]	BME	3	0
4	M	21[C]	BME	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	29	BME	1	0
4	M	36	BME	1	0
4	N	18	BME	8	0
4	N	32[A]	BME	3	0
4	N	32[B]	BME	2	0
4	N	44	BME	1	0
4	O	30	BME	1	0
4	O	33	BME	7	0
4	O	42	BME	1	0
4	O	45	BME	1	0
4	P	22[A]	BME	4	0
4	P	22[B]	BME	1	0
4	P	23	BME	1	0
4	P	31	BME	1	0
4	P	35	BME	1	0
4	P	40	BME	3	0
4	Q	19	BME	8	0
4	Q	34[A]	BME	2	0
4	Q	34[B]	BME	2	0
4	Q	46	BME	1	0
4	R	20	BME	9	0
4	R	26	BME	1	0
4	R	28	BME	2	0
4	R	43	BME	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	200/200 (100%)	0.03	8 (4%)	42	41	13, 18, 29, 38	6 (3%)
1	B	200/200 (100%)	0.32	16 (8%)	15	13	13, 21, 34, 42	5 (2%)
1	C	200/200 (100%)	0.07	9 (4%)	37	35	13, 18, 29, 37	4 (2%)
1	D	200/200 (100%)	0.05	8 (4%)	42	41	13, 18, 30, 42	2 (1%)
1	E	200/200 (100%)	0.34	15 (7%)	17	15	14, 21, 33, 45	4 (2%)
1	F	200/200 (100%)	0.09	8 (4%)	42	41	13, 18, 29, 38	4 (2%)
2	M	238/238 (100%)	-0.16	2 (0%)	87	88	13, 16, 26, 34	4 (1%)
2	N	238/238 (100%)	-0.07	9 (3%)	44	44	14, 17, 26, 38	4 (1%)
2	O	238/238 (100%)	-0.16	4 (1%)	73	76	13, 16, 25, 35	2 (0%)
2	P	238/238 (100%)	-0.13	4 (1%)	73	76	13, 16, 26, 34	1 (0%)
2	Q	238/238 (100%)	-0.07	9 (3%)	44	44	14, 17, 26, 37	3 (1%)
2	R	238/238 (100%)	-0.14	3 (1%)	79	82	13, 17, 25, 35	0
All	All	2628/2628 (100%)	0.00	95 (3%)	46	47	13, 18, 29, 45	39 (1%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	99[A]	PHE	7.7
1	C	99[A]	PHE	7.5
1	F	27	GLY	6.4
1	E	178	ASP	5.7
1	E	99	PHE	5.5
1	D	178	ASP	5.3
1	B	177	VAL	5.2
1	B	99	PHE	5.0
1	F	101[A]	ALA	4.9
1	C	101[A]	ALA	4.5
1	F	98[A]	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	99	PHE	4.3
1	C	98[A]	THR	4.2
1	B	100	ASP	4.2
1	B	178	ASP	4.1
1	E	179	GLY	4.0
1	E	177	VAL	4.0
1	B	43	ASP	3.9
1	C	27	GLY	3.9
1	E	43	ASP	3.9
2	Q	301	PRO	3.9
1	A	178	ASP	3.8
2	N	303	GLN	3.8
2	N	301	PRO	3.7
1	A	99	PHE	3.7
1	B	179	GLY	3.6
1	E	100	ASP	3.6
2	M	538	CYS	3.4
2	O	414	ARG	3.4
1	C	100[A]	ASP	3.3
2	Q	538	CYS	3.3
1	F	25	ALA	3.3
1	C	43	ASP	3.2
2	R	414	ARG	3.2
2	O	538	CYS	3.2
2	Q	303	GLN	3.2
2	R	538	CYS	3.2
1	A	43	ASP	3.2
1	D	100	ASP	3.1
1	A	179	GLY	3.0
2	P	538	CYS	3.0
1	E	176	GLU	3.0
1	F	100[A]	ASP	2.9
2	N	538	CYS	2.9
1	C	25	ALA	2.8
1	B	42	PRO	2.8
1	A	100	ASP	2.8
1	B	176	GLU	2.8
1	E	180	LYS	2.7
1	E	27	GLY	2.7
1	E	70	VAL	2.7
1	D	43	ASP	2.7
1	F	24	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	305	ASN	2.7
1	B	70	VAL	2.6
1	E	150	GLN	2.6
1	D	180	LYS	2.5
1	B	98	THR	2.5
1	E	98	THR	2.5
1	C	24	GLU	2.5
2	P	411	LYS	2.5
2	R	303	GLN	2.5
1	B	150	GLN	2.5
1	E	101	ALA	2.5
1	F	26	ALA	2.5
2	Q	305	ASN	2.4
1	E	32[A]	ASP	2.4
1	B	101	ALA	2.4
2	N	353	HIS	2.4
1	B	32	ASP	2.4
2	O	303	GLN	2.4
1	D	179	GLY	2.3
1	D	42	PRO	2.3
1	A	180	LYS	2.3
1	B	180	LYS	2.3
1	B	86	GLU	2.3
2	M	414	ARG	2.3
1	C	26	ALA	2.3
1	E	42	PRO	2.3
2	Q	353	HIS	2.2
2	N	470	ILE	2.2
2	N	370	GLY	2.2
2	Q	411	LYS	2.2
2	Q	302	ALA	2.2
1	A	42	PRO	2.1
2	Q	537	ASN	2.1
1	A	27	GLY	2.1
2	N	302	ALA	2.1
1	B	128	ILE	2.1
2	P	301	PRO	2.0
2	P	305	ASN	2.0
1	D	130	LEU	2.0
2	Q	370	GLY	2.0
2	N	537	ASN	2.0
2	O	305	ASN	2.0



## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BME	P	40	4/4	0.85	0.22	17.29	37,38,38,40	4
7	CL	M	7	1/1	0.97	0.16	14.97	38,38,38,38	0
4	BME	M	21[B]	4/4	0.88	0.18	13.84	17,18,19,25	4
4	BME	M	21[C]	4/4	0.88	0.18	13.84	18,21,21,22	4
4	BME	M	21[A]	4/4	0.88	0.18	13.44	28,30,30,31	4
4	BME	N	32[A]	4/4	0.92	0.16	11.69	42,43,43,44	4
4	BME	N	32[B]	4/4	0.92	0.16	11.16	17,17,18,23	4
4	BME	M	36	4/4	0.77	0.24	10.34	41,41,41,42	4
4	BME	Q	19	4/4	0.88	0.17	8.41	24,30,33,38	4
4	BME	R	28	4/4	0.96	0.17	7.98	14,14,15,18	0
4	BME	O	33	4/4	0.88	0.16	7.74	20,27,27,33	4
4	BME	Q	34[B]	4/4	0.94	0.17	7.45	56,57,57,57	4
4	BME	Q	34[A]	4/4	0.94	0.17	7.22	11,13,14,16	4
4	BME	N	18	4/4	0.89	0.15	6.89	23,27,30,36	4
4	BME	R	20	4/4	0.93	0.14	6.77	20,28,29,33	4
4	BME	P	22[A]	4/4	0.78	0.19	6.06	31,31,32,32	4
8	GOL	M	16	6/6	0.88	0.20	5.88	29,35,36,40	0
4	BME	O	42	4/4	0.93	0.16	5.78	28,32,33,36	4
5	TRS	D	202	8/8	0.71	0.25	4.94	34,35,37,38	8
4	BME	P	22[B]	4/4	0.78	0.19	4.89	21,29,29,35	4
5	TRS	F	202	8/8	0.72	0.29	4.84	41,41,42,43	8
5	TRS	A	203	8/8	0.68	0.26	4.79	36,37,39,40	0
4	BME	C	203	4/4	0.84	0.28	4.59	32,33,34,35	4
4	BME	N	44	4/4	0.87	0.15	4.41	35,37,38,40	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TRS	B	202	8/8	0.75	0.24	4.35	44,45,46,47	0
4	BME	Q	24	4/4	0.89	0.14	3.41	34,36,38,40	4
5	TRS	E	202	8/8	0.82	0.19	3.28	46,47,47,47	0
4	BME	O	45	4/4	0.87	0.16	3.27	32,33,34,35	4
4	BME	A	202	4/4	0.88	0.23	3.15	28,30,30,34	4
4	BME	R	43	4/4	0.87	0.19	3.10	34,36,36,37	4
4	BME	M	29	4/4	0.94	0.11	2.89	21,23,25,28	0
4	BME	P	31	4/4	0.95	0.10	1.72	23,24,26,28	0
8	GOL	C	202	6/6	0.87	0.13	0.92	36,41,42,43	0
4	BME	P	23	4/4	0.93	0.11	0.70	30,31,34,37	4
4	BME	O	30	4/4	0.96	0.09	0.56	23,24,26,28	0
6	FE	Q	600	1/1	1.00	0.04	-	16,16,16,16	0
7	CL	M	9	1/1	0.90	0.13	-	45,45,45,45	0
3	SO4	B	201	5/5	0.93	0.17	-	39,41,42,42	5
6	FE	O	600	1/1	1.00	0.04	-	15,15,15,15	0
3	SO4	A	201	5/5	0.96	0.15	-	36,37,38,38	5
6	FE	R	600	1/1	1.00	0.04	-	15,15,15,15	0
4	BME	P	41	4/4	0.84	0.16	-	44,45,45,45	4
7	CL	M	8	1/1	0.72	0.10	-	59,59,59,59	0
3	SO4	D	201	5/5	0.96	0.13	-	35,37,37,38	5
4	BME	Q	46	4/4	0.89	0.17	-	36,38,39,41	4
7	CL	M	14	1/1	0.90	0.07	-	61,61,61,61	0
6	FE	N	600	1/1	1.00	0.04	-	16,16,16,16	0
4	BME	P	25	4/4	0.83	0.17	-	32,34,34,36	4
6	FE	M	600	1/1	1.00	0.05	-	15,15,15,15	0
4	BME	N	37	4/4	0.68	0.18	-	56,58,59,62	0
7	CL	N	13	1/1	0.90	0.11	-	64,64,64,64	0
7	CL	R	10	1/1	0.88	0.19	-	68,68,68,68	0
7	CL	P	15	1/1	0.87	0.08	-	60,60,60,60	0
3	SO4	F	201	5/5	0.93	0.19	-	41,43,44,44	5
6	FE	P	600	1/1	1.00	0.05	-	15,15,15,15	0
7	CL	O	12	1/1	0.79	0.21	-	70,70,70,70	0
3	SO4	C	201	5/5	0.94	0.18	-	42,44,45,45	5
4	BME	P	35	4/4	0.93	0.11	-	37,37,37,37	4
4	BME	M	47	4/4	0.70	0.20	-	34,37,40,44	4
4	BME	R	26	4/4	0.78	0.13	-	47,48,49,49	4
7	CL	Q	11	1/1	0.90	0.11	-	68,68,68,68	0
4	BME	P	48	4/4	0.76	0.16	-	42,42,42,43	4
4	BME	O	49	4/4	0.91	0.10	-	37,38,38,38	4
3	SO4	E	201	5/5	0.95	0.19	-	38,39,40,41	5
4	BME	O	27	4/4	0.83	0.19	-	49,49,50,50	4

## 6.5 Other polymers

There are no such residues in this entry.