



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:17 AM GMT

PDB ID : 1D8C  
Title : MALATE SYNTHASE G COMPLEXED WITH MAGNESIUM AND GLY-  
OXYLATE  
Authors : Howard, B.R.; Endrizzi, J.A.; Remington, S.J.  
Deposited on : 1999-10-22  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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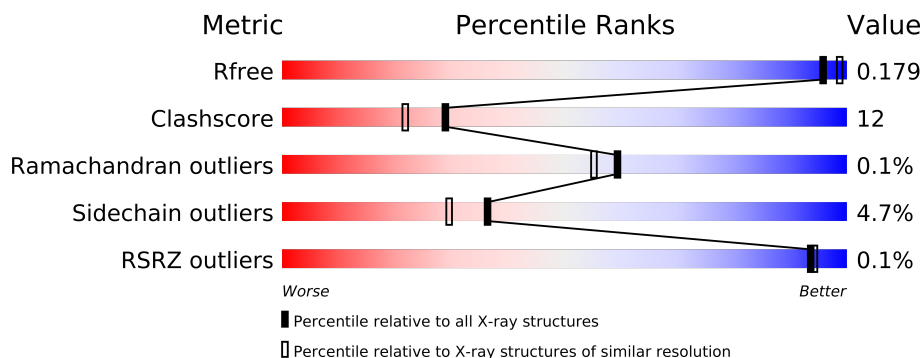
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	723	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SOR	A	4000	-	X
4	SO4	A	5000	-	X
4	SO4	A	6000	-	X
4	SO4	A	7000	-	X
4	SO4	A	8000	-	X
4	SO4	A	9000	-	X
5	GLV	A	2000	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5719 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

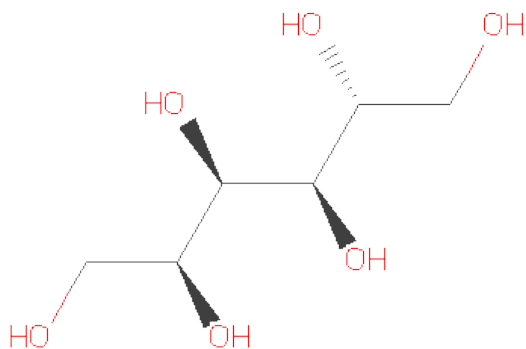
- Molecule 1 is a protein called MALATE SYNTHASE G.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	Se	0	0	0
			5331	3365	930	1009	6	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CONFLICT	UNP P37330
A	2	ALA	SER	ENGINEERED	UNP P37330
A	122	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	154	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	294	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	302	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	344	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	366	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	393	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	412	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	415	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	422	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	425	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	461	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	465	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	470	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	476	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	508	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	511	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	515	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	518	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	629	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	663	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	680	MSE	MET	MODIFIED RESIDUE	UNP P37330

- Molecule 2 is D-SORBITOL (three-letter code: SOR) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>6</sub>).

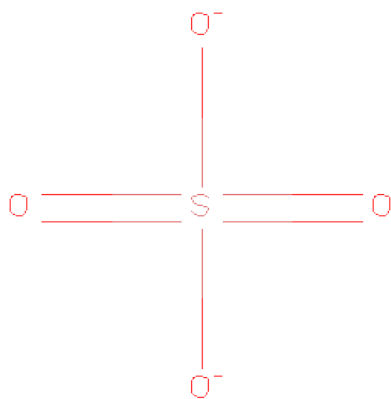


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

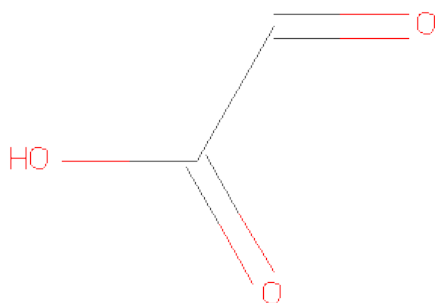
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C<sub>2</sub>H<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	2	3		

- Molecule 6 is water.

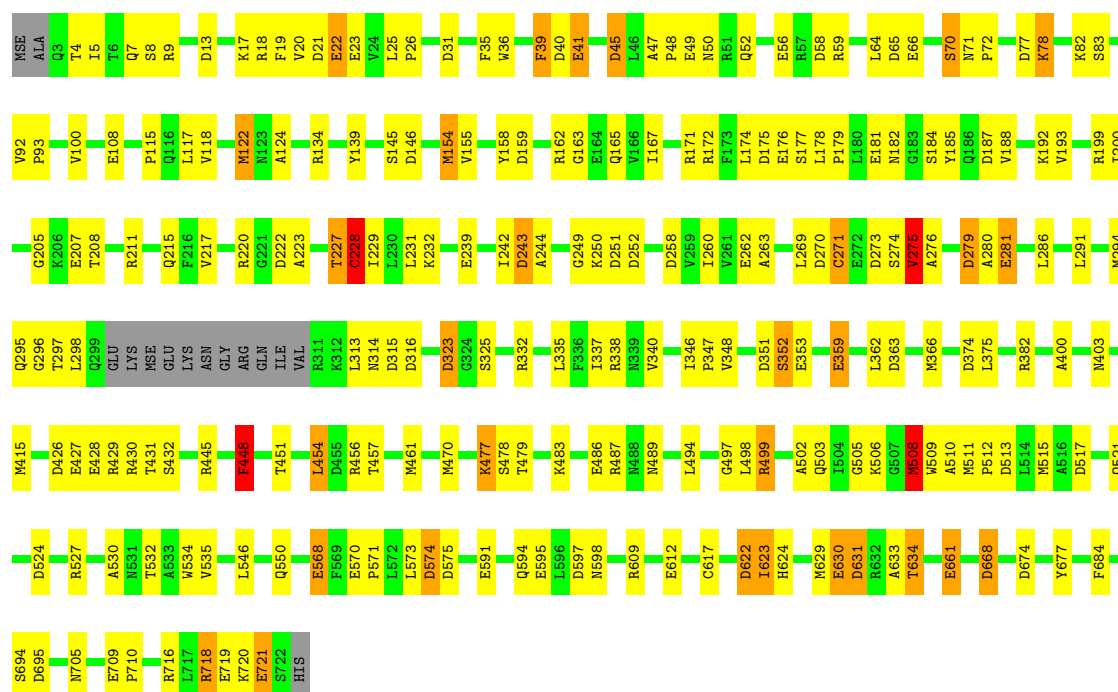
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	345	Total	O	0	0
			345	345		

### 3 Residue-property plots

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: MALATE SYNTHASE G

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.80Å 88.70Å 109.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.00) 99.5 (19.90-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.01Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.174 , 0.179	Depositor DCC
$R_{free}$ test set	2522 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 104.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49241 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SOR, SO4, GLV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.02	24/5416 (0.4%)	1.51	101/7345 (1.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CD-OE2	8.08	1.34	1.25
1	A	262	GLU	CD-OE2	7.75	1.34	1.25
1	A	630	GLU	CD-OE2	7.45	1.33	1.25
1	A	486	GLU	CD-OE2	6.82	1.33	1.25
1	A	41	GLU	CD-OE2	6.63	1.32	1.25
1	A	595	GLU	CD-OE2	6.61	1.32	1.25
1	A	23	GLU	CD-OE2	6.42	1.32	1.25
1	A	176	GLU	CD-OE2	6.29	1.32	1.25
1	A	49	GLU	CD-OE2	6.07	1.32	1.25
1	A	721	GLU	CD-OE2	6.04	1.32	1.25
1	A	353	GLU	CD-OE2	6.03	1.32	1.25
1	A	359	GLU	CD-OE2	5.80	1.32	1.25
1	A	108	GLU	CD-OE2	5.73	1.31	1.25
1	A	239	GLU	CD-OE2	5.73	1.31	1.25
1	A	281	GLU	CD-OE2	5.69	1.31	1.25
1	A	428	GLU	CD-OE2	5.51	1.31	1.25
1	A	612	GLU	CD-OE2	5.48	1.31	1.25
1	A	22	GLU	CD-OE2	5.39	1.31	1.25
1	A	591	GLU	CD-OE2	5.39	1.31	1.25
1	A	181	GLU	CD-OE2	5.22	1.31	1.25
1	A	568	GLU	CD-OE2	5.17	1.31	1.25
1	A	427	GLU	CD-OE1	-5.16	1.20	1.25
1	A	661	GLU	CD-OE2	5.08	1.31	1.25
1	A	207	GLU	CD-OE2	5.01	1.31	1.25

All (101) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	A	382	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	A	382	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	243	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	A	175	ASP	CB-CG-OD1	9.12	126.51	118.30
1	A	316	ASP	CB-CG-OD2	-9.04	110.17	118.30
1	A	279	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	A	315	ASP	CB-CG-OD1	8.74	126.17	118.30
1	A	13	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	A	426	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	175	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	609	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	674	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	258	ASP	CB-CG-OD1	8.18	125.66	118.30
1	A	187	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	A	631	ASP	CB-CG-OD1	8.07	125.56	118.30
1	A	574	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	45	ASP	CB-CG-OD1	7.85	125.37	118.30
1	A	251	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	716	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	A	448	PHE	CB-CG-CD1	7.76	126.24	120.80
1	A	21	ASP	CB-CG-OD2	-7.70	111.38	118.30
1	A	426	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	58	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	315	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	A	77	ASP	CB-CG-OD1	7.54	125.09	118.30
1	A	316	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	243	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	456	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	575	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	A	222	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	513	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	445	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	668	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	508	MSE	CA-CB-CG	-7.06	101.30	113.30
1	A	716	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	524	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	445	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	171	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	40	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	279	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	77	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	65	ASP	CB-CG-OD1	6.60	124.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	65	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	A	59	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	695	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	374	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	13	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	631	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	159	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	58	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	239	GLU	CB-CA-C	-6.27	97.86	110.40
1	A	363	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	674	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	275	VAL	N-CA-CB	-6.19	97.89	111.50
1	A	448	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	A	374	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	40	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	270	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	159	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	220	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	323	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	187	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	323	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	575	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	517	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	251	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	222	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	172	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	21	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	527	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	524	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	622	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	597	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	574	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	45	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	351	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	456	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	9	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	199	ARG	CB-CA-C	5.64	121.67	110.40
1	A	487	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	211	ARG	N-CA-CB	5.57	120.63	110.60
1	A	351	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	499	ARG	NE-CZ-NH1	5.53	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	134	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	634	THR	CA-CB-CG2	-5.42	104.81	112.40
1	A	508	MSE	N-CA-C	5.37	125.50	111.00
1	A	171	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	31	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	271	CYS	CB-CA-C	-5.27	99.86	110.40
1	A	668	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	517	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	228	CYS	CB-CA-C	5.11	120.63	110.40
1	A	695	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	454	LEU	CA-CB-CG	-5.06	103.66	115.30
1	A	227	THR	N-CA-CB	-5.05	100.70	110.30
1	A	448	PHE	CA-CB-CG	5.02	125.95	113.90
1	A	252	ASP	CB-CG-OD1	5.00	122.80	118.30
1	A	146	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5331	0	5096	130	0
2	A	12	0	14	0	0
3	A	1	0	0	0	0
4	A	25	0	0	1	0
5	A	5	0	1	0	0
6	A	345	0	0	9	0
All	All	5719	0	5111	130	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:ILE:HG13	1:A:347:PRO:HD2	1.40	1.03
1:A:122:MSE:HE2	1:A:276:ALA:H	1.23	1.00
1:A:508:MSE:HG3	1:A:534:TRP:HB3	1.51	0.91
1:A:7:GLN:HG2	1:A:36:TRP:HB3	1.53	0.91
1:A:508:MSE:HG3	1:A:534:TRP:CB	2.07	0.85
1:A:122:MSE:CE	1:A:276:ALA:H	1.92	0.82
1:A:269:LEU:HD12	1:A:337:ILE:CD1	2.12	0.80
1:A:7:GLN:HG2	1:A:36:TRP:CB	2.13	0.79
1:A:461:MSE:CE	1:A:470:MSE:HG3	2.13	0.78
1:A:269:LEU:HD12	1:A:337:ILE:HD13	1.66	0.77
1:A:228:CYS:C	1:A:229:ILE:HD13	2.06	0.76
1:A:457:THR:O	1:A:461:MSE:HG3	1.85	0.76
1:A:291:LEU:O	1:A:295:GLN:HG3	1.85	0.76
1:A:296:GLY:HA2	1:A:313:LEU:HD12	1.73	0.71
1:A:509:TRP:HZ3	1:A:521:GLN:NE2	1.88	0.71
1:A:479:THR:O	1:A:483:LYS:HG3	1.90	0.70
1:A:461:MSE:HE2	1:A:470:MSE:HG3	1.73	0.69
1:A:5:ILE:HG21	1:A:17:LYS:HD3	1.75	0.69
1:A:521:GLN:HB3	6:A:1216:HOH:O	1.92	0.69
1:A:82:LYS:NZ	1:A:573:LEU:HD23	2.08	0.68
1:A:280:ALA:HB2	1:A:348:VAL:HG22	1.75	0.68
1:A:271:CYS:HB2	1:A:338:ARG:O	1.92	0.68
1:A:167:ILE:N	1:A:167:ILE:HD13	2.08	0.67
1:A:82:LYS:NZ	1:A:574:ASP:OD1	2.30	0.65
1:A:193:VAL:HB	1:A:223:ALA:HB1	1.79	0.65
1:A:158:TYR:OH	1:A:163:GLY:HA3	1.99	0.63
1:A:228:CYS:O	1:A:229:ILE:HD13	1.99	0.63
1:A:375:LEU:HD11	1:A:415:MSE:HE2	1.80	0.63
1:A:200:ILE:HD12	1:A:200:ILE:N	2.13	0.62
1:A:205:GLY:HA2	6:A:1272:HOH:O	1.99	0.62
1:A:546:LEU:O	1:A:550:GLN:HG3	1.99	0.62
1:A:509:TRP:CE2	1:A:511:MSE:HE2	2.35	0.61
1:A:48:PRO:O	1:A:52:GLN:HG3	1.99	0.61
1:A:497:GLY:HA2	6:A:1061:HOH:O	2.01	0.61
1:A:508:MSE:HG2	1:A:534:TRP:O	2.00	0.60
1:A:185:TYR:HA	1:A:188:VAL:HG23	1.84	0.59
1:A:47:ALA:HB3	1:A:48:PRO:HD3	1.85	0.58
1:A:82:LYS:HZ2	1:A:573:LEU:HD23	1.68	0.57
1:A:122:MSE:HE3	1:A:275:VAL:HA	1.87	0.56
1:A:25:LEU:N	1:A:26:PRO:HD2	2.20	0.56
1:A:229:ILE:N	1:A:229:ILE:HD13	2.21	0.55
1:A:117:LEU:HD12	1:A:535:VAL:O	2.06	0.54
1:A:162:ARG:HA	1:A:165:GLN:HE21	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:594:GLN:O	1:A:598:ASN:HB2	2.08	0.54
1:A:295:GLN:HB2	1:A:297:THR:HG23	1.88	0.54
1:A:118:VAL:HG21	1:A:534:TRP:CE3	2.42	0.53
1:A:570:GLU:N	1:A:571:PRO:HD2	2.24	0.53
1:A:92:VAL:HB	1:A:93:PRO:HD2	1.91	0.53
1:A:122:MSE:HE2	1:A:276:ALA:N	2.07	0.53
1:A:498:LEU:HB3	1:A:502:ALA:HB3	1.91	0.52
1:A:145:SER:O	1:A:162:ARG:NH2	2.43	0.51
1:A:78:LYS:O	1:A:82:LYS:HG3	2.11	0.51
1:A:448:PHE:HB2	1:A:503:GLN:HB2	1.92	0.51
1:A:346:ILE:HG13	1:A:347:PRO:CD	2.26	0.51
1:A:5:ILE:CG2	1:A:17:LYS:HD3	2.41	0.50
1:A:509:TRP:CZ2	1:A:511:MSE:HE2	2.45	0.50
1:A:70:SER:C	1:A:72:PRO:HD3	2.31	0.50
1:A:35:PHE:HA	6:A:1290:HOH:O	2.12	0.50
1:A:82:LYS:HZ2	1:A:573:LEU:CD2	2.25	0.49
1:A:82:LYS:HZ3	1:A:573:LEU:HD23	1.77	0.49
1:A:630:GLU:HB3	1:A:634:THR:HG21	1.95	0.49
1:A:279:ASP:OD2	1:A:720:LYS:NZ	2.33	0.48
1:A:273:ASP:O	1:A:631:ASP:HB2	2.12	0.48
1:A:100:VAL:HG21	1:A:498:LEU:HD21	1.96	0.48
1:A:352:SER:HB2	6:A:1334:HOH:O	2.14	0.47
1:A:431:THR:O	1:A:432:SER:C	2.49	0.47
1:A:314:ASN:O	1:A:332:ARG:HD3	2.14	0.47
1:A:274:SER:HB2	1:A:617:CYS:HB2	1.96	0.47
1:A:661:GLU:HG2	1:A:684:PHE:CE2	2.50	0.47
1:A:47:ALA:N	1:A:48:PRO:CD	2.78	0.47
1:A:718:ARG:O	1:A:721:GLU:HB2	2.14	0.47
1:A:570:GLU:N	1:A:571:PRO:CD	2.78	0.47
1:A:340:VAL:HG21	1:A:359:GLU:HG2	1.97	0.46
1:A:178:LEU:N	1:A:179:PRO:CD	2.79	0.46
1:A:323:ASP:OD1	1:A:325:SER:OG	2.32	0.46
1:A:623:ILE:HG23	1:A:624:HIS:CD2	2.49	0.46
1:A:512:PRO:HG3	1:A:629:MSE:HG3	1.97	0.46
1:A:244:ALA:O	1:A:250:LYS:HA	2.16	0.46
1:A:25:LEU:N	1:A:26:PRO:CD	2.78	0.46
1:A:705:ASN:ND2	6:A:1042:HOH:O	2.49	0.45
1:A:505:GLY:HA2	1:A:532:THR:O	2.16	0.45
1:A:242:ILE:N	1:A:242:ILE:HD13	2.32	0.45
1:A:509:TRP:CZ2	1:A:511:MSE:CE	3.00	0.45
1:A:66:GLU:O	1:A:70:SER:OG	2.31	0.44
1:A:719:GLU:OE1	1:A:719:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:THR:HG23	1:A:489:ASN:CG	2.38	0.44
1:A:623:ILE:HG23	1:A:624:HIS:NE2	2.33	0.44
1:A:512:PRO:O	1:A:515:MSE:HE3	2.18	0.44
1:A:41:GLU:O	1:A:45:ASP:N	2.48	0.44
1:A:182:ASN:O	1:A:208:THR:HG21	2.17	0.44
1:A:115:PRO:HD2	1:A:263:ALA:O	2.18	0.44
1:A:7:GLN:O	1:A:8:SER:C	2.55	0.44
1:A:269:LEU:HD12	1:A:337:ILE:HD11	1.94	0.44
1:A:478:SER:HB2	6:A:1141:HOH:O	2.18	0.44
1:A:668:ASP:OD1	1:A:677:TYR:OH	2.31	0.44
1:A:630:GLU:HB2	6:A:1185:HOH:O	2.17	0.44
1:A:39:PHE:HZ	1:A:362:LEU:HD12	1.82	0.44
1:A:7:GLN:CG	1:A:36:TRP:HB3	2.38	0.43
1:A:494:LEU:HA	1:A:494:LEU:HD23	1.67	0.43
1:A:508:MSE:HG3	1:A:534:TRP:HB2	1.96	0.43
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.74	0.43
1:A:498:LEU:O	1:A:499:ARG:C	2.56	0.43
1:A:139:TYR:CZ	1:A:167:ILE:HD12	2.54	0.43
1:A:294:MSE:HE1	1:A:335:LEU:HD12	2.01	0.42
1:A:454:LEU:HB2	1:A:633:ALA:HB1	2.01	0.42
1:A:709:GLU:HB2	1:A:710:PRO:HD3	2.01	0.42
1:A:400:ALA:O	1:A:403:ASN:HB3	2.20	0.42
1:A:154:MSE:H	1:A:154:MSE:HG3	1.66	0.42
1:A:568:GLU:O	1:A:571:PRO:HD2	2.20	0.42
1:A:362:LEU:O	1:A:366:MSE:HG2	2.20	0.42
1:A:509:TRP:HZ3	1:A:521:GLN:CD	2.22	0.42
1:A:617:CYS:HA	6:A:1121:HOH:O	2.19	0.42
1:A:243:ASP:O	1:A:249:GLY:HA3	2.20	0.42
1:A:177:SER:C	1:A:178:LEU:HD12	2.40	0.42
1:A:185:TYR:HA	1:A:188:VAL:CG2	2.48	0.42
1:A:19:PHE:O	1:A:20:VAL:C	2.56	0.42
1:A:217:VAL:HG21	1:A:232:LYS:HB3	2.02	0.41
1:A:477:LYS:HE3	1:A:477:LYS:HB3	1.88	0.41
1:A:100:VAL:HG21	1:A:498:LEU:CD2	2.51	0.41
1:A:124:ALA:HB1	1:A:298:LEU:HD21	2.02	0.41
1:A:215:GLN:O	1:A:231:LEU:HA	2.20	0.41
1:A:18:ARG:O	1:A:22:GLU:N	2.34	0.41
1:A:508:MSE:HG2	1:A:509:TRP:H	1.86	0.41
1:A:448:PHE:CD1	1:A:448:PHE:C	2.94	0.41
1:A:510:ALA:O	1:A:512:PRO:HD3	2.20	0.41
1:A:174:LEU:HA	1:A:174:LEU:HD23	1.79	0.41
1:A:296:GLY:HA2	1:A:313:LEU:CD1	2.45	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:499:ARG:NH2	4:A:6000:SO4:O2	2.53	0.40
1:A:71:ASN:N	1:A:72:PRO:HD3	2.36	0.40
1:A:506:LYS:HG3	1:A:530:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	705/723 (98%)	684 (97%)	20 (3%)	1 (0%)	59 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL

### 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	531/576 (92%)	506 (95%)	25 (5%)	36 29

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	39	PHE
1	A	50	ASN
1	A	70	SER

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Mol	Chain	Res	Type
1	A	78	LYS
1	A	83	SER
1	A	122	MSE
1	A	154	MSE
1	A	184	SER
1	A	192	LYS
1	A	227	THR
1	A	228	CYS
1	A	260	ILE
1	A	275	VAL
1	A	281	GLU
1	A	286	LEU
1	A	352	SER
1	A	430	ARG
1	A	448	PHE
1	A	477	LYS
1	A	508	MSE
1	A	622	ASP
1	A	623	ILE
1	A	694	SER
1	A	718	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	165	GLN
1	A	295	GLN
1	A	418	ASN
1	A	441	GLN
1	A	521	GLN
1	A	705	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	GLV	A	2000	3	4,4,4	1.31	1 (25%)	3,4,4	1.55	1 (33%)
2	SOR	A	4000	-	11,11,11	0.37	0	14,14,14	1.08	0
4	SO4	A	5000	-	4,4,4	1.36	1 (25%)	6,6,6	0.21	0
4	SO4	A	6000	-	4,4,4	1.80	1 (25%)	6,6,6	0.43	0
4	SO4	A	7000	-	4,4,4	2.96	3 (75%)	6,6,6	0.44	0
4	SO4	A	8000	-	4,4,4	2.10	1 (25%)	6,6,6	0.26	0
4	SO4	A	9000	-	4,4,4	1.54	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLV	A	2000	3	-	0/0/2/2	0/0/0/0
2	SOR	A	4000	-	-	0/16/16/16	0/0/0/0
4	SO4	A	5000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	6000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	7000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	8000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	9000	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7000	SO4	O1-S	4.21	1.60	1.47
4	A	7000	SO4	O4-S	3.38	1.58	1.47
4	A	8000	SO4	O4-S	3.36	1.58	1.47
4	A	6000	SO4	O3-S	2.83	1.56	1.47
4	A	5000	SO4	O2-S	2.69	1.55	1.47
4	A	7000	SO4	O2-S	2.23	1.54	1.47
5	A	2000	GLV	C1-C2	2.19	1.50	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2000	GLV	O3-C2-C1	2.07	119.98	113.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	709/723 (98%)	-0.47	0 100 100	17, 29, 53, 71	0

There are no RSRZ outliers to report.

### 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	7000	5/5	0.35	8.33	100,100,100,100	0
2	SOR	A	4000	12/12	0.15	5.98	24,38,97,100	0
4	SO4	A	8000	5/5	0.20	5.21	98,98,100,100	0
4	SO4	A	6000	5/5	0.21	4.09	77,81,82,86	0
4	SO4	A	5000	5/5	0.18	3.62	88,88,89,91	0
4	SO4	A	9000	5/5	0.17	3.21	95,95,100,100	0
5	GLV	A	2000	5/5	0.12	3.12	21,23,33,33	0
3	MG	A	3001	1/1	0.03	-2.63	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.