



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:41 PM UTC

PDB ID : 1D8C / pdb_00001d8c
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

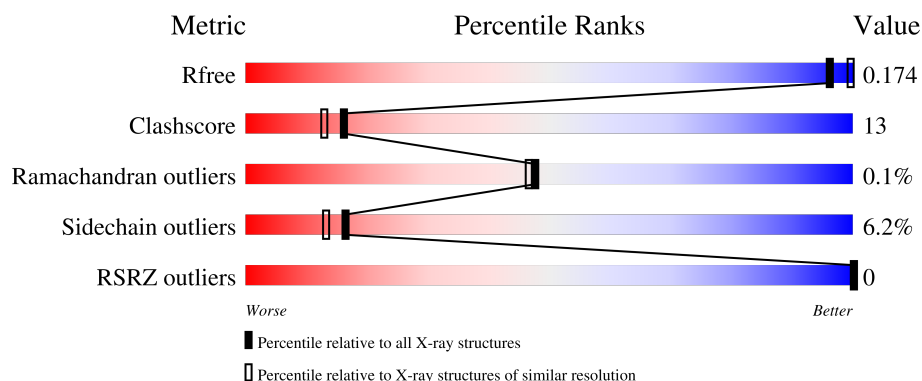
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	 67% 27% . . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5719 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.

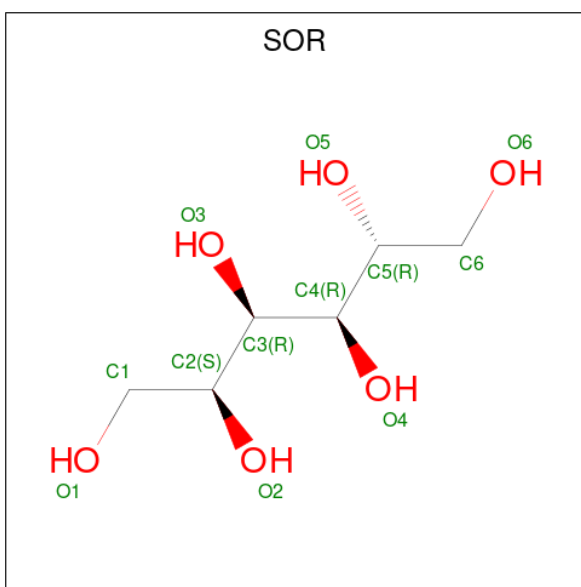
- Molecule 1 is a protein called MALATE SYNTHASE G.

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 mutation	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 sorbitol (CCD ID: SOR) (formula: C₆H₁₄O₆).

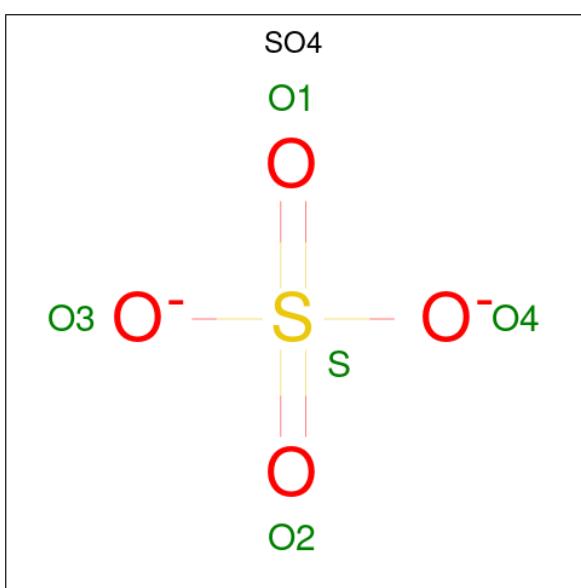


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

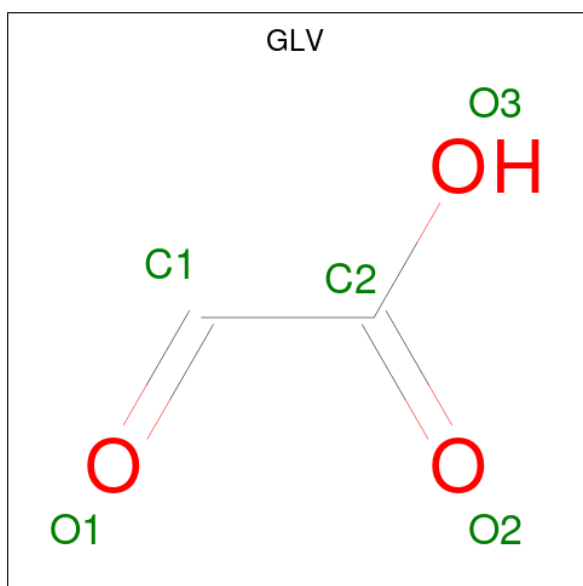
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is GLYOXYLIC ACID (CCD ID: GLV) (formula: $C_2H_2O_3$).



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

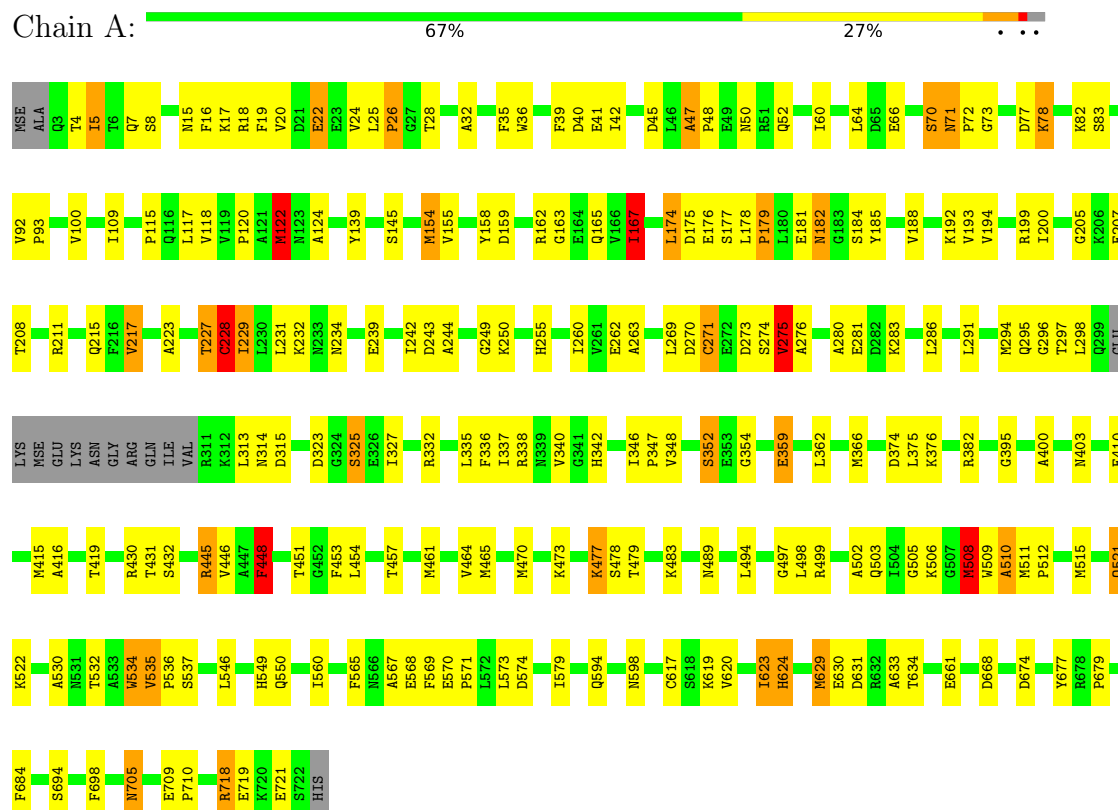
- Molecule 6 is water.

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

3 Residue-property plots

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: MALATE SYNTHASE G



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.80Å 88.70Å 109.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.00) 99.5 (20.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.01Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available) 0.168 , 0.174	Depositor DCC
R_{free} test set	2522 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 121.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	2/5416 (0.0%)	1.75	81/7345 (1.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	CYS	N-CA	-5.45	1.39	1.46
1	A	508	MSE	CA-CB	-5.38	1.45	1.53

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	PHE	CA-CB-CG	12.15	125.95	113.80
1	A	508	MSE	N-CA-C	9.73	125.50	110.42
1	A	619	LYS	CA-C-N	-8.66	115.07	123.04
1	A	619	LYS	C-N-CA	-8.66	115.07	123.04
1	A	535	VAL	CA-C-N	7.90	127.56	119.19
1	A	535	VAL	C-N-CA	7.90	127.56	119.19
1	A	624	HIS	CA-CB-CG	-7.80	106.00	113.80
1	A	255	HIS	CA-CB-CG	-7.69	106.11	113.80
1	A	522	LYS	N-CA-C	7.44	121.27	111.75
1	A	15	ASN	CA-CB-CG	-7.39	105.21	112.60
1	A	22	GLU	CA-C-N	-7.36	109.70	122.36
1	A	22	GLU	C-N-CA	-7.36	109.70	122.36
1	A	73	GLY	CA-C-N	7.31	127.35	119.89
1	A	73	GLY	C-N-CA	7.31	127.35	119.89
1	A	47	ALA	CA-C-O	7.08	124.85	118.33
1	A	24	VAL	N-CA-C	7.08	118.03	111.45
1	A	234	ASN	CA-CB-CG	-7.01	105.59	112.60
1	A	199	ARG	CB-CA-C	7.00	121.67	110.19
1	A	521	GLN	N-CA-C	7.00	122.07	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	VAL	N-CA-CB	-6.78	97.89	111.91
1	A	211	ARG	N-CA-CB	6.76	120.63	110.22
1	A	620	VAL	N-CA-C	6.65	115.89	108.05
1	A	674	ASP	CA-C-O	6.53	123.53	119.29
1	A	453	PHE	N-CA-C	6.46	120.26	112.38
1	A	508	MSE	CA-CB-CG	-6.40	101.30	114.10
1	A	262	GLU	N-CA-C	-6.38	100.20	109.59
1	A	534	TRP	N-CA-C	6.25	120.08	110.20
1	A	374	ASP	CA-C-N	-6.13	110.48	120.72
1	A	374	ASP	C-N-CA	-6.13	110.48	120.72
1	A	549	HIS	N-CA-C	-6.06	105.71	113.23
1	A	239	GLU	CB-CA-C	-6.02	97.86	109.37
1	A	40	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	270	ASP	N-CA-C	5.98	120.01	109.96
1	A	227	THR	N-CA-CB	-5.95	100.70	110.40
1	A	537	SER	N-CA-C	5.94	115.14	108.25
1	A	510	ALA	N-CA-C	5.91	120.62	113.17
1	A	174	LEU	N-CA-C	-5.87	104.80	111.14
1	A	315	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	120	PRO	N-CA-CB	5.80	108.47	103.36
1	A	271	CYS	CB-CA-C	-5.77	99.86	109.55
1	A	228	CYS	CB-CA-C	5.72	120.63	110.16
1	A	159	ASP	N-CA-CB	5.72	117.72	110.23
1	A	342	HIS	CA-CB-CG	5.71	119.51	113.80
1	A	60	ILE	N-CA-CB	-5.66	102.85	110.54
1	A	445	ARG	CB-CA-C	-5.58	100.43	109.13
1	A	359	GLU	N-CA-C	5.56	117.34	111.28
1	A	271	CYS	CA-C-O	5.55	125.16	119.05
1	A	336	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	508	MSE	N-CA-CB	-5.51	101.96	110.56
1	A	176	GLU	N-CA-CB	5.48	118.55	110.33
1	A	579	ILE	N-CA-C	5.47	114.11	109.02
1	A	679	PRO	CB-CA-C	-5.46	104.41	111.46
1	A	395	GLY	CA-C-N	5.45	124.79	118.85
1	A	395	GLY	C-N-CA	5.45	124.79	118.85
1	A	109	ILE	N-CA-C	5.45	116.49	111.81
1	A	536	PRO	N-CA-C	5.44	120.70	113.57
1	A	354	GLY	CA-C-N	-5.42	112.81	122.07
1	A	354	GLY	C-N-CA	-5.42	112.81	122.07
1	A	16	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	217	VAL	N-CA-CB	-5.39	102.81	111.82
1	A	698	PHE	CA-CB-CG	-5.39	108.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	569	PHE	N-CA-C	5.37	117.55	111.11
1	A	194	VAL	CB-CA-C	5.34	117.62	110.42
1	A	453	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	446	VAL	N-CA-C	5.33	115.87	108.84
1	A	26	PRO	CA-C-N	-5.30	114.06	119.94
1	A	26	PRO	C-N-CA	-5.30	114.06	119.94
1	A	122	MSE	CB-CA-C	-5.29	100.51	110.67
1	A	32	ALA	N-CA-C	5.27	116.71	111.07
1	A	376	LYS	CA-C-N	5.26	127.29	120.56
1	A	376	LYS	C-N-CA	5.26	127.29	120.56
1	A	181	GLU	CA-C-O	5.23	126.09	120.55
1	A	569	PHE	O-C-N	-5.18	116.70	122.09
1	A	705	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	167	ILE	CB-CA-C	-5.15	105.30	112.04
1	A	560	ILE	CB-CA-C	-5.13	105.32	112.04
1	A	71	ASN	CA-CB-CG	-5.12	107.48	112.60
1	A	382	ARG	N-CA-C	-5.09	106.48	113.30
1	A	179	PRO	N-CA-CB	5.04	107.69	103.25
1	A	28	THR	N-CA-C	5.03	121.51	110.80

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	5331	0	5096	137	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	137	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 13.

All (137) 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: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:228:CYS:C	1:A:229:ILE:HD13	2.06	0.80
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:291:LEU:O	1:A:295:GLN:HG3	1.85	0.76
1:A:457:THR:O	1:A:461:MSE: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:271:CYS:HB2	1:A:338:ARG:O	1.92	0.68
1:A:280:ALA:HB2	1:A:348:VAL:HG22	1.75	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:375:LEU:HD11	1:A:415:MSE:HE2	1.80	0.63
1:A:228:CYS:O	1:A:229:ILE:HD13	1.99	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:SER:C	1:A:72:PRO:HD3	2.31	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
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:283:LYS:NZ	1:A:359:GLU:OE2	2.32	0.53
1:A:92:VAL:HB	1:A:93:PRO:HD2	1.91	0.53
1:A:570:GLU:N	1:A:571:PRO:HD2	2.24	0.53
1:A:122:MSE:HE2	1:A:276:ALA:N	2.07	0.53
1:A:431:THR:O	1:A:432:SER:C	2.49	0.52
1:A:229:ILE:HD13	1:A:229:ILE:N	2.21	0.52
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: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:451:THR:HG23	1:A:489:ASN:CG	2.38	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:7:GLN:O	1:A:8:SER:C	2.55	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:416:ALA:O	1:A:419:THR:OG1	2.30	0.47
1:A:498:LEU:O	1:A:499:ARG:C	2.56	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:509:TRP:HZ3	1:A:521:GLN:CD	2.22	0.47
1:A:570:GLU:N	1:A:571:PRO:CD	2.78	0.47
1:A:177:SER:C	1:A:178:LEU:HD12	2.40	0.46
1:A:178:LEU:N	1:A:179:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:HG21	1:A:359:GLU:HG2	1.97	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:448:PHE:CD1	1:A:448:PHE:C	2.94	0.45
1:A:705:ASN:ND2	6:A:1042:HOH:O	2.49	0.45
1:A:19:PHE:O	1:A:20:VAL:C	2.56	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:HA	1:A:719:GLU:OE1	2.17	0.44
1:A:512:PRO:O	1:A:515:MSE:HE3	2.18	0.44
1:A:623:ILE:HG23	1:A:624:HIS:NE2	2.33	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:410:GLU:CD	1:A:445:ARG:HH12	2.24	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:39:PHE:HZ	1:A:362:LEU:HD12	1.82	0.44
1:A:630:GLU:HB2	6:A:1185:HOH:O	2.17	0.44
1:A:7:GLN:CG	1:A:36:TRP:HB3	2.38	0.43
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.67	0.43
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.74	0.43
1:A:508:MSE:HG3	1:A:534:TRP:HB2	1.96	0.43
1:A:139:TYR:CZ	1:A:167:ILE:HD12	2.54	0.43
1:A:448:PHE:C	1:A:448:PHE:HD1	2.26	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:400:ALA:O	1:A:403:ASN:HB3	2.20	0.42
1:A:709:GLU:HB2	1:A:710:PRO:HD3	2.01	0.42
1:A:154:MSE:H	1:A:154:MSE:HG3	1.66	0.42
1:A:362:LEU:O	1:A:366:MSE:HG2	2.20	0.42
1:A:568:GLU:O	1:A:571:PRO:HD2	2.20	0.42
1:A:243:ASP:O	1:A:249:GLY:HA3	2.20	0.42
1:A:617:CYS:HA	6:A:1121:HOH:O	2.19	0.42
1:A:185:TYR:HA	1:A:188:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:HG21	1:A:232:LYS:HB3	2.02	0.41
1:A:477:LYS:HB3	1:A:477:LYS:HE3	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:18:ARG:O	1:A:22:GLU:N	2.34	0.41
1:A:215:GLN:O	1:A:231:LEU:HA	2.20	0.41
1:A:174:LEU:O	1:A:175:ASP:C	2.62	0.41
1:A:174:LEU:HA	1:A:174:LEU:HD23	1.79	0.41
1:A:508:MSE:HG2	1:A:509:TRP:H	1.86	0.41
1:A:510:ALA:O	1:A:512:PRO:HD3	2.20	0.41
1:A:296:GLY:HA2	1:A:313:LEU:CD1	2.45	0.40
1:A:499:ARG:NH2	4:A:6000:SO4:O2	2.53	0.40
1:A:565:PHE:C	1:A:567:ALA:N	2.79	0.40
1:A:464:VAL:O	1:A:465:MSE:C	2.62	0.40
1:A:18:ARG:O	1:A:19:PHE:C	2.64	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%)	48	46

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%)	498 (94%)	33 (6%)	16	13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ILE
1	A	42	ILE
1	A	50	ASN
1	A	70	SER
1	A	78	LYS
1	A	83	SER
1	A	122	MSE
1	A	154	MSE
1	A	167	ILE
1	A	182	ASN
1	A	184	SER
1	A	192	LYS
1	A	207	GLU
1	A	227	THR
1	A	228	CYS
1	A	229	ILE
1	A	260	ILE
1	A	275	VAL
1	A	281	GLU
1	A	286	LEU
1	A	325	SER
1	A	327	ILE
1	A	352	SER
1	A	430	ARG
1	A	448	PHE
1	A	473	LYS
1	A	477	LYS
1	A	508	MSE
1	A	623	ILE

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Mol	Chain	Res	Type
1	A	629	MSE
1	A	694	SER
1	A	718	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	197	GLN
1	A	295	GLN
1	A	403	ASN
1	A	418	ASN
1	A	441	GLN
1	A	521	GLN
1	A	705	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
4	SO4	A	6000	-	4,4,4	0.97	0	6,6,6	0.38	0
4	SO4	A	8000	-	4,4,4	1.15	0	6,6,6	0.35	0
2	SOR	A	4000	-	11,11,11	0.42	0	14,14,14	1.14	1 (7%)
4	SO4	A	5000	-	4,4,4	0.93	0	6,6,6	0.16	0
4	SO4	A	9000	-	4,4,4	0.91	0	6,6,6	0.14	0
5	GLV	A	2000	3	4,4,4	1.58	1 (25%)	3,4,4	1.66	1 (33%)
4	SO4	A	7000	-	4,4,4	1.70	1 (25%)	6,6,6	0.37	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
2	SOR	A	4000	-	-	2/16/16/16	-
5	GLV	A	2000	3	-	0/0/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2000	GLV	C1-C2	2.82	1.50	1.44
4	A	7000	SO4	O1-S	2.68	1.60	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2000	GLV	O3-C2-C1	2.22	119.98	113.42
2	A	4000	SOR	C5-C4-C3	-2.06	109.31	112.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4000	SOR	O3-C3-C4-O4
2	A	4000	SOR	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6000	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	688/723 (95%)	-0.64	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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	7000	5/5	0.67	0.14	100,100,100,100	0
4	SO4	A	8000	5/5	0.75	0.13	98,98,100,100	0
4	SO4	A	9000	5/5	0.77	0.14	95,95,100,100	0
4	SO4	A	6000	5/5	0.79	0.11	77,81,82,86	0
4	SO4	A	5000	5/5	0.84	0.12	88,88,89,91	0
2	SOR	A	4000	12/12	0.94	0.08	24,38,97,100	0
5	GLV	A	2000	5/5	0.96	0.06	21,23,33,33	0
3	MG	A	3001	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.