



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:53 AM UTC

PDB ID : 1EF8 / pdb_00001ef8
Title : CRYSTAL STRUCTURE OF METHYLMALONYL COA DECARBOXY-
LASE
Authors : Benning, M.M.; Haller, T.; Gerlt, J.A.; Holden, H.M.
Deposited on : 2000-02-07
Resolution : 1.85 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

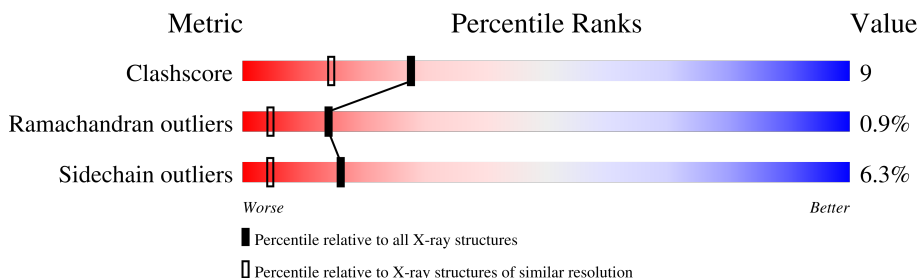
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	 81% 14% . .
1	B	261	 72% 20% 5% .
1	C	261	 74% 19% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6570 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 METHYLMALONYL COA DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2013	1282	343	376	12			
1	B	253	Total	C	N	O	S	0	0	0
			1985	1262	340	371	12			
1	C	250	Total	C	N	O	S	0	0	0
			1968	1253	337	366	12			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	189	Total	O	0	0
			189	189		
3	C	193	Total	O	0	0
			193	193		

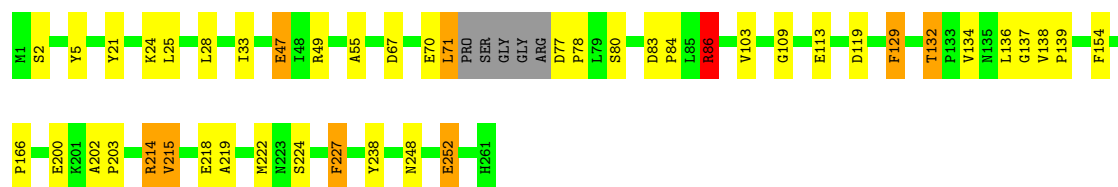
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

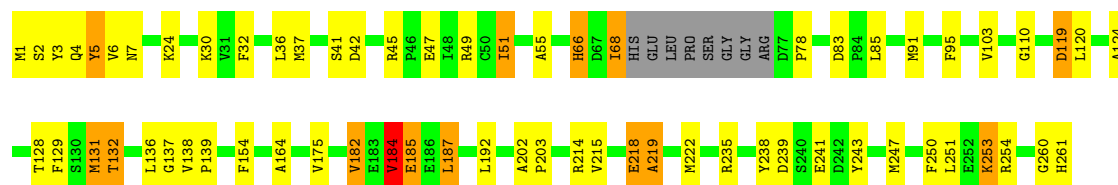
• Molecule 1: METHYLMALONYL COA DECARBOXYLASE

Chain A: 



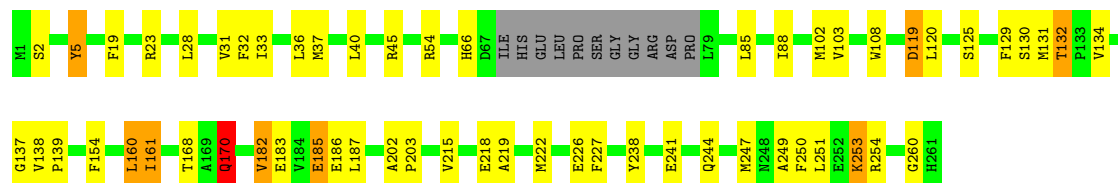
• Molecule 1: METHYLMALONYL COA DECARBOXYLASE

Chain B: 



• Molecule 1: METHYLMALONYL COA DECARBOXYLASE

Chain C: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.30Å 115.40Å 80.30Å 90.00° 127.80° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85	Depositor
% Data completeness (in resolution range)	89.0 (30.00-1.85)	Depositor
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.178 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6570	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
NI

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	1.23	2/2051 (0.1%)	1.29	11/2773 (0.4%)
1	B	1.20	3/2022 (0.1%)	1.25	11/2734 (0.4%)
1	C	1.21	1/2005 (0.0%)	1.26	9/2709 (0.3%)
All	All	1.22	6/6078 (0.1%)	1.27	31/8216 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	LYS	C-N	-6.71	1.25	1.33
1	C	130	SER	C-N	6.26	1.42	1.33
1	A	214	ARG	C-N	-5.72	1.26	1.33
1	B	175	VAL	CA-CB	-5.21	1.48	1.54
1	B	41	SER	N-CA	-5.12	1.40	1.46
1	A	86	ARG	CD-NE	-5.06	1.39	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	PHE	CA-CB-CG	10.81	124.61	113.80
1	A	103	VAL	N-CA-C	9.16	121.37	107.99
1	B	103	VAL	N-CA-C	9.03	121.27	108.36
1	A	5	TYR	N-CA-C	8.88	123.84	112.92
1	C	103	VAL	N-CA-C	8.83	120.99	108.36
1	C	138	VAL	N-CA-C	8.61	116.03	108.63
1	B	138	VAL	N-CA-C	7.99	115.50	108.63
1	B	119	ASP	N-CA-C	7.27	119.29	111.36
1	A	132	THR	N-CA-C	7.13	125.58	109.81
1	A	138	VAL	N-CA-C	6.94	114.60	108.63
1	C	132	THR	N-CA-C	6.85	124.95	109.81
1	B	132	THR	N-CA-C	6.69	124.60	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ASP	N-CA-C	6.45	118.39	111.36
1	C	170	GLN	N-CA-CB	6.41	120.21	110.28
1	B	5	TYR	N-CA-C	6.38	121.20	113.17
1	B	184	VAL	N-CA-CB	6.25	118.28	110.47
1	C	5	TYR	N-CA-C	6.24	120.89	113.28
1	B	83	ASP	CA-CB-CG	-5.89	106.71	112.60
1	C	227	PHE	CA-CB-CG	-5.71	108.08	113.80
1	B	66	HIS	N-CA-C	5.68	118.47	110.23
1	B	239	ASP	CA-CB-CG	5.47	118.08	112.60
1	A	55	ALA	N-CA-C	-5.45	103.27	110.40
1	A	119	ASP	N-CA-C	5.31	118.22	111.69
1	A	77	ASP	CA-CB-CG	5.25	117.86	112.60
1	C	161	ILE	N-CA-C	5.22	115.99	110.72
1	B	55	ALA	N-CA-C	-5.21	103.58	110.40
1	C	108	TRP	N-CA-C	5.19	117.90	109.24
1	A	28	LEU	N-CA-C	5.10	118.61	110.70
1	A	86	ARG	NE-CZ-NH2	-5.07	114.63	119.20
1	A	129	PHE	N-CA-C	5.06	117.31	108.76
1	B	219	ALA	N-CA-C	5.04	121.52	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	2013	0	2021	32	0
1	B	1985	0	1995	46	0
1	C	1968	0	1980	41	0
2	A	1	0	0	0	0
3	A	221	0	0	5	0
3	B	189	0	0	3	0
3	C	193	0	0	3	0
All	All	6570	0	5996	108	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 9.

All (108) 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:B:68:ILE:HD11	1:B:250:PHE:CE1	2.04	0.93
1:B:68:ILE:HD11	1:B:250:PHE:HE1	1.38	0.88
1:C:28:LEU:HB3	1:C:33:ILE:HD11	1.61	0.81
1:B:66:HIS:CE1	1:B:85:LEU:HD22	2.16	0.81
1:B:136:LEU:HB3	1:B:247:MET:HE2	1.68	0.76
1:C:131:MET:SD	1:C:161:ILE:HG12	2.28	0.73
1:C:37:MET:HG2	1:C:88:ILE:HD12	1.70	0.72
1:C:66:HIS:HE1	1:C:85:LEU:HD22	1.54	0.71
1:A:224:SER:HA	1:A:227:PHE:CD1	2.26	0.70
1:A:222:MET:HE1	1:B:215:VAL:HG12	1.75	0.68
1:B:78:PRO:HD2	1:B:238:TYR:OH	1.94	0.67
1:A:78:PRO:HD2	1:A:238:TYR:CZ	2.30	0.67
1:C:131:MET:HE3	1:C:160:LEU:HD23	1.79	0.64
1:C:28:LEU:HB3	1:C:33:ILE:CD1	2.28	0.64
1:B:136:LEU:HB3	1:B:247:MET:CE	2.29	0.62
1:C:66:HIS:CE1	1:C:85:LEU:HD22	2.33	0.62
1:A:222:MET:HG2	1:A:227:PHE:CE2	2.35	0.61
1:B:66:HIS:HE1	1:B:85:LEU:HD22	1.65	0.61
1:B:5:TYR:HB3	1:B:32:PHE:HD1	1.66	0.61
1:C:139:PRO:HG2	1:C:238:TYR:CZ	2.38	0.58
1:C:250:PHE:O	1:C:253:LYS:HD3	2.04	0.58
1:C:31:VAL:HG22	3:C:665:HOH:O	2.03	0.58
1:B:66:HIS:CE1	1:B:110:GLY:HA3	2.39	0.57
1:C:131:MET:SD	1:C:161:ILE:CG1	2.91	0.57
1:B:185:GLU:H	1:B:185:GLU:CD	2.12	0.57
1:B:49:ARG:NH1	3:B:785:HOH:O	2.29	0.57
1:B:68:ILE:HD11	1:B:250:PHE:CD1	2.40	0.56
1:B:42:ASP:O	1:B:45:ARG:HD3	2.07	0.55
1:A:214:ARG:O	1:A:218:GLU:HG2	2.07	0.54
1:B:6:VAL:HG11	1:B:36:LEU:HD23	1.89	0.54
1:A:248:ASN:O	1:A:252:GLU:HB2	2.07	0.54
1:C:182:VAL:HG21	1:C:187:LEU:HA	1.89	0.53
1:A:24:LYS:HG3	3:A:344:HOH:O	2.09	0.53
1:B:214:ARG:O	1:B:218:GLU:HG2	2.09	0.53
1:B:78:PRO:HD2	1:B:238:TYR:CZ	2.44	0.52
1:B:7:ASN:HB3	3:B:849:HOH:O	2.08	0.52
1:A:47:GLU:H	1:A:47:GLU:CD	2.19	0.51
1:B:37:MET:HE3	1:B:91:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ALA:HB1	1:C:254:ARG:O	2.11	0.51
1:B:254:ARG:HD2	3:B:679:HOH:O	2.10	0.51
1:C:139:PRO:HG2	1:C:238:TYR:CE1	2.47	0.50
1:B:139:PRO:HG2	1:B:238:TYR:CZ	2.47	0.50
1:B:243:TYR:CE1	1:B:247:MET:HE3	2.47	0.49
1:C:131:MET:HE3	1:C:160:LEU:HB3	1.94	0.49
1:B:137:GLY:HA2	1:C:202:ALA:CB	2.43	0.49
1:A:67:ASP:OD2	1:A:70:GLU:HG3	2.12	0.49
1:B:119:ASP:C	1:B:120:LEU:HD12	2.38	0.48
1:A:215:VAL:HG12	1:C:222:MET:HE1	1.96	0.48
1:A:137:GLY:HA2	1:B:202:ALA:CB	2.45	0.47
1:C:54:ARG:CZ	1:C:102:MET:HE1	2.44	0.47
1:A:80:SER:N	1:A:83:ASP:OD1	2.48	0.47
1:C:125:SER:HB3	3:C:820:HOH:O	2.15	0.47
1:B:51:ILE:CD1	1:B:95:PHE:CE2	2.98	0.47
1:A:224:SER:HA	1:A:227:PHE:HD1	1.76	0.46
1:B:51:ILE:CD1	1:B:95:PHE:HE2	2.28	0.46
1:C:182:VAL:HG23	1:C:183:GLU:O	2.16	0.46
1:B:222:MET:HE1	1:C:215:VAL:HG12	1.98	0.46
1:C:134:VAL:HG22	3:C:325:HOH:O	2.15	0.46
1:B:260:GLY:HA2	1:C:203:PRO:HG2	1.98	0.45
1:C:168:THR:HB	1:C:170:GLN:HE21	1.82	0.45
1:A:166:PRO:HD3	3:A:613:HOH:O	2.17	0.45
1:B:182:VAL:HG21	1:B:187:LEU:HA	1.98	0.44
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.59	0.44
1:C:129:PHE:N	1:C:129:PHE:CD1	2.86	0.44
1:A:222:MET:CG	1:A:227:PHE:CE2	3.00	0.44
1:B:124:ALA:HB1	1:B:184:VAL:HG13	1.99	0.44
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.80	0.44
1:C:185:GLU:CD	1:C:185:GLU:H	2.24	0.44
1:A:222:MET:HE1	1:B:215:VAL:CG1	2.44	0.44
1:A:83:ASP:HB3	1:A:84:PRO:HD2	2.00	0.44
1:B:3:TYR:OH	1:B:42:ASP:OD1	2.28	0.44
1:A:129:PHE:CD1	1:A:129:PHE:N	2.86	0.44
1:B:6:VAL:HG11	1:B:36:LEU:CD2	2.48	0.44
1:C:5:TYR:HB3	1:C:32:PHE:HD1	1.83	0.43
1:C:170:GLN:NE2	1:C:170:GLN:H	2.16	0.43
1:B:241:GLU:CD	1:B:261:HIS:CD2	2.97	0.43
1:C:170:GLN:H	1:C:170:GLN:CD	2.27	0.43
1:B:202:ALA:HA	1:B:203:PRO:HD2	1.91	0.43
1:A:86:ARG:HH22	1:A:113:GLU:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLU:OE2	1:C:226:GLU:HA	2.19	0.43
1:C:139:PRO:HD2	1:C:238:TYR:CE2	2.53	0.43
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.85	0.43
1:C:119:ASP:C	1:C:120:LEU:HD12	2.44	0.42
1:B:182:VAL:CG2	1:B:187:LEU:HA	2.49	0.42
1:A:24:LYS:O	1:A:25:LEU:HB2	2.20	0.42
1:A:200:GLU:HB2	3:A:730:HOH:O	2.18	0.42
1:C:19:PHE:CD1	1:C:32:PHE:HZ	2.37	0.42
1:A:203:PRO:HG2	1:C:260:GLY:HA2	2.02	0.42
1:A:222:MET:CE	1:B:215:VAL:CG1	2.97	0.42
1:A:248:ASN:O	1:A:252:GLU:N	2.36	0.42
1:A:86:ARG:NH2	1:A:113:GLU:OE2	2.41	0.42
1:B:131:MET:O	1:B:164:ALA:HA	2.19	0.42
1:B:128:THR:C	1:B:129:PHE:CD1	2.98	0.41
1:A:134:VAL:HG22	3:A:486:HOH:O	2.20	0.41
1:C:131:MET:HE3	1:C:160:LEU:CB	2.50	0.41
1:A:136:LEU:HD12	1:A:136:LEU:N	2.35	0.41
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.95	0.41
1:A:49:ARG:NH1	3:A:845:HOH:O	2.42	0.41
1:B:253:LYS:HD3	1:B:253:LYS:HA	1.88	0.41
1:B:66:HIS:NE2	1:B:85:LEU:HD22	2.36	0.41
1:A:202:ALA:CB	1:C:137:GLY:HA2	2.50	0.41
1:A:139:PRO:HD2	1:A:238:TYR:CE2	2.56	0.41
1:A:21:TYR:HH	1:A:24:LYS:HE3	1.86	0.40
1:B:222:MET:CE	1:C:215:VAL:HG12	2.51	0.40
1:C:40:LEU:HD23	1:C:40:LEU:HA	1.94	0.40
1:B:129:PHE:CD1	1:B:129:PHE:N	2.89	0.40
1:C:131:MET:CE	1:C:160:LEU:HD23	2.49	0.40
1:C:222:MET:HE2	1:C:222:MET:HB3	1.91	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	252/261 (97%)	242 (96%)	7 (3%)	3 (1%)	10	2
1	B	249/261 (95%)	240 (96%)	7 (3%)	2 (1%)	16	6
1	C	246/261 (94%)	234 (95%)	10 (4%)	2 (1%)	16	6
All	All	747/783 (95%)	716 (96%)	24 (3%)	7 (1%)	14	4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	ALA
1	A	219	ALA
1	C	219	ALA
1	B	132	THR
1	A	132	THR
1	C	132	THR
1	A	109	GLY

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	221/225 (98%)	213 (96%)	8 (4%)	31	16
1	B	218/225 (97%)	201 (92%)	17 (8%)	11	2
1	C	216/225 (96%)	200 (93%)	16 (7%)	13	3
All	All	655/675 (97%)	614 (94%)	41 (6%)	16	4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	33	ILE
1	A	47	GLU
1	A	71	LEU
1	A	86	ARG
1	A	154	PHE

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Mol	Chain	Res	Type
1	A	215	VAL
1	A	252	GLU
1	B	1	MET
1	B	2	SER
1	B	4	GLN
1	B	24	LYS
1	B	47	GLU
1	B	51	ILE
1	B	68	ILE
1	B	131	MET
1	B	154	PHE
1	B	182	VAL
1	B	184	VAL
1	B	185	GLU
1	B	187	LEU
1	B	218	GLU
1	B	235	ARG
1	B	251	LEU
1	B	253	LYS
1	C	2	SER
1	C	23	ARG
1	C	36	LEU
1	C	45	ARG
1	C	154	PHE
1	C	160	LEU
1	C	170	GLN
1	C	182	VAL
1	C	185	GLU
1	C	186	GLU
1	C	218	GLU
1	C	241	GLU
1	C	244	GLN
1	C	247	MET
1	C	251	LEU
1	C	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	ASN
1	A	44	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	248	ASN
1	B	4	GLN
1	B	7	ASN
1	B	44	ASN
1	B	66	HIS
1	B	248	ASN
1	C	7	ASN
1	C	12	ASN
1	C	44	ASN
1	C	66	HIS
1	C	170	GLN
1	C	248	ASN
1	C	261	HIS

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.