



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:44 PM GMT

PDB ID : 2X58
Title : THE CRYSTAL STRUCTURE OF MFE1 LIGANDED WITH COA
Authors : Kasaragod, P.; Venkatesan, R.; Kiema, T.R.; Hiltunen, J.K.; Wierenga, R.K.
Deposited on : 2010-02-05
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

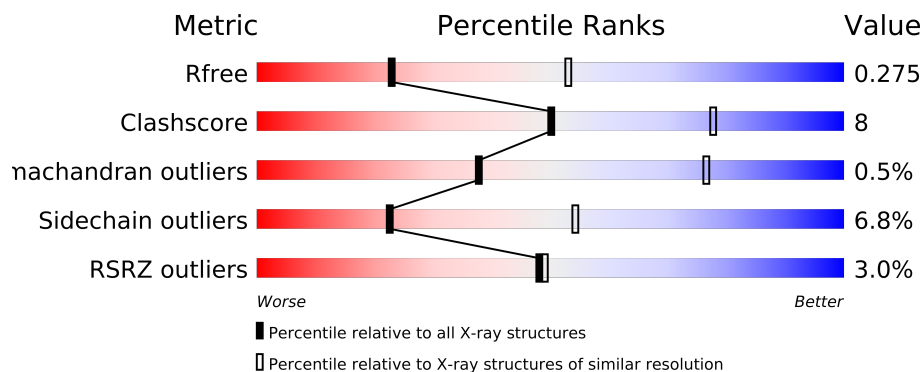
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 ≥ 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	727	
1	B	727	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	B	770	-	X
5	SO4	A	1722	-	X
5	SO4	A	1723	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11489 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5562	3553	976	1010	23			
1	B	721	Total	C	N	O	S	0	1	0
			5534	3537	969	1005	23			

There are 10 discrepancies between the modelled and reference sequences:

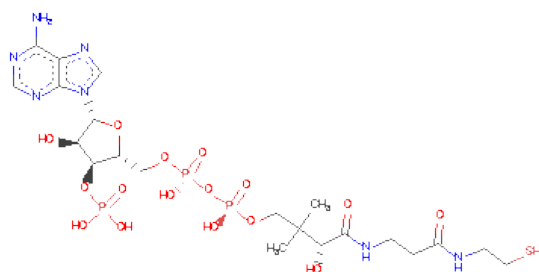
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	EXPRESSION TAG	UNP P07896
A	-3	ARG	-	EXPRESSION TAG	UNP P07896
A	-2	GLY	-	EXPRESSION TAG	UNP P07896
A	-1	SER	-	EXPRESSION TAG	UNP P07896
A	0	HIS	-	EXPRESSION TAG	UNP P07896
B	-4	PRO	-	EXPRESSION TAG	UNP P07896
B	-3	ARG	-	EXPRESSION TAG	UNP P07896
B	-2	GLY	-	EXPRESSION TAG	UNP P07896
B	-1	SER	-	EXPRESSION TAG	UNP P07896
B	0	HIS	-	EXPRESSION TAG	UNP P07896

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



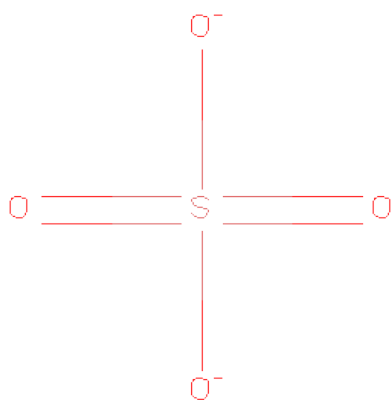
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

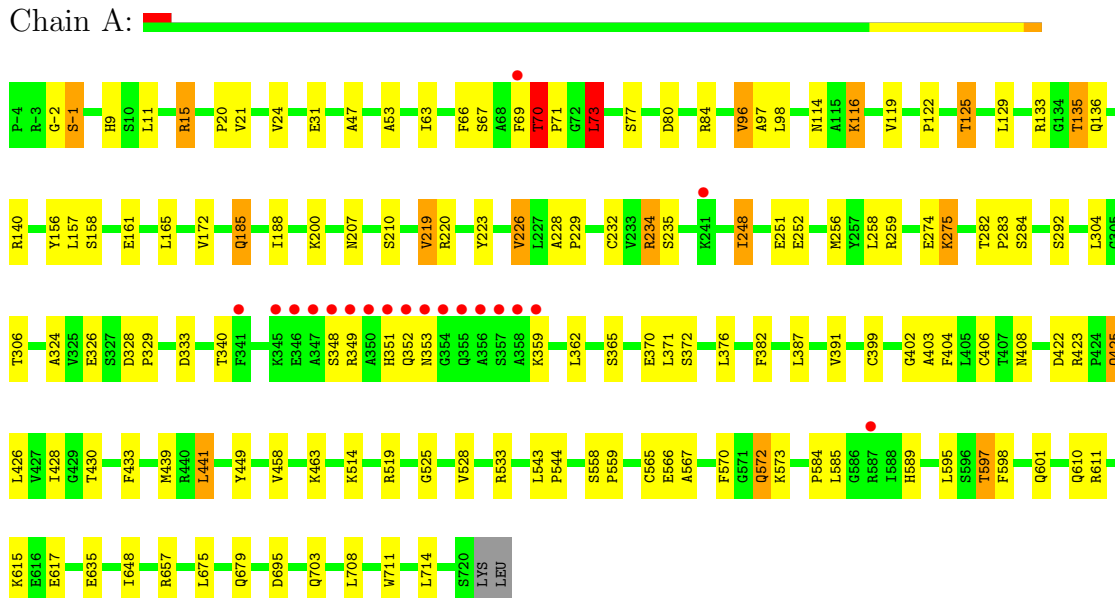
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total	O	0	0
			156	156		
6	B	71	Total	O	0	0
			71	71		

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.

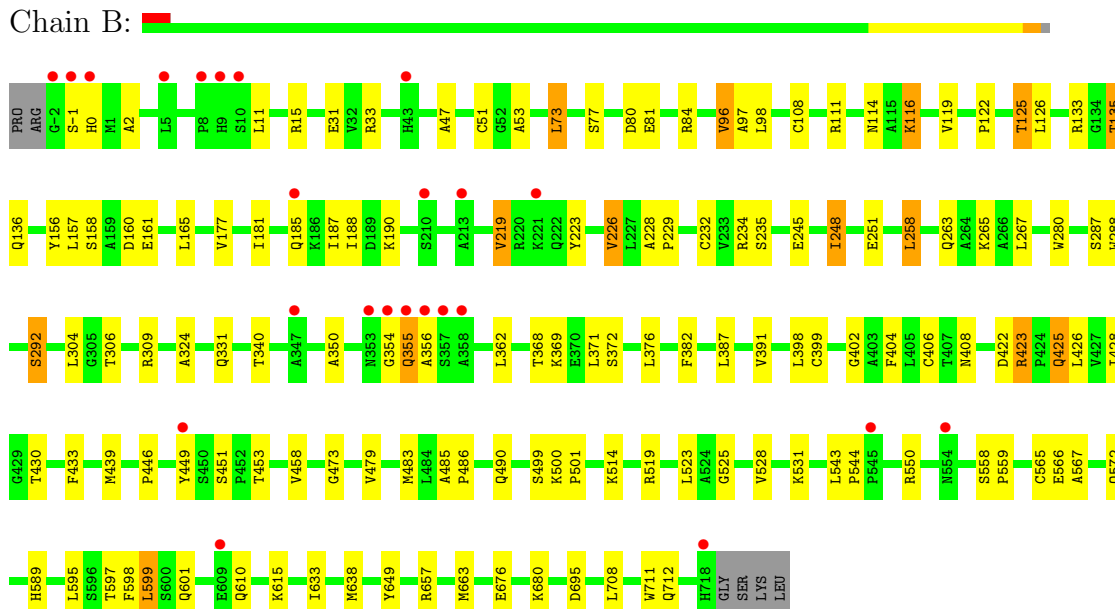
• Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

Chain A:



• Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.70Å 126.50Å 227.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.80 45.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.19-2.80) 97.9 (45.57-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.282 0.219 , 0.275	Depositor DCC
R_{free} test set	2364 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 11.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46591 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11489	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: COA, GOL, SO4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.66	0/5691	0.74	3/7709 (0.0%)
1	B	0.72	1/5662 (0.0%)	0.75	2/7671 (0.0%)
All	All	0.69	1/11353 (0.0%)	0.75	5/15380 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	CYS	CB-SG	-5.38	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	234	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	234	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	73	LEU	CB-CG-CD2	-5.47	101.71	111.00
1	B	676	GLU	CB-CA-C	-5.13	100.13	110.40

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	5562	0	5667	85	0
1	B	5534	0	5637	84	0
2	A	27	0	12	1	0
3	A	48	0	32	4	0
3	B	48	0	32	0	0
4	A	6	0	8	0	0
4	B	12	0	16	1	0
5	A	15	0	0	0	0
5	B	10	0	0	0	0
6	A	156	0	0	4	0
6	B	71	0	0	3	0
All	All	11489	0	11404	170	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 8.

All (170) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:597:THR:HG22	1:B:382:PHE:CE2	1.96	1.01
1:A:597:THR:HG22	1:B:382:PHE:HE2	1.39	0.88
1:B:96:VAL:HG13	1:B:98:LEU:HG	1.57	0.85
1:B:177:VAL:O	1:B:181:ILE:HD12	1.75	0.84
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.13	0.82
1:A:635:GLU:HG2	6:A:2144:HOH:O	1.78	0.81
1:B:368:THR:HG21	6:B:2041:HOH:O	1.85	0.76
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.20	0.76
1:A:122:PRO:O	1:A:125:THR:HB	1.87	0.75
1:A:282:THR:HG1	1:A:284:SER:HG	1.35	0.73
1:B:161:GLU:O	1:B:165:LEU:HB2	1.88	0.73
1:B:73:LEU:HD12	1:B:73:LEU:H	1.56	0.71
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.27	0.70
1:B:160:ASP:HB3	1:B:354:GLY:HA3	1.73	0.70
1:B:33:ARG:NH1	1:B:81:GLU:OE1	2.24	0.68
1:A:135:THR:HG21	1:A:235:SER:OG	1.92	0.67
1:A:133:ARG:HD2	1:A:248:ILE:CD1	2.23	0.67
1:A:73:LEU:HD21	1:A:252:GLU:OE2	1.95	0.67
1:B:372:SER:HA	1:B:399:CYS:HA	1.75	0.67
4:B:770:GOL:O1	4:B:770:GOL:O3	2.12	0.67
1:B:122:PRO:O	1:B:125:THR:HB	1.96	0.65
1:A:67:SER:HB2	1:A:70:THR:OG1	1.95	0.65
1:A:161:GLU:O	1:A:165:LEU:HB2	1.97	0.64
1:A:372:SER:HA	1:A:399:CYS:HA	1.78	0.64
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:595:LEU:HG	1:B:599:LEU:HD22	1.79	0.64
1:A:525:GLY:O	1:A:528:VAL:HG12	1.97	0.64
1:B:80:ASP:O	1:B:84:ARG:HG3	1.98	0.63
1:B:525:GLY:O	1:B:528:VAL:HG12	1.99	0.62
1:A:96:VAL:HG13	1:A:98:LEU:HG	1.83	0.60
1:B:158:SER:OG	1:B:161:GLU:HG2	2.02	0.59
1:B:15:ARG:CD	1:B:53:ALA:HB2	2.33	0.59
1:A:133:ARG:HD2	1:A:248:ILE:HD11	1.83	0.59
1:B:73:LEU:HD12	1:B:73:LEU:N	2.16	0.59
1:A:387:LEU:O	1:A:391:VAL:HG23	2.03	0.59
1:B:387:LEU:O	1:B:391:VAL:HG23	2.03	0.59
1:A:-2:GLY:HA2	1:A:31:GLU:OE2	2.02	0.59
1:A:403:ALA:HA	6:A:2099:HOH:O	2.02	0.58
1:B:595:LEU:HD12	1:B:598:PHE:HD2	1.69	0.58
1:A:223:TYR:HB3	1:A:226:VAL:HG13	1.87	0.57
1:A:349:ARG:HA	1:A:352:GLN:HG2	1.87	0.57
1:A:15:ARG:HD2	1:A:53:ALA:HB2	1.87	0.57
1:B:15:ARG:HD2	1:B:53:ALA:HB2	1.86	0.56
1:A:136:GLN:HG3	1:A:248:ILE:HD13	1.85	0.56
1:B:406:CYS:HA	1:B:428:ILE:O	2.04	0.56
1:B:663:MET:CE	1:B:663:MET:HA	2.36	0.56
1:B:473:GLY:HA3	1:B:638:MET:SD	2.46	0.56
1:A:63:ILE:HA	1:A:66:PHE:HD1	1.71	0.56
1:B:708:LEU:HA	1:B:711:TRP:CE2	2.42	0.55
1:B:2:ALA:HB3	1:B:31:GLU:HB3	1.89	0.55
1:B:304:LEU:HD11	1:B:324:ALA:HB1	1.87	0.55
1:A:63:ILE:HA	1:A:66:PHE:CD1	2.42	0.54
1:B:160:ASP:CB	1:B:354:GLY:HA3	2.36	0.54
3:A:760:COA:O9P	3:A:760:COA:H131	2.08	0.54
1:B:479:VAL:HG22	1:B:633:ILE:HG21	1.90	0.52
1:B:135:THR:HG22	1:B:251:GLU:OE2	2.09	0.52
1:A:135:THR:HG22	1:A:251:GLU:OE2	2.09	0.52
1:B:136:GLN:HG3	1:B:248:ILE:HD13	1.91	0.52
1:B:267:LEU:HD23	1:B:657:ARG:HG2	1.91	0.52
1:B:114:ASN:OD1	1:B:116:LYS:HG2	2.10	0.52
1:A:71:PRO:HD2	1:A:259:ARG:HD2	1.92	0.51
1:B:406:CYS:HB3	1:B:430:THR:HG23	1.90	0.51
1:B:219:VAL:HG22	1:B:229:PRO:HB2	1.93	0.51
1:B:425:GLN:HG3	1:B:449:TYR:O	2.09	0.51
1:B:228:ALA:HB3	1:B:229:PRO:HD3	1.94	0.50
3:A:760:COA:H62	3:A:760:COA:N7A	2.27	0.50
1:A:158:SER:OG	1:A:161:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:712:GLN:OE1	1:B:712:GLN:HA	2.11	0.50
1:B:565:CYS:C	1:B:567:ALA:H	2.15	0.50
1:B:408:ASN:CG	1:B:408:ASN:O	2.48	0.50
1:A:73:LEU:HD11	1:A:252:GLU:HG3	1.94	0.50
1:A:376:LEU:HD12	1:A:404:PHE:HB2	1.93	0.50
1:B:402:GLY:HA2	1:B:426:LEU:HD11	1.93	0.50
1:B:292:SER:O	1:B:453:THR:HG23	2.13	0.49
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.48	0.49
1:A:133:ARG:HD2	1:A:248:ILE:HD12	1.93	0.49
1:A:402:GLY:HA2	1:A:426:LEU:HD11	1.94	0.49
1:A:348:SER:HA	1:A:351:HIS:HB2	1.94	0.49
1:B:245:GLU:CD	1:B:245:GLU:H	2.15	0.49
1:B:223:TYR:HB3	1:B:226:VAL:HG13	1.94	0.48
1:B:226:VAL:HA	1:B:263:GLN:HE22	1.77	0.48
1:B:428:ILE:HG21	1:B:458:VAL:HG21	1.95	0.48
1:B:663:MET:HE2	1:B:663:MET:HA	1.95	0.48
1:A:15:ARG:CD	1:A:53:ALA:HB2	2.42	0.48
3:A:760:COA:O9P	3:A:760:COA:CDP	2.62	0.48
1:A:67:SER:H	1:A:71:PRO:HD3	1.79	0.47
1:A:533:ARG:HG3	1:A:533:ARG:HH11	1.78	0.47
1:A:274:GLU:OE2	1:A:657:ARG:NH2	2.47	0.47
1:A:597:THR:CG2	1:B:382:PHE:CE2	2.85	0.47
1:B:369:LYS:HA	1:B:398:LEU:HD21	1.97	0.47
1:B:433:PHE:O	1:B:439:MET:HB2	2.15	0.47
1:B:248:ILE:HD12	1:B:248:ILE:HA	1.75	0.47
1:A:441:LEU:HD11	1:A:648:ILE:HG23	1.97	0.47
1:A:463:LYS:HE3	6:A:2085:HOH:O	2.15	0.47
1:B:280:TRP:O	1:B:288:TRP:HD1	1.98	0.47
1:B:15:ARG:HD3	1:B:53:ALA:HB2	1.97	0.47
1:B:428:ILE:HG13	1:B:446:PRO:HA	1.97	0.46
1:A:408:ASN:CG	1:A:408:ASN:O	2.54	0.46
1:A:425:GLN:HG3	1:A:449:TYR:O	2.15	0.46
1:B:350:ALA:HB1	1:B:355:GLN:HB3	1.98	0.46
1:A:80:ASP:O	1:A:84:ARG:HG3	2.15	0.46
1:B:187:ILE:HG22	1:B:190:LYS:HD2	1.98	0.45
1:A:20:PRO:HG2	1:A:21:VAL:HG22	1.97	0.45
1:A:63:ILE:HB	3:A:760:COA:C6A	2.47	0.45
1:B:135:THR:HG21	1:B:235:SER:OG	2.16	0.45
1:B:425:GLN:HG2	1:B:451:SER:HB3	1.98	0.45
1:A:275:LYS:HD3	1:A:275:LYS:HA	1.62	0.45
1:A:226:VAL:HG22	1:A:229:PRO:HD3	1.99	0.45
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:543:LEU:HD12	1:A:544:PRO:HD2	1.99	0.44
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.98	0.44
1:A:-1:SER:N	1:A:31:GLU:OE2	2.51	0.44
1:A:220:ARG:O	6:A:2060:HOH:O	2.21	0.44
1:B:485:ALA:HB3	1:B:486:PRO:HD3	2.00	0.44
1:B:490:GLN:HA	1:B:490:GLN:OE1	2.17	0.44
1:B:228:ALA:N	1:B:229:PRO:CD	2.81	0.44
1:B:483:MET:O	1:B:486:PRO:HD2	2.18	0.44
1:A:129:LEU:C	1:A:129:LEU:HD12	2.38	0.43
1:B:125:THR:HG22	1:B:126:LEU:HG	2.00	0.43
1:B:595:LEU:HA	1:B:598:PHE:HB3	2.00	0.43
1:B:680:LYS:HA	6:B:2066:HOH:O	2.18	0.43
1:A:11:LEU:HD22	1:A:47:ALA:HB3	2.01	0.43
1:B:368:THR:O	1:B:398:LEU:HD21	2.19	0.43
1:B:531:LYS:HE2	1:B:531:LYS:HB3	1.93	0.43
1:A:406:CYS:HB3	1:A:430:THR:HG23	2.00	0.43
1:A:219:VAL:HG22	1:A:229:PRO:HB2	1.99	0.43
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.48	0.43
1:B:156:TYR:CD2	1:B:156:TYR:N	2.87	0.43
1:A:584:PRO:O	1:A:585:LEU:HB2	2.19	0.43
1:A:595:LEU:HD12	1:A:598:PHE:HD2	1.84	0.43
1:B:376:LEU:HD12	1:B:404:PHE:HB2	2.01	0.43
1:B:423:ARG:HA	6:B:2044:HOH:O	2.18	0.43
1:A:97:ALA:HB3	1:A:119:VAL:HG12	2.01	0.42
1:B:15:ARG:HA	1:B:51:CYS:O	2.20	0.42
1:A:9:HIS:HB3	1:A:185:GLN:HE22	1.84	0.42
1:A:133:ARG:CD	1:A:248:ILE:HD12	2.50	0.42
1:B:133:ARG:HD2	1:B:248:ILE:CD1	2.50	0.42
1:A:573:LYS:HA	1:A:585:LEU:HD12	2.00	0.42
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.94	0.42
1:A:703:GLN:OE1	1:A:714:LEU:HB3	2.20	0.42
1:A:565:CYS:C	1:A:567:ALA:H	2.23	0.42
1:A:229:PRO:O	1:A:232:CYS:HB2	2.20	0.42
1:B:108:CYS:O	1:B:111:ARG:NH1	2.53	0.42
1:A:365:SER:CB	1:A:370:GLU:HG3	2.50	0.42
1:A:326:GLU:OE1	2:A:750:ADP:H1'	2.20	0.42
1:B:11:LEU:HD22	1:B:47:ALA:HB3	2.01	0.42
1:A:428:ILE:HG21	1:A:458:VAL:HG21	2.02	0.41
1:B:309:ARG:NH2	1:B:331:GLN:OE1	2.53	0.41
1:A:226:VAL:HG22	1:A:229:PRO:CD	2.49	0.41
1:A:185:GLN:H	1:A:185:GLN:HG2	1.71	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:ASN:OD1	1:A:116:LYS:HG2	2.21	0.41
1:B:350:ALA:HB1	1:B:355:GLN:HG2	2.03	0.41
1:A:207:ASN:O	1:A:210:SER:HB3	2.20	0.41
1:A:433:PHE:O	1:A:439:MET:HB2	2.20	0.41
1:A:140:ARG:NE	1:A:200:LYS:O	2.53	0.41
1:A:525:GLY:HA2	1:A:570:PHE:O	2.21	0.41
1:B:499:SER:OG	1:B:500:LYS:N	2.54	0.41
1:A:611:ARG:NH2	1:A:617:GLU:OE1	2.54	0.41
1:B:558:SER:HA	1:B:559:PRO:HD3	1.89	0.41
1:A:156:TYR:CD2	1:A:156:TYR:N	2.89	0.41
1:A:558:SER:HA	1:A:559:PRO:HD3	1.86	0.41
1:A:228:ALA:HB3	1:A:229:PRO:HD3	2.02	0.40
1:B:156:TYR:HD2	1:B:156:TYR:N	2.19	0.40
1:A:349:ARG:O	1:A:353:ASN:ND2	2.54	0.40
1:A:533:ARG:HG3	1:A:533:ARG:NH1	2.37	0.40
1:A:406:CYS:HA	1:A:428:ILE:O	2.21	0.40
1:B:483:MET:HE2	1:B:649:TYR:CE1	2.56	0.40
1:A:223:TYR:HB3	1:A:226:VAL:CG1	2.51	0.40
1:A:572:GLN:HE21	1:A:572:GLN:HB3	1.63	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	723/727 (99%)	669 (92%)	50 (7%)	4 (1%)	33	72
1	B	719/727 (99%)	664 (92%)	52 (7%)	3 (0%)	43	80
All	All	1442/1454 (99%)	1333 (92%)	102 (7%)	7 (0%)	38	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	566	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	-1	SER
1	A	382	PHE
1	B	356	ALA
1	A	566	GLU
1	A	70	THR
1	B	544	PRO

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	594/596 (100%)	552 (93%)	42 (7%)	21	51
1	B	591/596 (99%)	553 (94%)	38 (6%)	25	58
All	All	1185/1192 (99%)	1105 (93%)	80 (7%)	22	54

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	24	VAL
1	A	69	PHE
1	A	70	THR
1	A	73	LEU
1	A	77	SER
1	A	96	VAL
1	A	116	LYS
1	A	125	THR
1	A	135	THR
1	A	157	LEU
1	A	172	VAL
1	A	185	GLN
1	A	188	ILE
1	A	219	VAL
1	A	226	VAL
1	A	234	ARG
1	A	248	ILE
1	A	256	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	258	LEU
1	A	275	LYS
1	A	283	PRO
1	A	292	SER
1	A	306	THR
1	A	333	ASP
1	A	340	THR
1	A	359	LYS
1	A	362	LEU
1	A	371	LEU
1	A	422	ASP
1	A	423	ARG
1	A	425	GLN
1	A	441	LEU
1	A	514	LYS
1	A	572	GLN
1	A	597	THR
1	A	601	GLN
1	A	610	GLN
1	A	615	LYS
1	A	675	LEU
1	A	679	GLN
1	A	695	ASP
1	B	-1	SER
1	B	0	HIS
1	B	73	LEU
1	B	77	SER
1	B	96	VAL
1	B	116	LYS
1	B	125	THR
1	B	135	THR
1	B	157	LEU
1	B	185	GLN
1	B	188	ILE
1	B	219	VAL
1	B	226	VAL
1	B	248	ILE
1	B	258	LEU
1	B	265	LYS
1	B	287	SER
1	B	292	SER
1	B	306	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	340	THR
1	B	355	GLN
1	B	362	LEU
1	B	371	LEU
1	B	422	ASP
1	B	423	ARG
1	B	425	GLN
1	B	501	PRO
1	B	514	LYS
1	B	523	LEU
1	B	543	LEU
1	B	550	ARG
1	B	572	GLN
1	B	597	THR
1	B	599	LEU
1	B	601	GLN
1	B	610	GLN
1	B	615	LYS
1	B	695	ASP

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

Mol	Chain	Res	Type
1	A	353	ASN
1	A	572	GLN
1	A	601	GLN
1	B	278	ASN
1	B	572	GLN
1	B	589	HIS
1	B	679	GLN
1	B	718	HIS

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 ⓘ

11 ligands are modelled in this entry.

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	SO4	A	1721	-	4,4,4	0.13	0	6,6,6	0.22	0
5	SO4	A	1722	-	4,4,4	0.20	0	6,6,6	0.35	0
5	SO4	A	1723	-	4,4,4	0.16	0	6,6,6	0.20	0
2	ADP	A	750	-	29,29,29	1.34	3 (10%)	45,45,45	2.19	12 (26%)
3	COA	A	760	-	50,50,50	1.56	3 (6%)	75,75,75	2.07	11 (14%)
4	GOL	A	770	-	5,5,5	0.26	0	5,5,5	0.84	0
5	SO4	B	1719	-	4,4,4	0.11	0	6,6,6	0.11	0
5	SO4	B	1720	-	4,4,4	0.26	0	6,6,6	0.48	0
3	COA	B	760	-	50,50,50	1.53	3 (6%)	75,75,75	1.81	12 (16%)
4	GOL	B	770	-	5,5,5	0.33	0	5,5,5	0.63	0
4	GOL	B	780	-	5,5,5	0.29	0	5,5,5	0.32	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	SO4	A	1721	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1722	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1723	-	-	0/0/0/0	0/0/0/0
2	ADP	A	750	-	-	0/16/32/32	0/1/3/3
3	COA	A	760	-	-	0/48/64/64	0/1/3/3
4	GOL	A	770	-	-	0/4/4/4	0/0/0/0
5	SO4	B	1719	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1720	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	760	-	-	0/48/64/64	0/1/3/3
4	GOL	B	770	-	-	0/4/4/4	0/0/0/0
4	GOL	B	780	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	760	COA	O9P-C9P	9.21	1.41	1.23
3	B	760	COA	O9P-C9P	8.80	1.40	1.23
2	A	750	ADP	C5-C4	4.23	1.50	1.40
3	B	760	COA	C2A-N3A	3.49	1.39	1.32
2	A	750	ADP	C4-N9	-3.46	1.32	1.37
3	A	760	COA	C2A-N3A	3.20	1.38	1.32
3	A	760	COA	C2A-N1A	2.75	1.39	1.33
3	B	760	COA	C2A-N1A	2.62	1.39	1.33
2	A	750	ADP	C2-N3	2.18	1.36	1.32

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	COA	N3A-C2A-N1A	-11.60	119.01	128.71
3	B	760	COA	N3A-C2A-N1A	-11.17	119.37	128.71
3	A	760	COA	CBP-CAP-C9P	8.79	121.25	112.73
2	A	750	ADP	O4'-C1'-N9	5.91	113.94	108.44
2	A	750	ADP	C2'-C1'-N9	5.39	127.10	113.27
2	A	750	ADP	N3-C4-N9	5.14	134.72	125.43
2	A	750	ADP	C4'-O4'-C1'	-4.73	104.61	109.75
2	A	750	ADP	N3-C2-N1	-4.45	124.99	128.71
3	A	760	COA	P2A-O3A-P1A	-4.30	119.07	131.68
3	A	760	COA	O4B-C1B-N9A	4.14	112.29	108.44
3	B	760	COA	N3A-C4A-N9A	3.64	132.01	125.43
3	A	760	COA	N3A-C4A-N9A	3.50	131.76	125.43
2	A	750	ADP	C1'-N9-C4	3.50	132.68	126.64
3	B	760	COA	CBP-CAP-C9P	3.33	115.95	112.73
2	A	750	ADP	C8-N9-C1'	-2.96	120.56	126.38
2	A	750	ADP	O4'-C1'-C2'	-2.89	102.34	106.77
2	A	750	ADP	C5-C4-N3	-2.79	119.62	125.70
3	A	760	COA	CDP-CBP-CAP	2.72	113.54	108.82
3	B	760	COA	P3B-O3B-C3B	2.62	127.46	121.96
3	B	760	COA	C1B-N9A-C4A	-2.59	122.16	126.64
3	B	760	COA	O6A-CCP-CBP	-2.55	106.31	110.57
3	B	760	COA	P2A-O3A-P1A	-2.52	124.30	131.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	COA	C4A-C5A-N7A	-2.43	107.44	109.52
2	A	750	ADP	N6-C6-N1	2.38	124.03	119.36
3	B	760	COA	C2A-N3A-C4A	2.30	120.54	114.01
3	B	760	COA	C5A-C4A-N3A	-2.29	120.72	125.70
2	A	750	ADP	O2B-PB-O1B	2.20	117.62	110.44
3	A	760	COA	C2A-N3A-C4A	2.19	120.25	114.01
2	A	750	ADP	O3'-C3'-C4'	-2.18	104.66	111.08
3	A	760	COA	N7A-C8A-N9A	-2.13	108.35	114.36
3	A	760	COA	CEP-CBP-CCP	-2.12	105.70	108.76
3	A	760	COA	C4A-C5A-N7A	-2.11	107.71	109.52
3	A	760	COA	C5A-C4A-N3A	-2.10	121.14	125.70
3	B	760	COA	N7A-C8A-N9A	-2.05	108.55	114.36
3	B	760	COA	CDP-CBP-CAP	2.00	112.29	108.82

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, 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	725/727 (99%)	-0.17	19 (2%) 53 54	9, 36, 68, 107	0
1	B	721/727 (99%)	-0.19	24 (3%) 44 45	12, 38, 69, 105	0
All	All	1446/1454 (99%)	-0.18	43 (2%) 48 49	9, 37, 69, 107	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	6.4
1	B	-1	SER	5.5
1	B	356	ALA	4.7
1	B	-2	GLY	4.3
1	A	356	ALA	4.2
1	A	359	LYS	3.9
1	B	718	HIS	3.8
1	B	355	GLN	3.8
1	B	357	SER	3.8
1	A	351	HIS	3.7
1	A	357	SER	3.7
1	A	358	ALA	3.5
1	B	545	PRO	3.5
1	B	358	ALA	3.4
1	B	213	ALA	3.4
1	A	348	SER	3.4
1	B	43	HIS	3.2
1	A	347	ALA	3.1
1	B	185	GLN	3.1
1	A	352	GLN	3.1
1	A	349	ARG	3.0
1	A	354	GLY	3.0
1	B	5	LEU	2.9
1	A	355	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	9	HIS	2.8
1	B	221	LYS	2.6
1	A	353	ASN	2.6
1	B	10	SER	2.5
1	A	350	ALA	2.5
1	A	346	GLU	2.5
1	B	609	GLU	2.5
1	B	554	ASN	2.5
1	A	345	LYS	2.4
1	B	347	ALA	2.4
1	A	587	ARG	2.4
1	A	69	PHE	2.4
1	B	210	SER	2.3
1	B	354	GLY	2.3
1	A	241	LYS	2.2
1	A	341	PHE	2.2
1	B	353	ASN	2.1
1	B	449	TYR	2.0
1	B	8	PRO	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	A	1722	5/5	0.41	7.30	97,97,98,99	0
5	SO4	A	1723	5/5	0.24	6.44	83,83,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	B	770	6/6	0.17	2.46	32,36,37,38	0
3	COA	A	760	48/48	0.25	1.53	54,92,100,100	0
5	SO4	B	1720	5/5	0.17	0.64	79,80,80,81	0
3	COA	B	760	48/48	0.16	0.45	59,64,69,69	0
2	ADP	A	750	27/27	0.17	-0.27	33,48,52,56	0
5	SO4	B	1719	5/5	0.17	-0.29	91,91,92,92	0
4	GOL	A	770	6/6	0.13	-0.47	21,25,26,27	0
4	GOL	B	780	6/6	0.20	-1.63	72,74,74,74	0
5	SO4	A	1721	5/5	0.12	-3.23	49,50,51,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.