



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

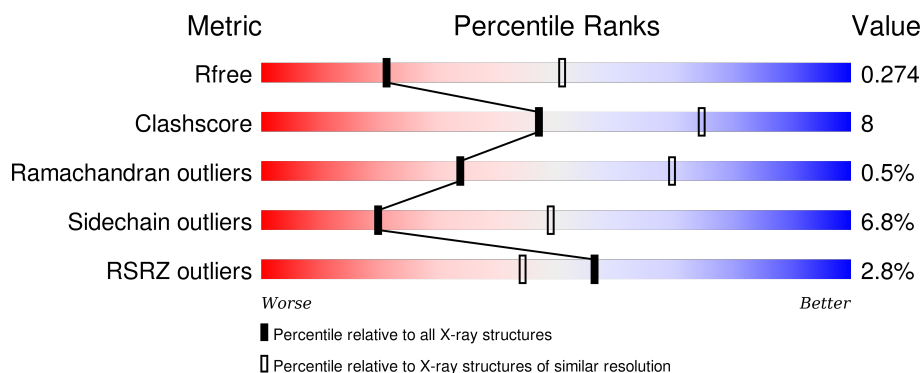
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	B	727	<div> <div>3%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	770	-	-	-	X

## 2 Entry composition

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

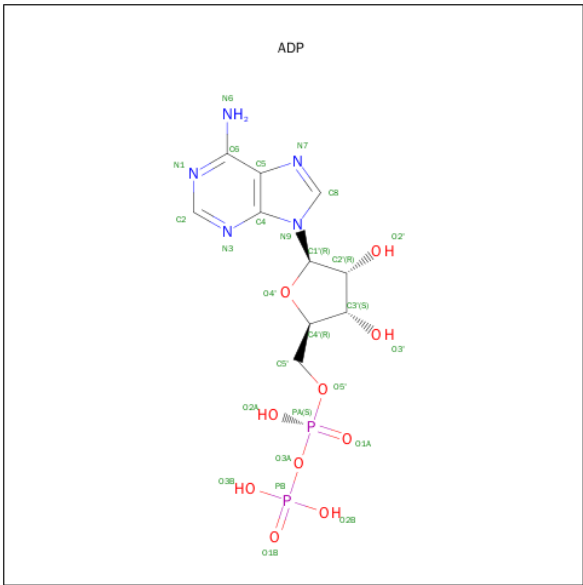
- Molecule 1 is a protein called PEROXISOMAL BIFUNCTIONAL ENZYME.

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:

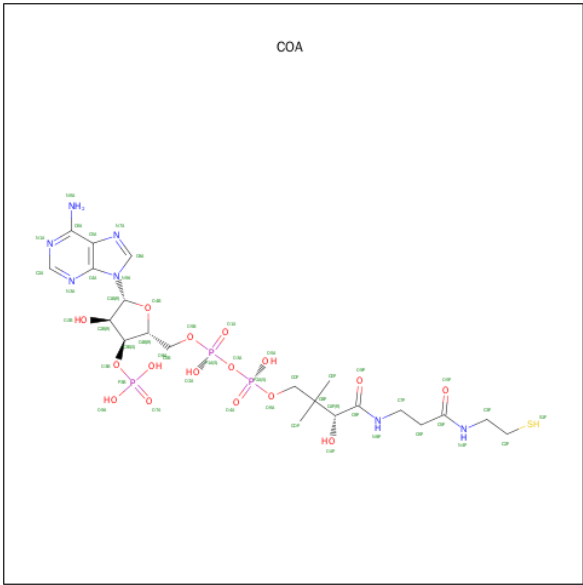
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	EXPRESSION TAG	UNP P07896
A	-3	ARG	-	EXPRESSION TAG	UNP P07896
A	-2	GLY	-	EXPRESSION TAG	UNP P07896
A	-1	SER	-	EXPRESSION TAG	UNP P07896
A	0	HIS	-	EXPRESSION TAG	UNP P07896
B	-4	PRO	-	EXPRESSION TAG	UNP P07896
B	-3	ARG	-	EXPRESSION TAG	UNP P07896
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:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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: O<sub>4</sub>S).



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		

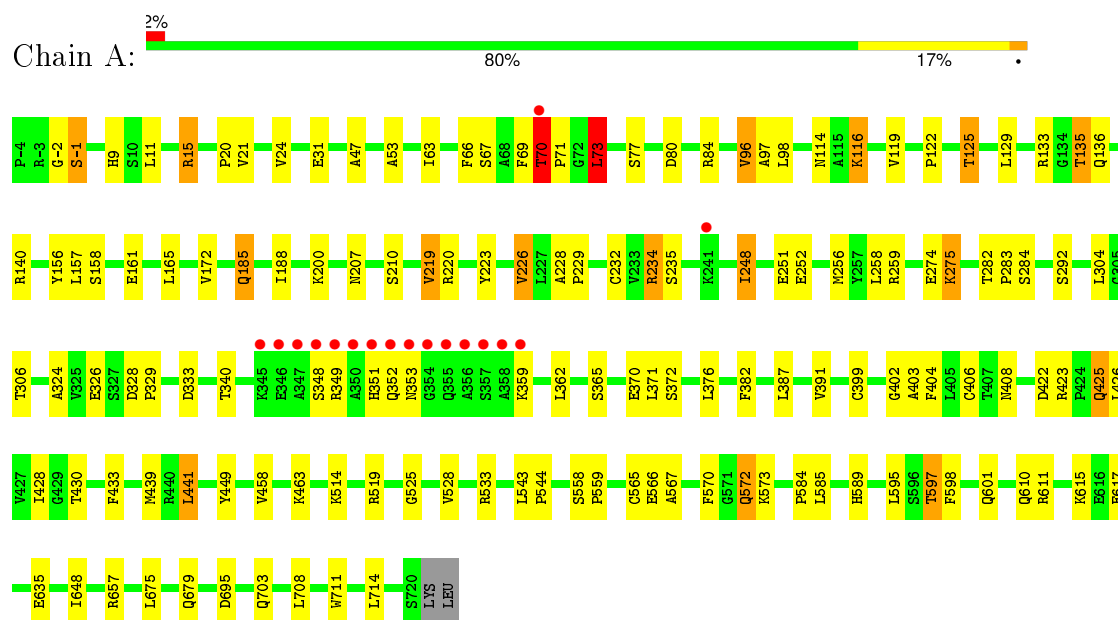
- Molecule 6 is water.

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

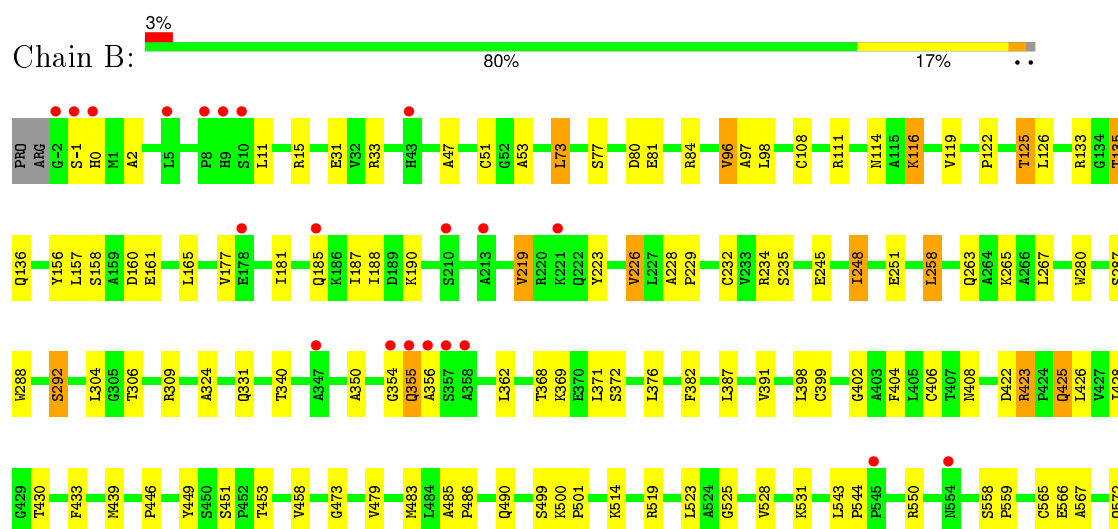
### 3 Residue-property plots

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



#### • Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.224 , 0.282 0.219 , 0.274	Depositor DCC
$R_{free}$ test set	2364 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	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

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 8.

All (170) 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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	723/727 (99%)	669 (92%)	50 (7%)	4 (1%)	30 65

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	719/727 (99%)	664 (92%)	52 (7%)	3 (0%)	39 74
All	All	1442/1454 (99%)	1333 (92%)	102 (7%)	7 (0%)	34 69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	566	GLU
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%)	18 46
1	B	591/596 (99%)	553 (94%)	38 (6%)	22 52
All	All	1185/1192 (99%)	1105 (93%)	80 (7%)	20 49

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.22	0	6,6,6	0.36	0
5	SO4	A	1723	-	4,4,4	0.16	0	6,6,6	0.21	0
2	ADP	A	750	-	22,29,29	1.29	2 (9%)	27,45,45	2.56	8 (29%)
3	COA	A	760	-	40,50,50	1.75	3 (7%)	50,75,75	2.17	5 (10%)
4	GOL	A	770	-	5,5,5	0.27	0	5,5,5	0.82	0
5	SO4	B	1719	-	4,4,4	0.11	0	6,6,6	0.12	0
5	SO4	B	1720	-	4,4,4	0.28	0	6,6,6	0.49	0
3	COA	B	760	-	40,50,50	1.70	3 (7%)	50,75,75	2.12	6 (12%)
4	GOL	B	770	-	5,5,5	0.37	0	5,5,5	0.57	0
4	GOL	B	780	-	5,5,5	0.30	0	5,5,5	0.28	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	-	-	0/12/32/32	0/3/3/3
3	COA	A	760	-	-	0/44/64/64	0/3/3/3
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
3	COA	B	760	-	-	0/44/64/64	0/3/3/3
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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	ADP	C2-N3	2.43	1.36	1.32
3	B	760	COA	C2A-N1A	2.72	1.39	1.33
3	A	760	COA	C2A-N1A	2.86	1.39	1.33
3	A	760	COA	C2A-N3A	3.57	1.38	1.32
3	B	760	COA	C2A-N3A	3.89	1.39	1.32
2	A	750	ADP	C5-C4	4.23	1.50	1.40
3	B	760	COA	O9P-C9P	8.90	1.40	1.23
3	A	760	COA	O9P-C9P	9.31	1.41	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	COA	N3A-C2A-N1A	-12.91	119.01	128.89
3	B	760	COA	N3A-C2A-N1A	-12.44	119.37	128.89
2	A	750	ADP	N3-C2-N1	-5.10	124.99	128.89
3	A	760	COA	P2A-O3A-P1A	-4.87	119.07	132.73
2	A	750	ADP	C4'-O4'-C1'	-4.65	104.61	109.72
3	B	760	COA	C1B-N9A-C4A	-3.17	122.16	126.94
3	B	760	COA	P2A-O3A-P1A	-3.00	124.30	132.73
3	B	760	COA	O6A-CCP-CBP	-2.63	106.31	110.55
3	B	760	COA	C4A-C5A-N7A	-2.21	107.44	109.48
3	A	760	COA	CEP-CBP-CCP	-2.16	105.70	108.50
2	A	750	ADP	O3'-C3'-C4'	-2.13	104.66	111.05
3	A	760	COA	O4B-C1B-N9A	2.00	112.29	108.10
2	A	750	ADP	O2B-PB-O1B	2.19	117.62	110.58
2	A	750	ADP	N6-C6-N1	2.25	124.03	119.20
3	A	760	COA	CDP-CBP-CAP	2.30	113.54	109.34
3	B	760	COA	P3B-O3B-C3B	2.46	127.46	121.56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	ADP	O4'-C1'-N9	2.79	113.94	108.10
2	A	750	ADP	C1'-N9-C4	3.80	132.68	126.94
2	A	750	ADP	C2'-C1'-N9	8.38	127.10	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	ADP	1	0
3	A	760	COA	4	0
4	B	770	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	725/727 (99%)	-0.11	17 (2%) 64 52	9, 36, 68, 107	0
1	B	721/727 (99%)	-0.15	23 (3%) 51 39	12, 38, 69, 105	0
All	All	1446/1454 (99%)	-0.13	40 (2%) 56 44	9, 37, 69, 107	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	5.4
1	A	356	ALA	4.3
1	B	-1	SER	4.0
1	A	357	SER	3.9
1	A	359	LYS	3.9
1	A	348	SER	3.8
1	A	352	GLN	3.8
1	A	351	HIS	3.6
1	B	718	HIS	3.5
1	A	358	ALA	3.4
1	B	609	GLU	3.3
1	B	357	SER	3.2
1	B	213	ALA	3.1
1	A	347	ALA	3.1
1	B	-2	GLY	3.1
1	A	353	ASN	3.0
1	B	356	ALA	3.0
1	B	5	LEU	2.9
1	A	346	GLU	2.9
1	B	185	GLN	2.9
1	A	354	GLY	2.9
1	B	545	PRO	2.8
1	A	349	ARG	2.8
1	A	355	GLN	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	43	HIS	2.7
1	B	347	ALA	2.7
1	A	241	LYS	2.6
1	B	178	GLU	2.6
1	A	345	LYS	2.6
1	B	355	GLN	2.5
1	B	10	SER	2.5
1	B	554	ASN	2.5
1	B	221	LYS	2.4
1	B	9	HIS	2.4
1	B	358	ALA	2.4
1	B	210	SER	2.4
1	A	350	ALA	2.2
1	B	8	PRO	2.2
1	B	354	GLY	2.1
1	A	70	THR	2.1

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	770	6/6	0.94	0.18	2.12	32,36,37,38	0
3	COA	A	760	48/48	0.81	0.27	1.91	54,92,100,100	0
3	COA	B	760	48/48	0.91	0.18	0.49	59,64,69,69	0
5	SO4	B	1719	5/5	0.88	0.19	-0.07	91,91,92,92	0
2	ADP	A	750	27/27	0.92	0.18	-0.16	33,48,52,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1720	5/5	0.91	0.16	-0.25	79,80,80,81	0
4	GOL	A	770	6/6	0.96	0.14	-0.27	21,25,26,27	0
5	SO4	A	1721	5/5	0.96	0.14	-2.04	49,50,51,52	0
5	SO4	A	1722	5/5	0.90	0.47	-	97,97,98,99	0
4	GOL	B	780	6/6	0.74	0.21	-	72,74,74,74	0
5	SO4	A	1723	5/5	0.90	0.27	-	83,83,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.