



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 08:14 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 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

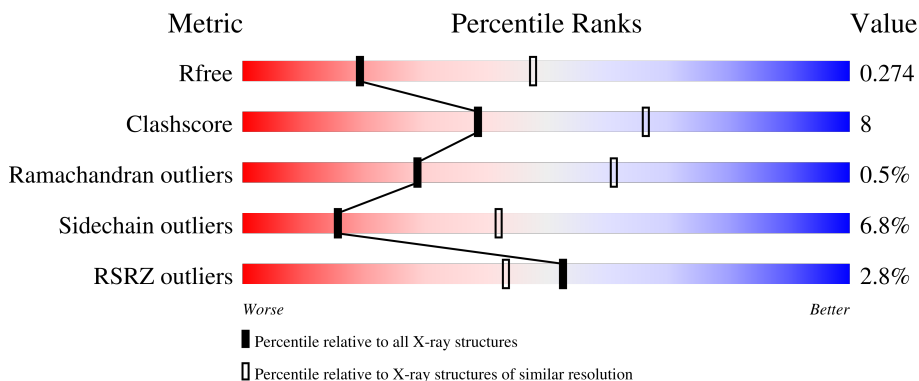
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	727	
1	B	727	

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
			Total	C	N	O	S			
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:

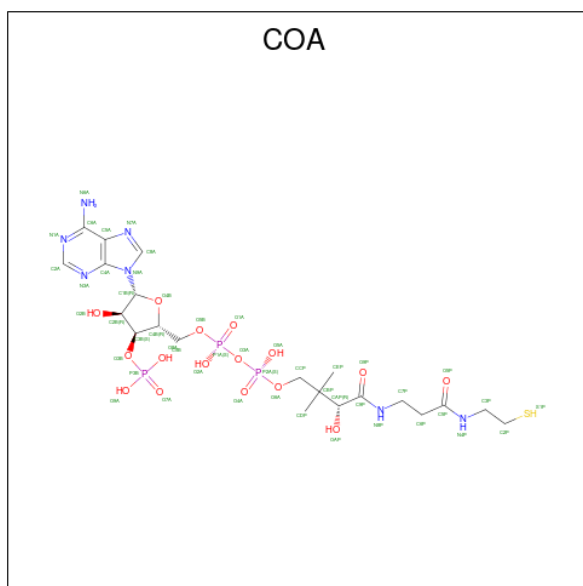
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
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
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

- 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	
			Total	C	N	O	P			S
3	A	1	48	21	7	16	3	1	0	0
3	B	1	48	21	7	16	3	1	0	0

- 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 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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



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

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		

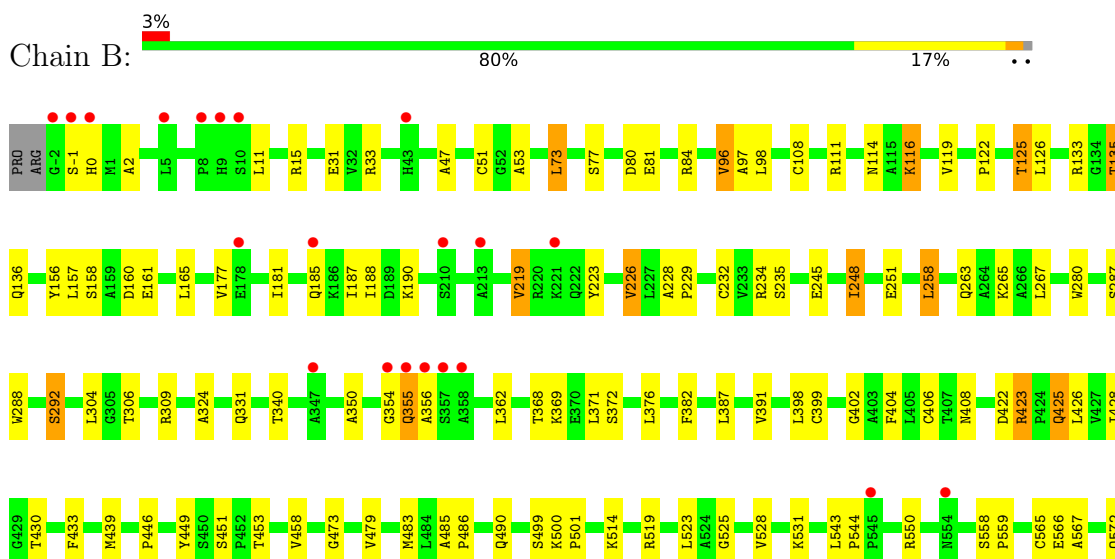
3 Residue-property plots [i](#)

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: 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, 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)	Xtrriage
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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, ADP, SO4, GOL

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:H	1:B:73:LEU:HD12	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:133:ARG:HD2	1:A:248:ILE:CD1	2.23	0.67
1:A:135:THR:HG21	1:A:235:SER:OG	1.92	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:O3	4:B:770:GOL:O1	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:15:ARG:CD	1:B:53:ALA:HB2	2.33	0.59
1:B:158:SER:OG	1:B:161:GLU:HG2	2.02	0.59
1:A:133:ARG:HD2	1:A:248:ILE:HD11	1.83	0.59
1:A:387:LEU:O	1:A:391:VAL:HG23	2.03	0.59
1:B:73:LEU:HD12	1:B:73:LEU:N	2.16	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:HA	1:B:663:MET:CE	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:2:ALA:HB3	1:B:31:GLU:HB3	1.89	0.55
1:B:708:LEU:HA	1:B:711:TRP:CE2	2.42	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:H131	3:A:760:COA:O9P	2.08	0.54
1:B:135:THR:HG22	1:B:251:GLU:OE2	2.09	0.52
1:B:479:VAL:HG22	1:B:633:ILE:HG21	1.90	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:N7A	3:A:760:COA:H62	2.27	0.50
1:A:158:SER:OG	1:A:161:GLU:HG2	2.11	0.50
1:B:712:GLN:HA	1:B:712:GLN:OE1	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:H	1:B:245:GLU:CD	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:HA	1:B:663:MET:HE2	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:274:GLU:OE2	1:A:657:ARG:NH2	2.47	0.47
1:A:533:ARG:HG3	1:A:533:ARG:HH11	1.78	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:A:408:ASN:O	1:A:408:ASN:CG	2.54	0.46
1:B:428:ILE:HG13	1:B:446:PRO:HA	1.97	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:HA	1:A:275:LYS:HD3	1.62	0.45
1:A:226:VAL:HG22	1:A:229:PRO:HD3	1.99	0.45
1:A:543:LEU:HD12	1:A:544:PRO:HD2	1.99	0.44
1:B:633:ILE:HG23	1:B:638:MET:HB2	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:OE1	1:B:490:GLN:HA	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:A:11:LEU:HD22	1:A:47:ALA:HB3	2.01	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:406:CYS:HB3	1:A:430:THR:HG23	2.00	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:219:VAL:HG22	1:A:229:PRO:HB2	1.99	0.43
1:B:156:TYR:N	1:B:156:TYR:CD2	2.87	0.43
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.48	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:A:9:HIS:HB3	1:A:185:GLN:HE22	1.84	0.42
1:B:15:ARG:HA	1:B:51:CYS:O	2.20	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:565:CYS:C	1:A:567:ALA:H	2.23	0.42
1:A:573:LYS:HA	1:A:585:LEU:HD12	2.00	0.42
1:A:703:GLN:OE1	1:A:714:LEU:HB3	2.20	0.42
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.94	0.42
1:A:229:PRO:O	1:A:232:CYS:HB2	2.20	0.42
1:A:365:SER:CB	1:A:370:GLU:HG3	2.50	0.42
1:B:108:CYS:O	1:B:111:ARG:NH1	2.53	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:185:GLN:H	1:A:185:GLN:HG2	1.71	0.41
1:A:226:VAL:HG22	1:A:229:PRO:CD	2.49	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:A:207:ASN:O	1:A:210:SER:HB3	2.20	0.41
1:B:350:ALA:HB1	1:B:355:GLN:HG2	2.03	0.41
1:A:140:ARG:NE	1:A:200:LYS:O	2.53	0.41
1:A:433:PHE:O	1:A:439:MET:HB2	2.20	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:156:TYR:N	1:A:156:TYR:CD2	2.89	0.41
1:A:558:SER:HA	1:A:559:PRO:HD3	1.86	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:228:ALA:HB3	1:A:229:PRO:HD3	2.02	0.40
1:B:156:TYR:N	1:B:156:TYR:HD2	2.19	0.40
1:A:349:ARG:O	1:A:353:ASN:ND2	2.54	0.40
1:A:406:CYS:HA	1:A:428:ILE:O	2.21	0.40
1:A:533:ARG:HG3	1:A:533:ARG:NH1	2.37	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%)	25 56

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%)	34 66
All	All	1442/1454 (99%)	1333 (92%)	102 (7%)	7 (0%)	29 61

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 [i](#)

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%)	14 39
1	B	591/596 (99%)	553 (94%)	38 (6%)	17 45
All	All	1185/1192 (99%)	1105 (93%)	80 (7%)	16 42

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

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	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 [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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	COA	B	760	-	41,50,50	1.72	3 (7%)	52,75,75	1.35	5 (9%)
5	SO4	B	1719	-	4,4,4	0.19	0	6,6,6	0.11	0
3	COA	A	760	-	41,50,50	1.76	3 (7%)	52,75,75	1.35	3 (5%)
5	SO4	A	1721	-	4,4,4	0.16	0	6,6,6	0.30	0
5	SO4	A	1723	-	4,4,4	0.16	0	6,6,6	0.19	0
4	GOL	B	770	-	5,5,5	0.43	0	5,5,5	0.57	0
5	SO4	A	1722	-	4,4,4	0.11	0	6,6,6	0.33	0
2	ADP	A	750	-	24,29,29	1.20	2 (8%)	29,45,45	1.56	6 (20%)
5	SO4	B	1720	-	4,4,4	0.13	0	6,6,6	0.62	0
4	GOL	A	770	-	5,5,5	0.29	0	5,5,5	0.82	0
4	GOL	B	780	-	5,5,5	0.34	0	5,5,5	0.26	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
3	COA	B	760	-	-	18/44/64/64	0/3/3/3
3	COA	A	760	-	-	20/44/64/64	0/3/3/3
4	GOL	B	770	-	-	2/4/4/4	-
2	ADP	A	750	-	-	2/12/32/32	0/3/3/3
4	GOL	A	770	-	-	2/4/4/4	-
4	GOL	B	780	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	760	COA	O9P-C9P	9.19	1.41	1.23
3	B	760	COA	O9P-C9P	8.78	1.40	1.23
3	B	760	COA	C2A-N3A	4.33	1.39	1.32
3	A	760	COA	C2A-N3A	3.98	1.38	1.32
2	A	750	ADP	C5-C4	3.44	1.50	1.40
3	A	760	COA	C2A-N1A	2.91	1.39	1.33
3	B	760	COA	C2A-N1A	2.78	1.39	1.33
2	A	750	ADP	C2-N3	2.73	1.36	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	COA	N3A-C2A-N1A	-6.18	119.01	128.68
3	B	760	COA	N3A-C2A-N1A	-5.95	119.37	128.68
3	A	760	COA	P2A-O3A-P1A	-4.01	119.07	132.83
2	A	750	ADP	C1'-N9-C4	3.44	132.68	126.64
2	A	750	ADP	O4'-C1'-C2'	-3.14	102.34	106.93
3	A	760	COA	CDP-CBP-CAP	2.72	113.54	108.82
3	B	760	COA	O6A-CCP-CBP	-2.63	106.31	110.55
2	A	750	ADP	N6-C6-N1	2.63	124.03	118.57
3	B	760	COA	C1B-N9A-C4A	-2.55	122.16	126.64
3	B	760	COA	P2A-O3A-P1A	-2.48	124.30	132.83
2	A	750	ADP	N3-C2-N1	-2.36	124.99	128.68
2	A	750	ADP	O3'-C3'-C4'	-2.21	104.66	111.05
2	A	750	ADP	O2B-PB-O3A	-2.09	97.62	104.64
3	B	760	COA	CDP-CBP-CAP	2.00	112.29	108.82

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	760	COA	C5B-O5B-P1A-O2A
3	A	760	COA	C5B-O5B-P1A-O3A
3	A	760	COA	C9P-CAP-CBP-CCP
3	A	760	COA	C9P-CAP-CBP-CDP
3	A	760	COA	OAP-CAP-CBP-CEP
3	A	760	COA	C9P-CAP-CBP-CEP
3	A	760	COA	O9P-C9P-CAP-CBP
3	A	760	COA	N8P-C9P-CAP-CBP
3	A	760	COA	O9P-C9P-CAP-OAP
3	A	760	COA	N8P-C9P-CAP-OAP
3	A	760	COA	CAP-C9P-N8P-C7P
3	A	760	COA	O9P-C9P-N8P-C7P
3	B	760	COA	C9P-CAP-CBP-CCP
3	B	760	COA	C9P-CAP-CBP-CDP
3	B	760	COA	C9P-CAP-CBP-CEP
3	B	760	COA	N8P-C9P-CAP-OAP
3	B	760	COA	CAP-C9P-N8P-C7P
3	B	760	COA	C5P-C6P-C7P-N8P
3	B	760	COA	C6P-C5P-N4P-C3P
3	B	760	COA	O5P-C5P-N4P-C3P
4	B	780	GOL	O1-C1-C2-C3
3	B	760	COA	O9P-C9P-N8P-C7P
4	B	780	GOL	O1-C1-C2-O2
3	A	760	COA	C4B-C3B-O3B-P3B
4	A	770	GOL	O1-C1-C2-C3
4	B	770	GOL	O1-C1-C2-C3
3	B	760	COA	O9P-C9P-CAP-OAP
3	A	760	COA	OAP-CAP-CBP-CDP
3	B	760	COA	OAP-CAP-CBP-CDP
3	B	760	COA	OAP-CAP-CBP-CEP
3	B	760	COA	P1A-O3A-P2A-O6A
3	A	760	COA	C3B-O3B-P3B-O9A
3	B	760	COA	C3B-O3B-P3B-O8A
3	A	760	COA	O5P-C5P-N4P-C3P
3	A	760	COA	C4B-C5B-O5B-P1A
3	A	760	COA	OAP-CAP-CBP-CCP
3	B	760	COA	OAP-CAP-CBP-CCP
3	A	760	COA	C2B-C3B-O3B-P3B
3	B	760	COA	P2A-O3A-P1A-O2A
3	A	760	COA	C6P-C5P-N4P-C3P
2	A	750	ADP	O4'-C4'-C5'-O5'
3	B	760	COA	P2A-O3A-P1A-O1A
3	B	760	COA	C3B-O3B-P3B-O9A

Continued on next page...

Continued from previous page...

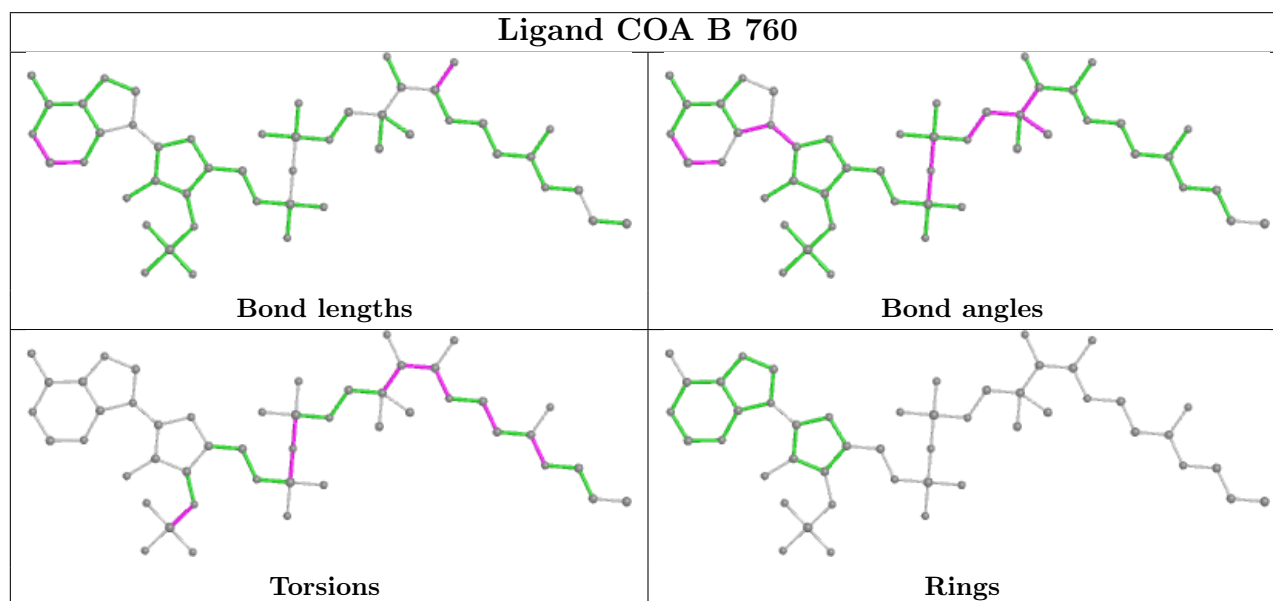
Mol	Chain	Res	Type	Atoms
4	A	770	GOL	O1-C1-C2-O2
4	B	770	GOL	O1-C1-C2-O2
2	A	750	ADP	PB-O3A-PA-O2A

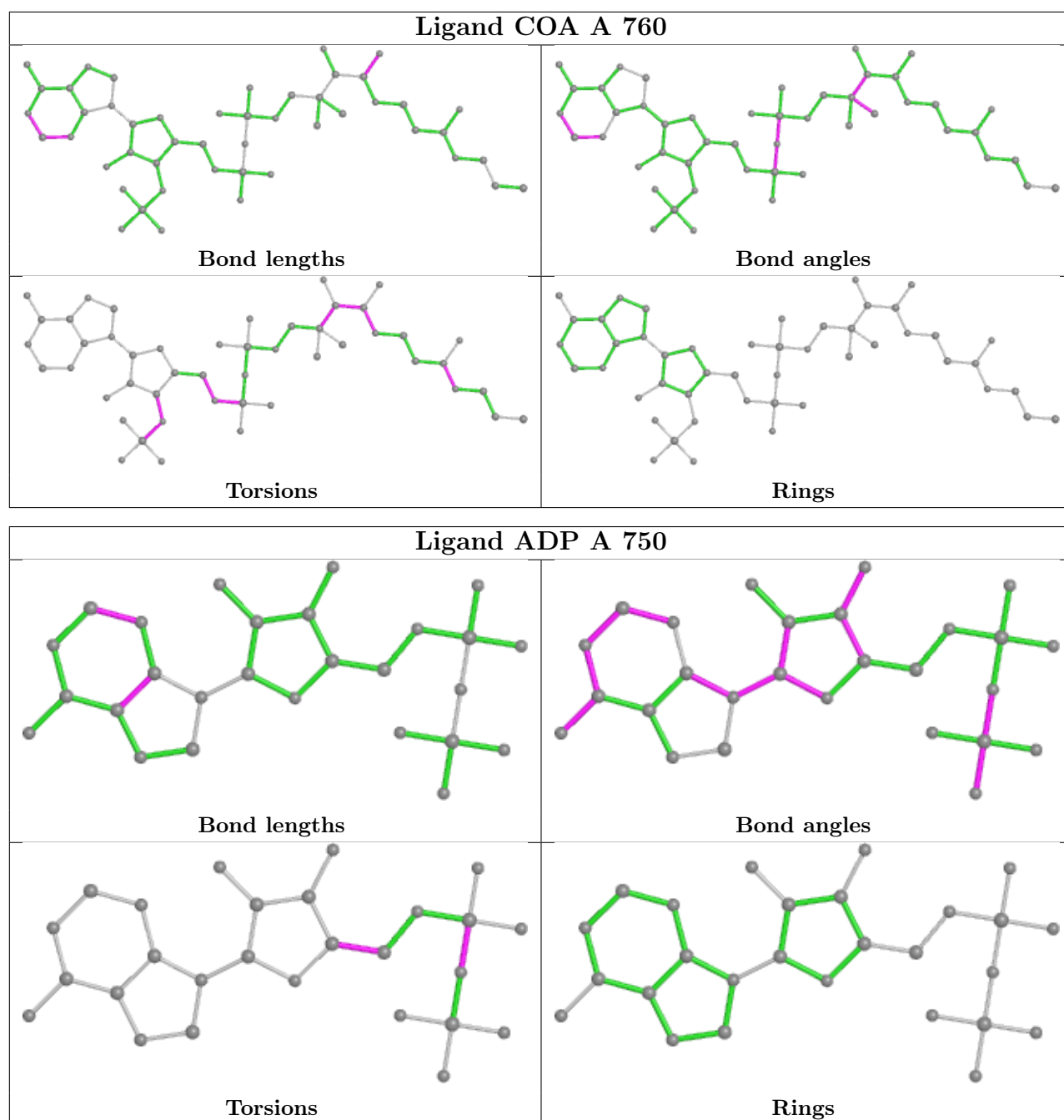
There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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%)	-0.12	17 (2%) 60 51	9, 36, 68, 107	0
1	B	721/727 (99%)	-0.16	23 (3%) 47 37	12, 38, 69, 105	0
All	All	1446/1454 (99%)	-0.14	40 (2%) 53 43	9, 37, 69, 107	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	5.3
1	A	356	ALA	4.4
1	B	-1	SER	3.9
1	A	357	SER	3.9
1	A	359	LYS	3.7
1	A	348	SER	3.7
1	A	352	GLN	3.7
1	A	351	HIS	3.5
1	B	718	HIS	3.4
1	A	358	ALA	3.4
1	B	609	GLU	3.2
1	B	357	SER	3.2
1	A	347	ALA	3.1
1	B	213	ALA	3.1
1	B	356	ALA	3.0
1	B	-2	GLY	3.0
1	A	353	ASN	2.9
1	B	5	LEU	2.9
1	A	346	GLU	2.8
1	A	349	ARG	2.8
1	A	354	GLY	2.8
1	B	185	GLN	2.8
1	B	43	HIS	2.7
1	A	355	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	545	PRO	2.6
1	B	347	ALA	2.6
1	A	241	LYS	2.6
1	B	178	GLU	2.5
1	A	345	LYS	2.5
1	B	10	SER	2.4
1	B	554	ASN	2.4
1	B	355	GLN	2.4
1	B	358	ALA	2.4
1	B	9	HIS	2.4
1	B	221	LYS	2.4
1	B	210	SER	2.3
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 monosaccharides 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.

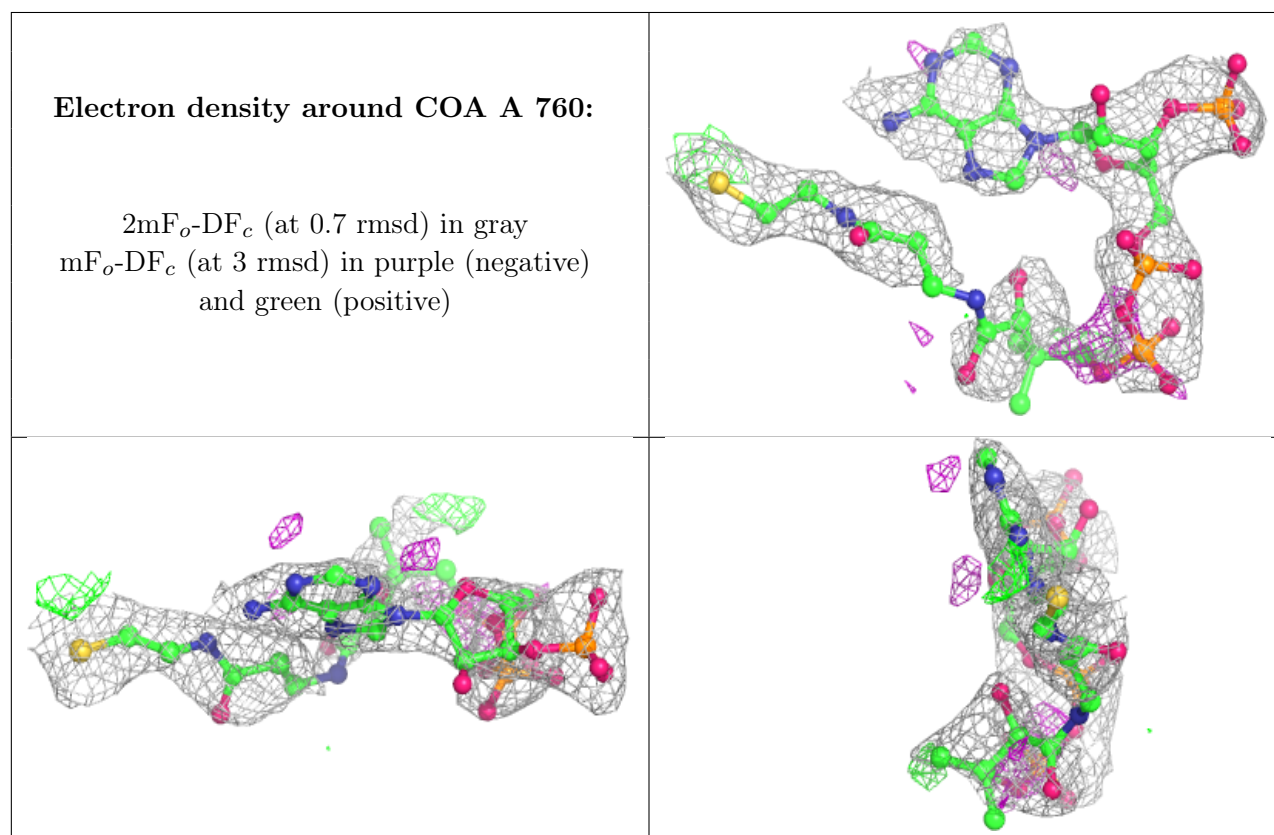
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	780	6/6	0.74	0.21	72,74,74,74	0
3	COA	A	760	48/48	0.80	0.27	54,92,100,100	0
5	SO4	B	1719	5/5	0.88	0.19	91,91,92,92	0
5	SO4	A	1723	5/5	0.90	0.27	83,83,84,84	0
5	SO4	A	1722	5/5	0.90	0.48	97,97,98,99	0
3	COA	B	760	48/48	0.91	0.18	59,64,69,69	0
5	SO4	B	1720	5/5	0.91	0.16	79,80,80,81	0

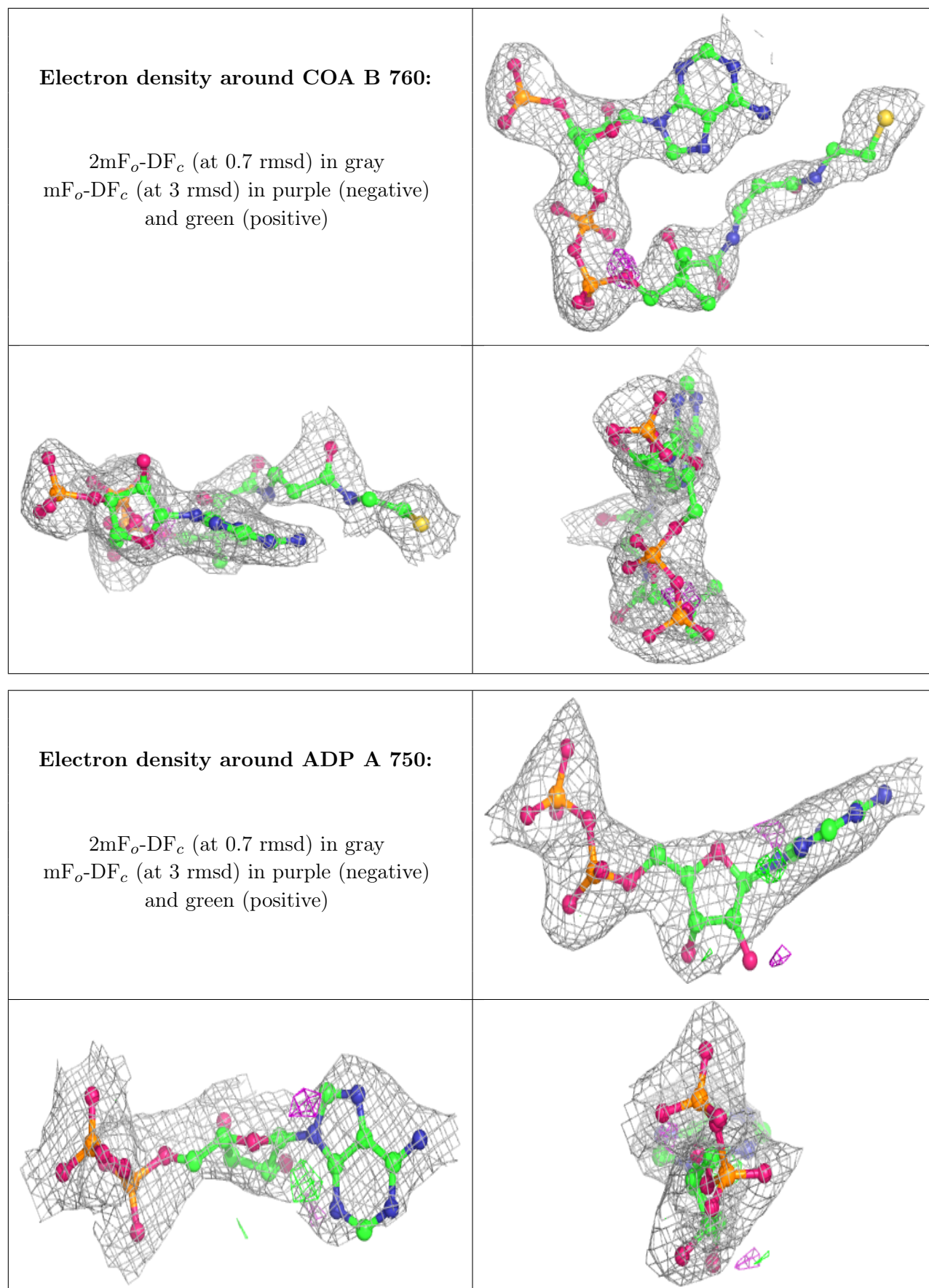
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	A	750	27/27	0.92	0.18	33,48,52,56	0
4	GOL	B	770	6/6	0.94	0.18	32,36,37,38	0
4	GOL	A	770	6/6	0.96	0.14	21,25,26,27	0
5	SO4	A	1721	5/5	0.96	0.14	49,50,51,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.