Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:07 am BST

PDB ID	:	1SG4
Title	:	Crystal structure of human mitochondrial delta3-delta2-enoyl-CoA isomerase
Authors	:	Partanen, S.T.; Novikov, D.K.; Popov, A.N.; Mursula, A.M.; Hiltunen, J.K.; Wierenga, R.K.
Deposited on	:	2004-02-23
Resolution	:	1.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

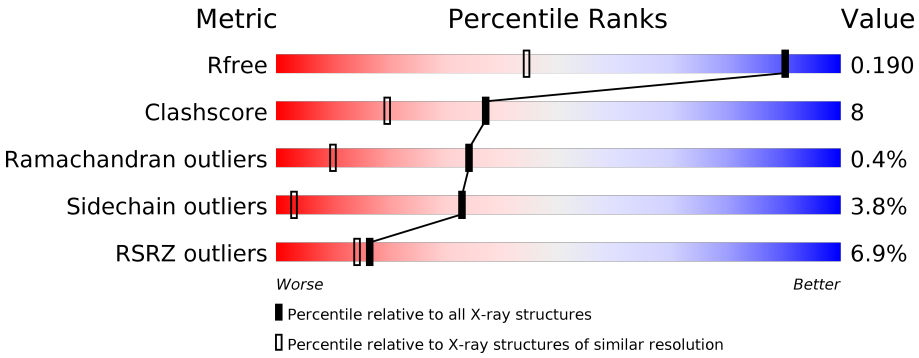
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 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 <=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	260	9% 74% 18%
1	B	260	6% 81% 17%
1	C	260	5% 82% 13%

2 Entry composition

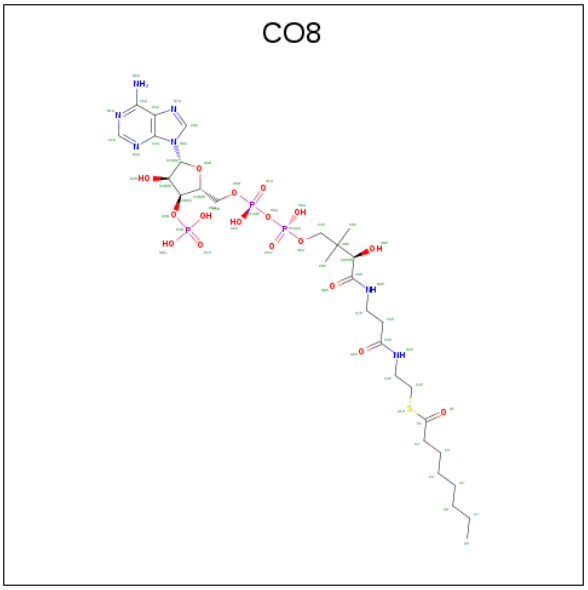
There are 3 unique types of molecules in this entry. The entry contains 6800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3,2-trans-enoyl-CoA isomerase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	28	0
			2061	1316	349	379	17			
1	B	258	Total	C	N	O	S	0	13	0
			2047	1304	350	377	16			
1	C	250	Total	C	N	O	S	0	9	0
			1968	1258	339	359	12			

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

- Molecule 3 is water.

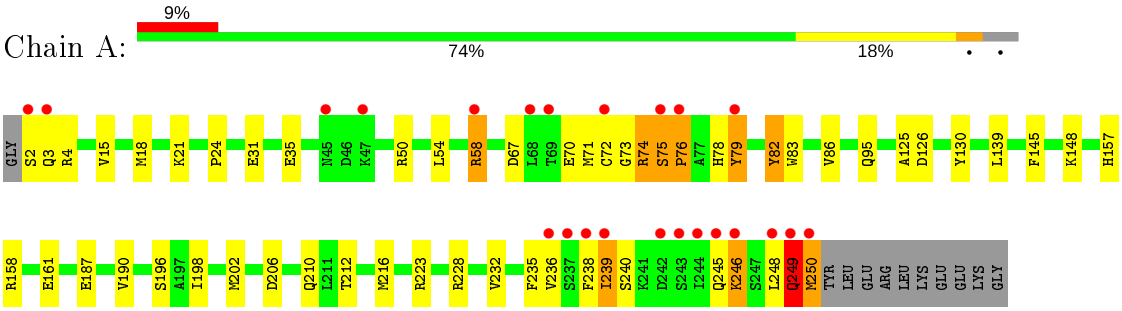
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	212	Total O 212 212	0	0
3	B	222	Total O 223 223	0	1
3	C	232	Total O 232 232	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

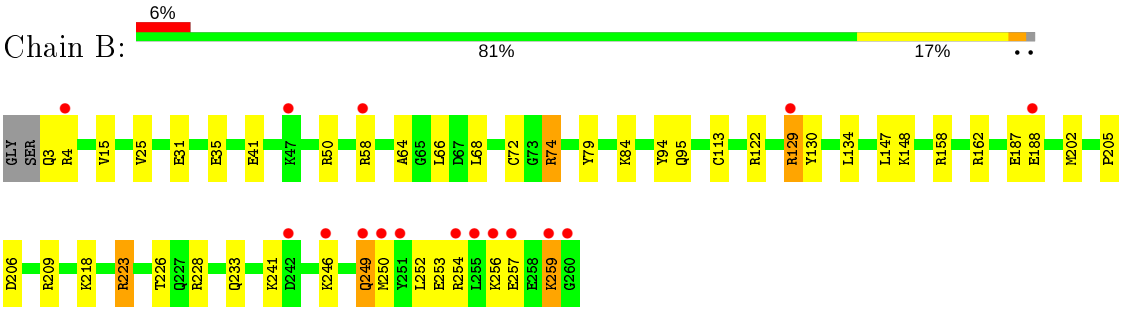
- Molecule 1: 3,2-trans-enoyl-CoA isomerase, mitochondrial

Chain A:



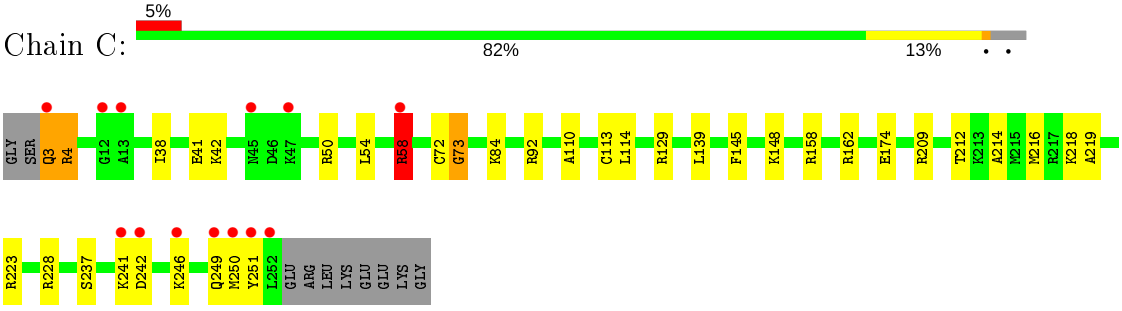
- Molecule 1: 3,2-trans-enoyl-CoA isomerase, mitochondrial

Chain B:



- Molecule 1: 3,2-trans-enoyl-CoA isomerase, mitochondrial

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.98Å 78.29Å 113.21Å 90.00° 116.39° 90.00°	Depositor
Resolution (Å)	20.00 – 1.30 19.73 – 1.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.30) 91.0 (19.73-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.157 , 0.202 0.151 , 0.190	Depositor DCC
R_{free} test set	9150 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6800	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO8

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	0.59	0/2177	1.39	28/2952 (0.9%)
1	B	0.66	1/2134 (0.0%)	1.36	19/2892 (0.7%)
1	C	0.69	1/2041 (0.0%)	1.35	18/2769 (0.7%)
All	All	0.65	2/6352 (0.0%)	1.37	65/8613 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	CYS	CB-SG	-8.46	1.67	1.82
1	B	113	CYS	CB-SG	-6.32	1.71	1.82

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	ARG	CG-CD-NE	14.83	142.95	111.80
1	B	228	ARG	NE-CZ-NH1	-14.55	113.03	120.30
1	B	228	ARG	NE-CZ-NH2	14.26	127.43	120.30
1	B	223[A]	ARG	NE-CZ-NH2	-13.59	113.51	120.30
1	B	223[B]	ARG	NE-CZ-NH2	-13.59	113.51	120.30
1	B	223[A]	ARG	NE-CZ-NH1	12.93	126.76	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	223[B]	ARG	NE-CZ-NH1	12.93	126.76	120.30
1	A	223	ARG	CD-NE-CZ	11.54	139.75	123.60
1	C	92	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	B	50	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	A	50	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	C	58	ARG	CA-CB-CG	9.06	133.33	113.40
1	C	223[A]	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	223[B]	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	228	ARG	NE-CZ-NH1	-8.77	115.91	120.30
1	C	223[A]	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	C	223[B]	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	254	ARG	CD-NE-CZ	8.15	135.01	123.60
1	A	228	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	C	72	CYS	C-N-CA	-7.59	106.36	122.30
1	A	238	PHE	CA-C-O	7.11	135.04	120.10
1	A	126	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	50	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	50	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	145	PHE	CB-CG-CD1	6.81	125.56	120.80
1	C	174	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	C	92	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	74[A]	ARG	CD-NE-CZ	6.64	132.90	123.60
1	A	74[B]	ARG	CD-NE-CZ	6.64	132.90	123.60
1	B	130	TYR	CB-CG-CD1	6.53	124.92	121.00
1	A	83	TRP	CE3-CZ3-CH2	6.50	128.35	121.20
1	B	74	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	254	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	206	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	209	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	83	TRP	CA-C-N	6.18	130.80	117.20
1	A	73	GLY	O-C-N	-6.14	112.88	122.70
1	A	58	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	228	ARG	NH1-CZ-NH2	6.01	126.01	119.40
1	A	79[A]	TYR	CB-CG-CD1	5.95	124.57	121.00
1	A	79[B]	TYR	CB-CG-CD1	5.95	124.57	121.00
1	B	122	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	74[A]	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	74[B]	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	67	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	162	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	223	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	94	TYR	CB-CG-CD2	5.68	124.41	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	50	ARG	CD-NE-CZ	5.67	131.54	123.60
1	A	58	ARG	CA-CB-CG	5.58	125.69	113.40
1	A	83	TRP	O-C-N	-5.57	113.79	122.70
1	B	122	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	B	233	GLN	CA-CB-CG	5.38	125.24	113.40
1	C	174	GLU	CG-CD-OE1	5.38	129.06	118.30
1	A	79[A]	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	79[B]	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	228	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	C	73	GLY	CA-C-N	5.13	128.48	117.20
1	A	130	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	C	114	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	129	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	A	145	PHE	CB-CG-CD1	5.05	124.33	120.80
1	A	82[A]	TYR	CA-C-O	-5.03	109.54	120.10
1	A	82[B]	TYR	CA-C-O	-5.03	109.54	120.10
1	C	209	ARG	CD-NE-CZ	5.02	130.62	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	GLN	Peptide
1	C	73	GLY	Peptide

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	2061	0	2081	46	0
1	B	2047	0	2081	29	0
1	C	1968	0	2016	20	0
2	B	57	0	46	6	0
3	A	212	0	0	7	0
3	B	223	0	0	13	0
3	C	232	0	0	7	0
All	All	6800	0	6224	97	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 (97) 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:253:GLU:O	1:B:257:GLU:HG3	1.85	0.77
1:B:147:LEU:HD21	3:B:741:HOH:O	1.86	0.75
1:A:235:PHE:O	1:A:239:ILE:HG22	1.88	0.74
1:A:72[B]:CYS:SG	1:A:248:LEU:HD13	2.27	0.74
1:A:212:THR:O	1:A:216[B]:MET:HG2	1.89	0.73
1:C:214:ALA:O	1:C:218[B]:LYS:HG3	1.91	0.71
1:A:187[A]:GLU:HG3	3:A:445:HOH:O	1.90	0.71
1:A:31:GLU:O	1:A:35:GLU:HG3	1.90	0.70
1:A:239:ILE:HD12	1:A:239:ILE:O	1.92	0.69
1:B:41:GLU:HG3	3:B:871:HOH:O	1.92	0.69
1:B:66:LEU:HD12	2:B:701:CO8:H3'1	1.73	0.69
1:B:218:LYS:HD2	3:B:920:HOH:O	1.91	0.69
1:C:246:LYS:O	1:C:250:MET:HG3	1.94	0.68
1:C:3:GLN:HB2	3:C:439:HOH:O	1.95	0.66
1:A:232:VAL:O	1:A:236:VAL:HG23	1.96	0.65
2:B:701:CO8:H8A	2:B:701:CO8:OAP	1.97	0.64
1:C:84:LYS:HD2	3:C:332:HOH:O	1.98	0.63
1:A:76[B]:PRO:HD3	3:A:367:HOH:O	1.98	0.62
1:C:242:ASP:O	1:C:246:LYS:HG3	1.98	0.62
1:B:223[B]:ARG:HG3	3:B:862:HOH:O	1.99	0.62
1:A:202[A]:MET:HE2	3:A:354:HOH:O	1.99	0.61
1:B:15[B]:VAL:HG22	1:B:202:MET:SD	2.40	0.61
1:C:212:THR:O	1:C:216[B]:MET:HG2	2.00	0.61
1:A:246:LYS:O	1:A:249:GLN:HB2	2.01	0.60
1:B:72[B]:CYS:SG	1:B:249:GLN:HG2	2.42	0.60
1:B:25:VAL:HG11	2:B:701:CO8:H143	1.84	0.60
1:A:74[B]:ARG:HG3	1:A:78[B]:HIS:ND1	2.18	0.59
1:A:198:ILE:O	1:A:202[A]:MET:HG3	2.02	0.59
1:B:187:GLU:HG3	3:B:749:HOH:O	2.03	0.59
1:A:249:GLN:NE2	1:A:249:GLN:HA	2.16	0.58
1:B:134:LEU:HD22	3:B:741:HOH:O	2.05	0.57
1:C:237:SER:O	1:C:241:LYS:HD2	2.04	0.57
1:A:79[B]:TYR:CG	1:A:239:ILE:HG23	2.40	0.56
1:B:241:LYS:HE3	3:B:866:HOH:O	2.05	0.55
1:A:235:PHE:CE2	1:A:239:ILE:HG21	2.42	0.53
1:A:15:VAL:HG22	1:A:202[A]:MET:SD	2.49	0.53
2:B:701:CO8:O2A	2:B:701:CO8:OAP	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:OE1	1:B:253:GLU:HA	2.08	0.53
1:A:82[B]:TYR:O	1:A:86:VAL:HG23	2.08	0.52
1:A:198:ILE:HG12	1:A:202[A]:MET:SD	2.50	0.51
1:A:79[B]:TYR:CD2	1:A:239:ILE:HG13	2.44	0.51
1:A:74[B]:ARG:O	1:A:75[B]:SER:O	2.28	0.51
1:A:79[B]:TYR:CE1	1:A:240:SER:HA	2.46	0.51
1:C:41:GLU:HG3	3:C:464:HOH:O	2.10	0.51
1:A:79[B]:TYR:OH	1:A:245[B]:GLN:HG2	2.12	0.50
1:A:239:ILE:HD12	1:A:245[A]:GLN:OE1	2.11	0.50
1:A:74[B]:ARG:HB3	1:A:78[B]:HIS:HD1	1.76	0.50
1:B:259:LYS:HB3	2:B:701:CO8:O1A	2.10	0.50
1:A:206:ASP:OD2	1:A:210:GLN:OE1	2.30	0.50
1:A:74[B]:ARG:N	1:A:74[B]:ARG:HD2	2.25	0.50
1:C:218[A]:LYS:HG3	1:C:219:ALA:N	2.25	0.49
1:B:129:ARG:HD2	3:B:769:HOH:O	2.11	0.49
1:B:95:GLN:HA	3:B:904:HOH:O	2.13	0.49
1:A:79[B]:TYR:CE2	1:A:239:ILE:HG13	2.48	0.48
1:C:218[B]:LYS:CE	1:C:219:ALA:H	2.27	0.47
1:A:157:HIS:HE1	1:A:161[A]:GLU:OE2	1.96	0.47
1:B:31:GLU:OE2	1:B:35:GLU:OE2	2.33	0.47
1:C:38:ILE:O	1:C:42[A]:LYS:HG3	2.14	0.47
1:A:250:MET:HG2	3:A:451:HOH:O	2.15	0.46
1:A:70:GLU:O	1:A:78[B]:HIS:ND1	2.49	0.46
1:A:3:GLN:OE1	1:A:4:ARG:NH2	2.49	0.46
1:B:4:ARG:HB2	1:B:35:GLU:OE1	2.17	0.45
1:C:249:GLN:O	1:C:249:GLN:NE2	2.50	0.45
1:B:58:ARG:NE	3:B:882:HOH:O	2.50	0.45
1:C:58:ARG:NH1	3:C:423:HOH:O	2.50	0.45
1:A:24:PRO:O	1:A:58:ARG:NH1	2.48	0.45
1:B:162:ARG:NH1	3:B:787:HOH:O	2.48	0.45
1:A:15:VAL:HG22	1:A:202[B]:MET:SD	2.56	0.44
1:B:223[B]:ARG:NE	3:B:862:HOH:O	2.51	0.44
1:C:218[B]:LYS:HD2	1:C:219:ALA:N	2.33	0.44
1:A:24:PRO:O	1:A:58:ARG:NH2	2.49	0.44
1:C:129:ARG:NE	3:C:397:HOH:O	2.50	0.44
1:A:125:ALA:HB2	1:A:190[B]:VAL:HG21	2.00	0.44
1:A:95:GLN:HA	3:A:425:HOH:O	2.18	0.44
1:B:129:ARG:NH1	3:B:769:HOH:O	2.50	0.44
1:A:74[B]:ARG:HG3	1:A:78[B]:HIS:HD1	1.82	0.43
1:A:70:GLU:HA	1:A:78[B]:HIS:HE1	1.82	0.43
1:C:246:LYS:NZ	3:C:453:HOH:O	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245[B]:GLN:NE2	3:A:470:HOH:O	2.50	0.43
1:A:76[B]:PRO:HA	3:A:367:HOH:O	2.18	0.43
1:C:139:LEU:HD21	1:C:251:TYR:CD1	2.53	0.42
1:A:54:LEU:N	1:A:54:LEU:HD12	2.33	0.42
1:B:202:MET:HE2	1:B:202:MET:HB3	1.95	0.42
1:A:235:PHE:CZ	1:A:239:ILE:HG21	2.55	0.42
1:B:246:LYS:HG2	1:B:250:MET:SD	2.59	0.42
1:C:3:GLN:HG2	1:C:4:ARG:N	2.34	0.42
1:B:74:ARG:HB2	1:B:79:TYR:CE1	2.53	0.42
1:B:246:LYS:O	1:B:250:MET:HG3	2.20	0.41
1:A:3:GLN:HG2	1:A:4:ARG:CZ	2.50	0.41
1:B:64:ALA:O	2:B:701:CO8:H62	2.20	0.41
1:C:58:ARG:HG2	3:C:317:HOH:O	2.20	0.41
1:A:71[B]:MET:SD	1:A:82[B]:TYR:CE2	3.14	0.41
1:A:2:SER:OG	1:A:3:GLN:N	2.50	0.40
1:B:72[A]:CYS:SG	1:B:252:LEU:HD12	2.61	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	275/260 (106%)	264 (96%)	7 (2%)	4 (2%)	10 1
1	B	269/260 (104%)	262 (97%)	7 (3%)	0	100 100
1	C	257/260 (99%)	249 (97%)	7 (3%)	1 (0%)	34 10
All	All	801/780 (103%)	775 (97%)	21 (3%)	5 (1%)	34 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75[A]	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75[B]	SER
1	C	110	ALA
1	A	76[A]	PRO
1	A	76[B]	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	232/216 (107%)	220 (95%)	12 (5%)	23 2
1	B	228/216 (106%)	217 (95%)	11 (5%)	25 2
1	C	217/216 (100%)	213 (98%)	4 (2%)	59 24
All	All	677/648 (104%)	650 (96%)	27 (4%)	33 3

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18[A]	MET
1	A	18[B]	MET
1	A	21	LYS
1	A	139	LEU
1	A	148	LYS
1	A	158	ARG
1	A	196[A]	SER
1	A	196[B]	SER
1	A	239	ILE
1	A	246	LYS
1	A	249	GLN
1	A	250	MET
1	B	3	GLN
1	B	68[A]	LEU
1	B	68[B]	LEU
1	B	84	LYS
1	B	148	LYS
1	B	158	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	188	GLU
1	B	205	PRO
1	B	249	GLN
1	B	256	LYS
1	B	259	LYS
1	C	3	GLN
1	C	58	ARG
1	C	148	LYS
1	C	158	ARG

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	157	HIS
1	A	191	GLN
1	A	249	GLN
1	B	3	GLN
1	B	165	GLN
1	B	191	GLN
1	C	87	GLN
1	C	200	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	CO8	B	701	-	51,59,59	1.35	5 (9%)	62,85,85	2.36	19 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO8	B	701	-	-	22/54/74/74	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	CO8	P3B-O3B	-4.09	1.51	1.59
2	B	701	CO8	C1'-S1P	-4.08	1.66	1.76
2	B	701	CO8	O1'-C1'	3.62	1.26	1.21
2	B	701	CO8	C2'-C1'	3.41	1.54	1.50
2	B	701	CO8	C5A-C4A	2.55	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	CO8	C2'-C1'-S1P	9.76	124.82	113.46
2	B	701	CO8	C4'-C3'-C2'	6.48	136.48	113.19
2	B	701	CO8	O1'-C1'-S1P	-4.91	116.24	122.61
2	B	701	CO8	O1'-C1'-C2'	-4.28	118.94	123.99
2	B	701	CO8	C7P-N8P-C9P	3.90	129.54	122.59
2	B	701	CO8	N3A-C2A-N1A	-3.64	122.98	128.68
2	B	701	CO8	C6'-C5'-C4'	3.49	132.15	114.42
2	B	701	CO8	O5B-C5B-C4B	3.36	120.54	108.99
2	B	701	CO8	CDP-CBP-CAP	3.19	114.34	108.82
2	B	701	CO8	C6P-C7P-N8P	-3.06	105.71	111.90
2	B	701	CO8	C2P-S1P-C1'	2.75	110.44	101.87
2	B	701	CO8	C3'-C2'-C1'	2.63	118.16	112.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	CO8	O4B-C1B-C2B	-2.61	103.11	106.93
2	B	701	CO8	C4A-C5A-N7A	2.58	112.09	109.40
2	B	701	CO8	P2A-O3A-P1A	2.44	141.19	132.83
2	B	701	CO8	C6P-C5P-N4P	-2.41	112.37	116.42
2	B	701	CO8	O6A-CCP-CBP	2.35	114.32	110.55
2	B	701	CO8	O5P-C5P-N4P	2.22	127.20	123.01
2	B	701	CO8	O9P-C9P-N8P	2.03	127.36	122.99

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	CO8	C2B-C3B-O3B-P3B
2	B	701	CO8	O4B-C4B-C5B-O5B
2	B	701	CO8	C5B-O5B-P1A-O1A
2	B	701	CO8	C5B-O5B-P1A-O2A
2	B	701	CO8	C5B-O5B-P1A-O3A
2	B	701	CO8	CDP-CBP-CCP-O6A
2	B	701	CO8	CAP-CBP-CCP-O6A
2	B	701	CO8	OAP-CAP-CBP-CCP
2	B	701	CO8	C9P-CAP-CBP-CCP
2	B	701	CO8	OAP-CAP-CBP-CDP
2	B	701	CO8	C9P-CAP-CBP-CDP
2	B	701	CO8	OAP-CAP-CBP-CEP
2	B	701	CO8	C9P-CAP-CBP-CEP
2	B	701	CO8	C3B-C4B-C5B-O5B
2	B	701	CO8	CEP-CBP-CCP-O6A
2	B	701	CO8	P2A-O3A-P1A-O5B
2	B	701	CO8	S1P-C1'-C2'-C3'
2	B	701	CO8	O1'-C1'-C2'-C3'
2	B	701	CO8	C3B-O3B-P3B-O9A
2	B	701	CO8	C4'-C5'-C6'-C7'
2	B	701	CO8	C4B-C5B-O5B-P1A
2	B	701	CO8	P2A-O3A-P1A-O2A

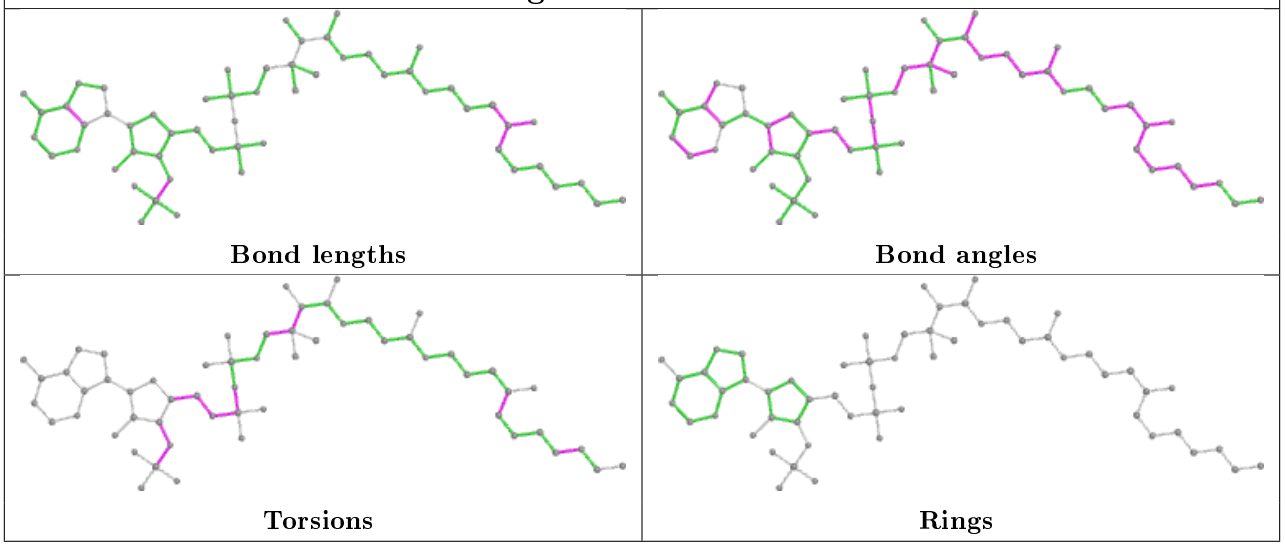
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	CO8	6	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 then 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.

Ligand CO8 B 701



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^{th} 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	249/260 (95%)	0.33	23 (9%)	9	6	12, 22, 45, 80	0
1	B	258/260 (99%)	0.08	16 (6%)	20	18	12, 20, 41, 87	0
1	C	250/260 (96%)	0.00	13 (5%)	27	24	12, 19, 39, 64	0
All	All	757/780 (97%)	0.13	52 (6%)	16	14	12, 20, 43, 87	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	7.5
1	A	2	SER	6.7
1	B	251[A]	TYR	6.1
1	B	260	GLY	5.6
1	B	259	LYS	5.5
1	A	244	ILE	5.1
1	A	76[A]	PRO	4.9
1	A	246	LYS	4.5
1	C	251	TYR	4.2
1	B	255	LEU	4.1
1	A	75[A]	SER	4.1
1	A	58	ARG	4.0
1	A	72[A]	CYS	4.0
1	C	246	LYS	3.9
1	A	47	LYS	3.9
1	B	256	LYS	3.9
1	C	249	GLN	3.9
1	C	252	LEU	3.8
1	A	249	GLN	3.8
1	A	239	ILE	3.5
1	A	68	LEU	3.3
1	C	58	ARG	3.3
1	A	250	MET	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	250	MET	3.3
1	A	69	THR	3.3
1	C	3	GLN	3.3
1	B	254	ARG	3.1
1	A	45	ASN	3.1
1	A	238	PHE	3.0
1	B	47	LYS	3.0
1	B	129	ARG	3.0
1	B	249	GLN	2.7
1	C	45	ASN	2.6
1	A	245[A]	GLN	2.6
1	B	250	MET	2.5
1	A	79[A]	TYR	2.5
1	B	246	LYS	2.4
1	C	241	LYS	2.4
1	B	242[A]	ASP	2.4
1	A	3	GLN	2.3
1	B	188	GLU	2.3
1	B	257	GLU	2.3
1	A	242	ASP	2.2
1	C	13	ALA	2.2
1	C	47	LYS	2.2
1	B	4	ARG	2.2
1	A	236	VAL	2.2
1	B	58	ARG	2.2
1	A	237[A]	SER	2.1
1	C	242	ASP	2.1
1	C	12	GLY	2.1
1	A	243	SER	2.0

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

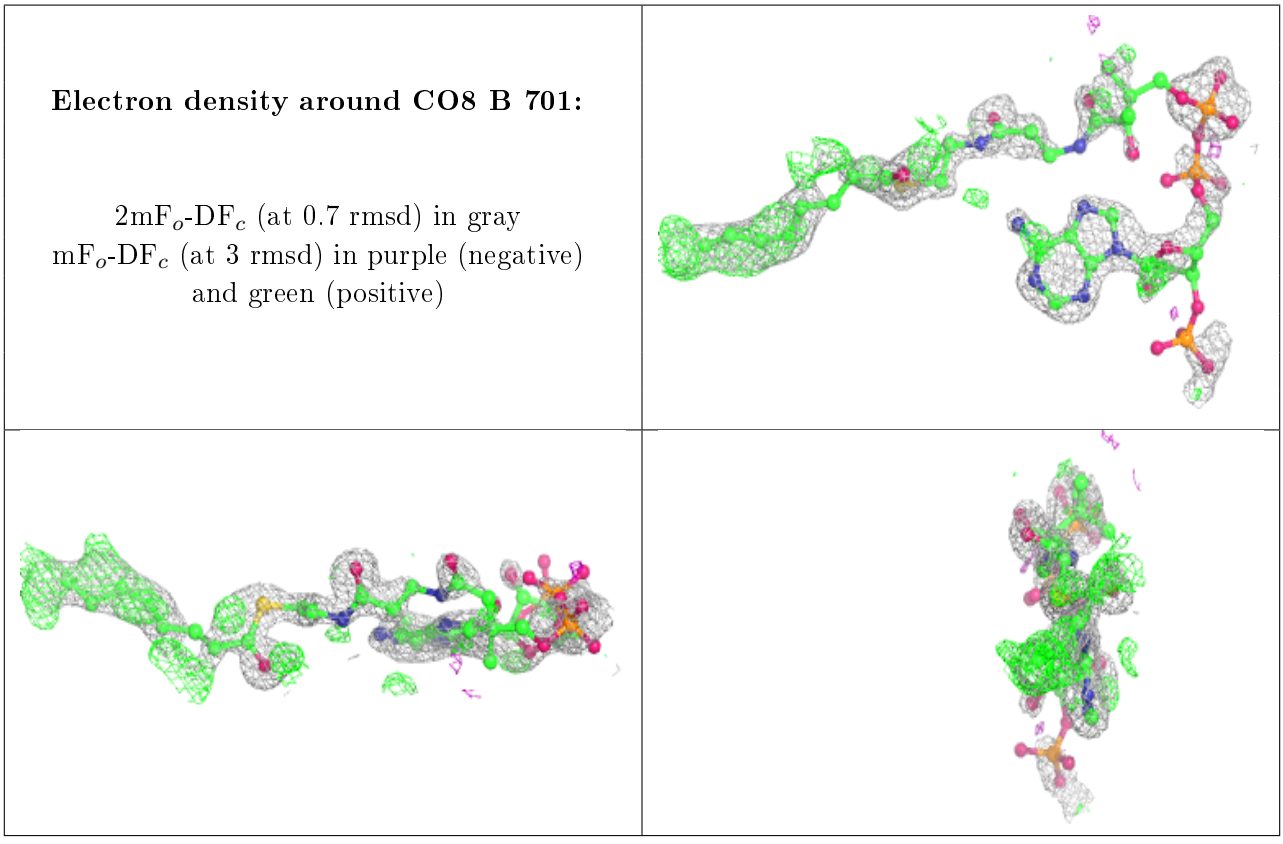
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	CO8	B	701	57/57	0.48	0.34	18,34,64,74	57

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.

Electron density around CO8 B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.