Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:47 AM GMT

PDB ID	:	3Q0G
Title	:	Crystal Structure of the Mycobacterium tuberculosis Crotonase Bound to a Reaction Intermediate Derived from Crotonyl CoA
Authors	:	Bruning, J.B.; Delgado, E.; Ghosh, S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2010-12-15
Resolution	:	2.38 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

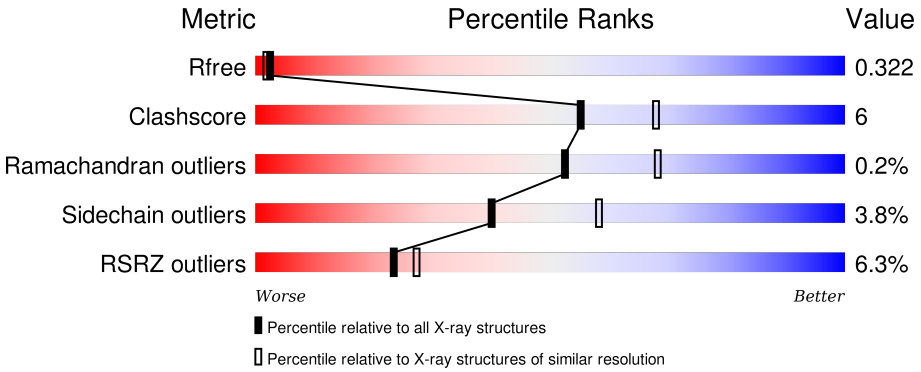
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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. 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	257	6% 84% 12%
1	B	257	5% 82% 16%
1	C	257	7% 86% 13%
1	D	257	4% 87% 9%
1	E	257	8% 85% 12%

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Mol	Chain	Length	Quality of chain
1	F	257	6% 81% 18%

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	COA	C	258	-	-	-	X
5	BCO	F	259	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12127 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.

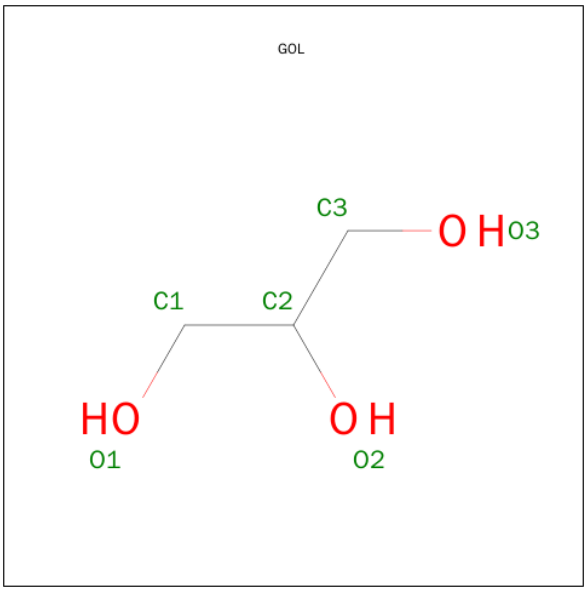
- Molecule 1 is a protein called enoyl-CoA hydratase echA8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	1	0
			1840	1147	321	361	11			
1	B	253	Total	C	N	O	S	0	0	0
			1866	1164	322	368	12			
1	C	255	Total	C	N	O	S	0	1	0
			1878	1172	324	370	12			
1	D	250	Total	C	N	O	S	0	1	0
			1831	1140	318	362	11			
1	E	253	Total	C	N	O	S	0	2	0
			1857	1158	323	364	12			
1	F	254	Total	C	N	O	S	0	3	0
			1885	1176	326	371	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

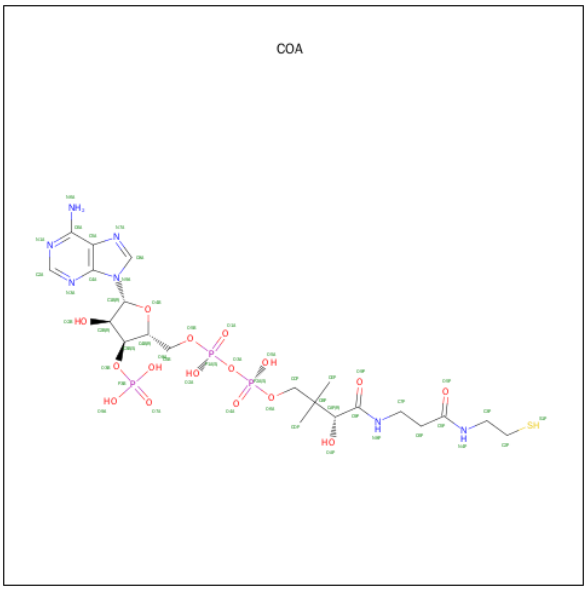
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



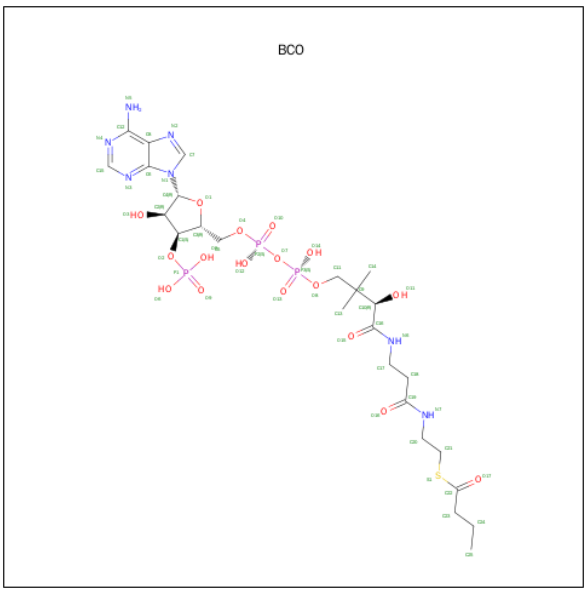
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 5 is BUTYRYL COENZYME A (three-letter code: BCO) (formula: $C_{25}H_{42}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		

- Molecule 6 is water.

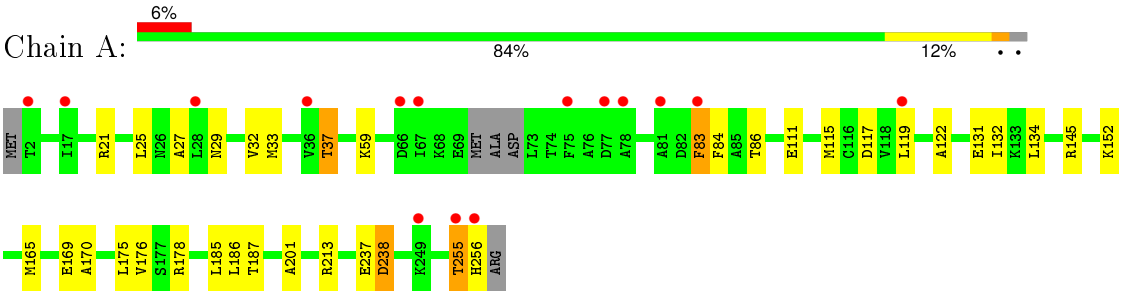
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	140	Total	O	0	0
			140	140		
6	C	152	Total	O	0	0
			152	152		
6	D	141	Total	O	0	0
			141	141		
6	E	144	Total	O	0	0
			144	144		
6	F	149	Total	O	0	0
			149	149		

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 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.

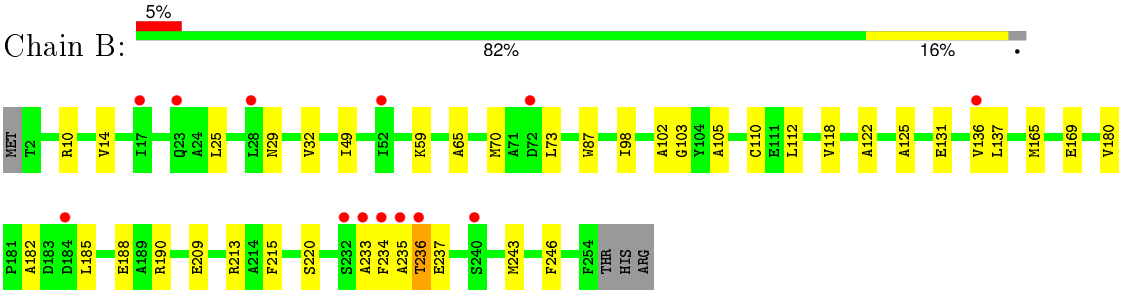
- Molecule 1: enoyl-CoA hydratase echA8

Chain A:



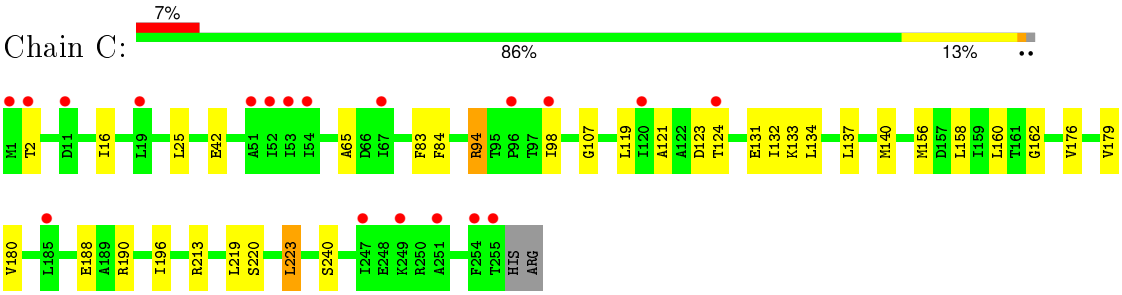
- Molecule 1: enoyl-CoA hydratase echA8

Chain B:



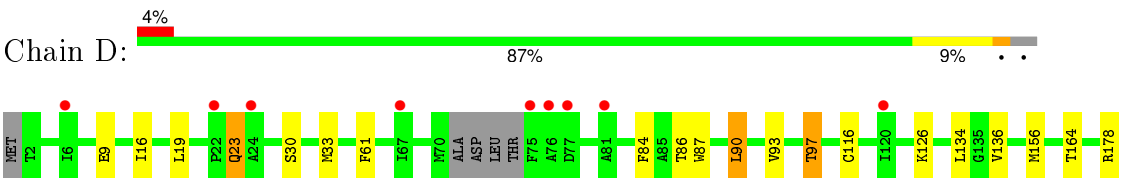
- Molecule 1: enoyl-CoA hydratase echA8

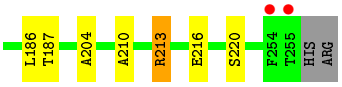
Chain C:



- Molecule 1: enoyl-CoA hydratase echA8

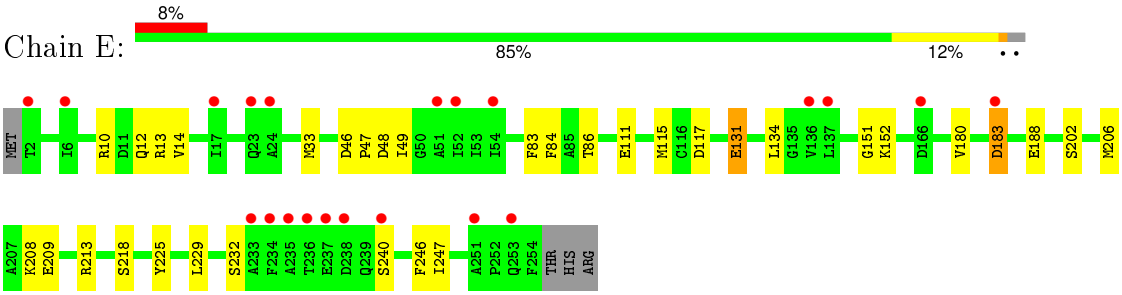
Chain D:





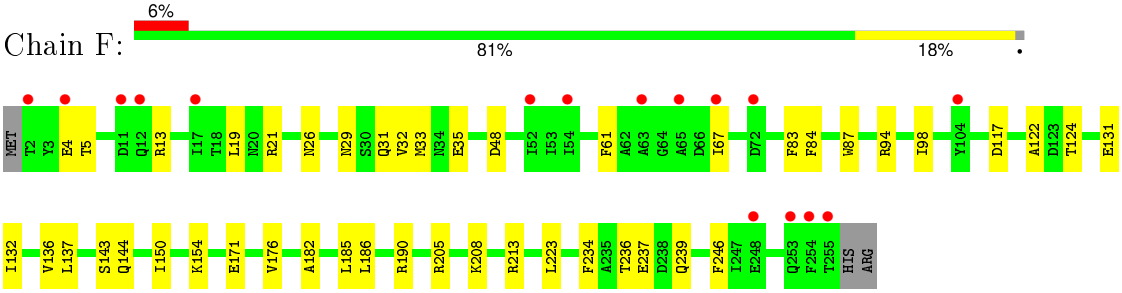
• Molecule 1: enoyl-CoA hydratase echA8

Chain E:



• Molecule 1: enoyl-CoA hydratase echA8

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.64Å 133.17Å 133.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.38 19.87 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.87-2.38) 93.1 (19.87-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.233 , 0.288 0.270 , 0.322	Depositor DCC
R_{free} test set	3444 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 27.5	EDS
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	5 of 67951 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12127	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.46 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8312e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: COA, GOL, MG, BCO

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	0.50	0/1866	0.62	0/2524
1	B	0.48	0/1889	0.63	0/2555
1	C	0.51	0/1904	0.64	1/2576 (0.0%)
1	D	0.49	0/1856	0.61	0/2510
1	E	0.49	0/1885	0.61	0/2549
1	F	0.50	0/1917	0.63	0/2592
All	All	0.49	0/11317	0.62	1/15306 (0.0%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	123	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	234	PHE	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	1840	0	1807	23	0
1	B	1866	0	1861	23	0
1	C	1878	0	1876	26	0
1	D	1831	0	1804	23	0
1	E	1857	0	1857	24	0
1	F	1885	0	1886	26	0
2	A	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	3	0
3	D	6	0	8	0	0
4	C	48	0	31	8	0
5	F	53	0	34	7	0
6	A	123	0	0	2	0
6	B	140	0	0	3	0
6	C	152	0	0	1	0
6	D	141	0	0	0	0
6	E	144	0	0	4	0
6	F	149	0	0	4	0
All	All	12127	0	11180	141	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 6.

All (141) 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)
5:F:259:BCO:C24	6:F:1000:HOH:O	2.04	1.06
1:E:206:MET:HE1	6:E:502:HOH:O	1.54	1.05
1:C:156:MET:HE3	1:C:160:LEU:HD11	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:HH11	1:C:94:ARG:HG2	1.28	0.95
1:C:132:ILE:O	1:C:133:LYS:HG2	1.68	0.93
1:C:134:LEU:HD12	4:C:258:COA:S1P	2.09	0.92
1:C:156:MET:CE	1:C:160:LEU:HD11	2.02	0.90
1:B:131:GLU:HG2	3:B:402:GOL:O1	1.70	0.89
1:C:94:ARG:NH1	6:C:533:HOH:O	2.10	0.83
1:D:33:MET:HE1	1:D:84:PHE:HA	1.64	0.79
1:B:180:VAL:HG11	1:B:188:GLU:HG2	1.67	0.76
1:D:33:MET:CE	1:D:84:PHE:HA	2.17	0.74
1:F:131:GLU:OE2	5:F:259:BCO:H34	1.87	0.74
1:F:186:LEU:O	1:F:190:ARG:HG2	1.87	0.74
1:C:94:ARG:NH1	1:C:94:ARG:HG2	2.02	0.71
1:B:70:MET:HA	1:B:73:LEU:HD13	1.74	0.70
1:C:132:ILE:O	1:C:133:LYS:CG	2.40	0.69
1:A:119:LEU:HD22	1:A:176:VAL:HG12	1.76	0.67
1:C:180:VAL:HG11	1:C:188:GLU:HG3	1.77	0.66
4:C:258:COA:H131	4:C:258:COA:O9P	1.97	0.65
1:A:237:GLU:O	1:A:238:ASP:HB2	1.97	0.64
1:F:83:PHE:O	1:F:84:PHE:HB2	1.96	0.64
1:D:33:MET:CE	1:D:87:TRP:CD1	2.82	0.63
1:D:33:MET:HE3	1:D:87:TRP:CD1	2.33	0.63
1:D:23:GLN:OE1	1:D:23:GLN:HA	1.98	0.62
1:E:83:PHE:O	1:E:84:PHE:HB2	2.00	0.62
1:C:65:ALA:HB2	1:C:140:MET:HE1	1.82	0.60
1:A:117:ASP:HB3	1:C:156:MET:CE	2.32	0.60
1:A:201:ALA:H	1:A:256:HIS:HB3	1.67	0.59
4:C:258:COA:H8A	4:C:258:COA:H52A	1.86	0.57
1:E:232:SER:HB3	6:E:502:HOH:O	2.05	0.56
1:C:25:LEU:HD12	4:C:258:COA:H8A	1.87	0.56
5:F:259:BCO:C25	6:F:1000:HOH:O	2.46	0.56
1:A:131:GLU:HA	1:A:131:GLU:OE2	2.07	0.55
1:C:83:PHE:O	1:C:84:PHE:HB2	2.08	0.54
1:B:209:GLU:O	1:B:213:ARG:HG2	2.07	0.54
1:A:122:ALA:HB2	1:A:185:LEU:HD22	1.89	0.54
1:A:237:GLU:O	1:A:238:ASP:CB	2.55	0.54
1:F:131:GLU:CD	5:F:259:BCO:H34	2.29	0.53
1:C:119:LEU:HD22	1:C:176:VAL:HG12	1.90	0.53
1:F:19:LEU:HD12	1:F:61:PHE:O	2.08	0.53
1:C:131:GLU:HA	4:C:258:COA:S1P	2.49	0.53
1:C:156:MET:CE	1:C:160:LEU:CD1	2.83	0.52
1:E:225:TYR:HE2	1:E:229:LEU:HD22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:MET:HE3	1:E:117:ASP:OD1	2.10	0.52
1:E:209:GLU:O	1:E:213:ARG:HG2	2.10	0.52
1:B:131:GLU:HB3	1:B:136:VAL:HG23	1.91	0.51
1:D:33:MET:HE2	1:D:87:TRP:CD1	2.46	0.51
1:F:4:GLU:HB3	1:F:31:GLN:HE22	1.75	0.51
1:B:131:GLU:CG	3:B:402:GOL:O1	2.53	0.51
1:D:33:MET:CE	1:D:84:PHE:HD1	2.24	0.51
1:A:111:GLU:O	1:A:115:MET:HG3	2.11	0.51
1:D:33:MET:HE3	1:D:87:TRP:NE1	2.25	0.51
1:C:132:ILE:O	1:C:133:LYS:CB	2.60	0.50
1:B:122:ALA:HB1	1:B:182:ALA:HA	1.93	0.50
1:F:29:ASN:OD1	1:F:32:VAL:HG23	2.11	0.50
1:D:97:THR:CG2	1:D:116:CYS:HA	2.41	0.50
1:F:131:GLU:CG	5:F:259:BCO:H34	2.42	0.49
1:C:16:ILE:HD11	1:C:190:ARG:HD3	1.95	0.49
1:B:87:TRP:CZ3	1:B:112:LEU:HD13	2.48	0.49
1:B:102:ALA:HB2	1:B:185:LEU:HD22	1.95	0.48
1:F:21:ARG:HB2	1:F:26:ASN:HA	1.93	0.48
1:E:111:GLU:O	1:E:115:MET:HG3	2.13	0.48
5:F:259:BCO:H31	5:F:259:BCO:O17	2.10	0.48
1:A:33:MET:O	1:A:37:THR:HB	2.13	0.48
1:D:33:MET:HE2	1:D:84:PHE:HA	1.95	0.48
1:E:13:ARG:HG3	1:E:48:ASP:O	2.14	0.48
1:D:216:GLU:HA	1:E:218[A]:SER:OG	2.14	0.48
1:A:21:ARG:HH12	1:A:27:ALA:HB3	1.79	0.48
1:D:33:MET:SD	1:D:86:THR:HB	2.54	0.47
1:E:225:TYR:CE2	1:E:229:LEU:HD22	2.48	0.47
1:E:183:ASP:N	1:E:183:ASP:OD2	2.44	0.47
1:F:150:ILE:HD12	1:F:154:LYS:HB3	1.97	0.47
1:B:98:ILE:HD12	1:B:118:VAL:HB	1.95	0.46
1:F:33:MET:HG3	1:F:87:TRP:CE2	2.50	0.46
1:F:67:ILE:H	5:F:259:BCO:C15	2.28	0.46
1:F:124:THR:HG23	1:F:182:ALA:HB2	1.97	0.46
1:D:33:MET:HE1	1:D:84:PHE:HD1	1.81	0.46
1:B:131:GLU:HG2	3:B:402:GOL:HO1	1.78	0.46
1:C:156:MET:HE2	1:C:156:MET:HB3	1.90	0.45
1:D:126:LYS:HD3	1:D:126:LYS:HA	1.79	0.45
1:A:33:MET:SD	1:A:86:THR:HB	2.57	0.45
1:E:134:LEU:HD22	1:F:246:PHE:HB2	1.99	0.45
1:F:5:THR:OG1	1:F:35:GLU:OE1	2.27	0.44
1:B:29:ASN:OD1	1:B:32:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:GLU:HB3	1:F:136:VAL:HG23	2.00	0.44
4:C:258:COA:H52A	4:C:258:COA:C8A	2.47	0.44
1:C:107:GLY:HA2	1:C:131:GLU:OE2	2.17	0.44
1:B:105:ALA:O	1:B:110:CYS:HB2	2.18	0.43
1:B:233:ALA:HB3	6:B:594:HOH:O	2.17	0.43
1:C:219:LEU:HG	1:C:223:LEU:HD22	1.99	0.43
1:F:94:ARG:HE	1:F:205:ARG:NH1	2.16	0.43
1:E:117:ASP:OD2	1:E:208:LYS:NZ	2.50	0.43
1:E:46:ASP:HA	1:E:47:PRO:HD3	1.84	0.43
1:F:171:GLU:HA	1:F:176:VAL:HG22	2.01	0.43
1:C:121:ALA:O	1:C:179:VAL:HA	2.19	0.43
1:F:236:THR:HB	6:F:505:HOH:O	2.19	0.43
1:B:25:LEU:HD21	1:B:59:LYS:HE2	2.01	0.43
1:D:9:GLU:HB3	1:D:16:ILE:HG23	2.01	0.42
1:D:19:LEU:HD12	1:D:61:PHE:O	2.19	0.42
1:A:201:ALA:CB	1:A:256:HIS:HB3	2.49	0.42
1:A:178:ARG:HA	6:A:575:HOH:O	2.19	0.42
1:B:65:ALA:HB2	6:B:623:HOH:O	2.19	0.42
1:A:134:LEU:HD21	1:B:246:PHE:HB2	2.01	0.42
1:F:234:PHE:CD2	1:F:239:GLN:NE2	2.87	0.42
1:E:152:LYS:HD2	6:F:545:HOH:O	2.19	0.42
1:F:13:ARG:HA	1:F:48:ASP:O	2.19	0.42
1:A:29:ASN:OD1	1:A:32:VAL:HG23	2.19	0.42
1:A:83:PHE:O	1:A:84:PHE:HB2	2.19	0.42
1:B:103:GLY:O	1:B:125:ALA:HA	2.19	0.42
1:B:165:MET:HG3	1:B:169:GLU:HB3	2.01	0.42
1:F:143:SER:OG	1:F:144:GLN:NE2	2.51	0.42
1:E:10:ARG:HG2	1:E:49:ILE:HD11	2.02	0.42
1:C:131:GLU:HA	4:C:258:COA:C2P	2.49	0.42
4:C:258:COA:O9P	4:C:258:COA:CDP	2.63	0.42
1:B:235:ALA:O	1:B:236:THR:HG23	2.20	0.41
1:D:204:ALA:HA	1:F:132:ILE:HD11	2.03	0.41
1:D:134:LEU:HD22	1:E:246:PHE:HB2	2.02	0.41
1:E:180:VAL:HG11	1:E:188:GLU:HG2	2.02	0.41
1:C:158:LEU:O	1:C:162:GLY:HA2	2.19	0.41
1:A:25:LEU:HD11	1:E:247:ILE:HD13	2.01	0.41
1:E:151:GLY:HA2	6:E:569:HOH:O	2.20	0.41
1:E:33:MET:SD	1:E:86:THR:HB	2.60	0.41
1:D:90:LEU:O	1:D:93:VAL:HB	2.21	0.41
1:F:117:ASP:OD2	1:F:208:LYS:HD2	2.20	0.41
1:B:190:ARG:NH2	6:B:524:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:HD2	6:A:527:HOH:O	2.21	0.41
1:D:210:ALA:O	1:D:213:ARG:HB2	2.19	0.41
1:B:10:ARG:HG2	1:B:49:ILE:HD11	2.01	0.41
1:E:202:SER:O	1:E:206:MET:HG3	2.21	0.41
1:A:117:ASP:HB3	1:C:156:MET:HE2	2.03	0.41
1:D:156:MET:HE3	1:E:208:LYS:HG3	2.03	0.41
1:A:152:LYS:HB2	1:B:215:PHE:CZ	2.56	0.41
1:D:97:THR:HG23	1:D:116:CYS:HA	2.02	0.41
1:A:170:ALA:HB1	1:A:175:LEU:HB3	2.03	0.41
1:A:165:MET:HG3	1:A:169:GLU:HB3	2.03	0.40
1:C:98:ILE:HD11	1:C:196:ILE:HD12	2.03	0.40
1:E:131:GLU:HB2	6:E:632:HOH:O	2.22	0.40
1:F:132:ILE:HA	1:F:136:VAL:O	2.21	0.40
1:A:201:ALA:HB3	1:A:256:HIS:HB3	2.03	0.40
1:F:122:ALA:HB2	1:F:185:LEU:HD22	2.03	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	249/257 (97%)	241 (97%)	7 (3%)	1 (0%)	39	53
1	B	251/257 (98%)	240 (96%)	10 (4%)	1 (0%)	39	53
1	C	254/257 (99%)	243 (96%)	11 (4%)	0	100	100
1	D	247/257 (96%)	240 (97%)	7 (3%)	0	100	100
1	E	253/257 (98%)	242 (96%)	10 (4%)	1 (0%)	39	53
1	F	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
All	All	1509/1542 (98%)	1452 (96%)	54 (4%)	3 (0%)	52	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	B	236	THR
1	E	12	GLN

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	180/192 (94%)	172 (96%)	8 (4%)	35	51
1	B	186/192 (97%)	181 (97%)	5 (3%)	52	71
1	C	187/192 (97%)	178 (95%)	9 (5%)	31	47
1	D	181/192 (94%)	170 (94%)	11 (6%)	23	34
1	E	185/192 (96%)	181 (98%)	4 (2%)	60	78
1	F	189/192 (98%)	184 (97%)	5 (3%)	54	73
All	All	1108/1152 (96%)	1066 (96%)	42 (4%)	40	58

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	59	LYS
1	A	83	PHE
1	A	132	ILE
1	A	186	LEU
1	A	187	THR
1	A	213	ARG
1	A	255	THR
1	B	14	VAL
1	B	137	LEU
1	B	220	SER
1	B	237	GLU
1	B	243	MET
1	C	2	THR
1	C	42	GLU
1	C	94	ARG

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Mol	Chain	Res	Type
1	C	124	THR
1	C	137	LEU
1	C	213	ARG
1	C	220	SER
1	C	223	LEU
1	C	240	SER
1	D	23	GLN
1	D	30	SER
1	D	90	LEU
1	D	97	THR
1	D	136	VAL
1	D	164	THR
1	D	178	ARG
1	D	186	LEU
1	D	187	THR
1	D	213	ARG
1	D	220	SER
1	E	14	VAL
1	E	131	GLU
1	E	183	ASP
1	E	240	SER
1	F	98	ILE
1	F	137	LEU
1	F	213	ARG
1	F	223	LEU
1	F	237	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	31	GLN
1	F	31	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)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	GOL	A	401	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	B	402	-	5,5,5	0.34	0	5,5,5	0.63	0
4	COA	C	258	-	40,50,50	2.84	20 (50%)	50,75,75	4.15	28 (56%)
3	GOL	D	403	-	5,5,5	0.33	0	5,5,5	0.25	0
5	BCO	F	259	2	43,55,55	2.56	17 (39%)	55,81,81	3.88	30 (54%)

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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
4	COA	C	258	-	-	0/44/64/64	0/3/3/3
3	GOL	D	403	-	-	0/4/4/4	0/0/0/0
5	BCO	F	259	2	1/1/12/14	1/49/70/70	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	258	COA	P1A-O5B	-7.29	1.25	1.59
5	F	259	BCO	P2-O4	-6.29	1.30	1.59
4	C	258	COA	O4B-C4B	-5.87	1.31	1.45
4	C	258	COA	P3B-O3B	-5.47	1.43	1.60
5	F	259	BCO	O1-C3	-4.76	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	258	COA	O3B-C3B	-4.58	1.30	1.44
4	C	258	COA	P3B-O9A	-4.52	1.38	1.54
5	F	259	BCO	P3-O14	-4.34	1.36	1.54
4	C	258	COA	O5B-C5B	-4.18	1.27	1.44
4	C	258	COA	P1A-O1A	-3.98	1.36	1.51
5	F	259	BCO	O4-C5	-3.90	1.28	1.44
5	F	259	BCO	P1-O6	-3.89	1.40	1.54
4	C	258	COA	P1A-O2A	-3.76	1.38	1.54
5	F	259	BCO	P2-O10	-3.69	1.37	1.51
5	F	259	BCO	P3-O8	-3.67	1.42	1.59
4	C	258	COA	P2A-O5A	-3.57	1.39	1.54
5	F	259	BCO	C7-N2	-3.28	1.28	1.34
4	C	258	COA	C8A-N7A	-3.20	1.28	1.34
5	F	259	BCO	P1-O2	-3.13	1.50	1.60
5	F	259	BCO	C8-N2	-3.07	1.29	1.39
4	C	258	COA	CDP-CBP	-2.97	1.47	1.53
5	F	259	BCO	P3-O13	-2.90	1.40	1.51
5	F	259	BCO	C6-N3	-2.78	1.31	1.35
4	C	258	COA	C5A-C4A	-2.76	1.34	1.40
4	C	258	COA	C5A-N7A	-2.61	1.30	1.39
4	C	258	COA	P2A-O4A	-2.60	1.41	1.51
4	C	258	COA	C2A-N3A	-2.49	1.27	1.32
4	C	258	COA	C6A-N6A	-2.40	1.27	1.34
5	F	259	BCO	P2-O12	-2.33	1.45	1.54
4	C	258	COA	C5B-C4B	-2.26	1.44	1.51
4	C	258	COA	O9P-C9P	-2.05	1.19	1.23
4	C	258	COA	CEP-CBP	-2.01	1.49	1.53
5	F	259	BCO	C1-C3	-2.01	1.47	1.52
5	F	259	BCO	C17-N6	2.60	1.47	1.40
4	C	258	COA	O4B-C1B	3.11	1.45	1.41
5	F	259	BCO	C17-C18	3.99	1.53	1.36
5	F	259	BCO	C23-C24	5.70	1.51	1.30

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	259	BCO	C10-C16-N6	-15.56	99.12	115.58
4	C	258	COA	N3A-C2A-N1A	-14.28	117.96	128.89
4	C	258	COA	C4B-O4B-C1B	-9.10	99.72	109.72
5	F	259	BCO	C25-C24-C23	-8.37	109.62	125.27
4	C	258	COA	C2B-C3B-C4B	-7.33	89.53	103.29
5	F	259	BCO	C2-C1-C3	-6.66	90.78	103.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	258	COA	O3A-P1A-O5B	-6.25	86.35	102.94
4	C	258	COA	O4B-C4B-C5B	-6.04	87.70	109.32
5	F	259	BCO	C3-O1-C4	-5.59	103.57	109.72
5	F	259	BCO	C6-C8-N2	-5.13	104.76	109.48
5	F	259	BCO	O2-P1-O9	-4.66	95.47	107.11
5	F	259	BCO	O7-P2-O4	-4.62	90.68	102.94
4	C	258	COA	O3B-P3B-O7A	-4.54	95.77	107.11
4	C	258	COA	O8A-P3B-O7A	-4.32	96.69	110.58
5	F	259	BCO	N3-C15-N4	-4.02	125.82	128.89
4	C	258	COA	C2B-C1B-N9A	-3.95	108.26	114.29
5	F	259	BCO	C2-C4-N1	-3.93	108.28	114.29
5	F	259	BCO	C18-C17-N6	-3.65	113.02	123.18
5	F	259	BCO	O12-P2-O4	-3.41	91.26	108.46
4	C	258	COA	C1B-N9A-C4A	-3.33	121.92	126.94
4	C	258	COA	O5B-P1A-O1A	-3.23	97.07	109.62
5	F	259	BCO	O17-C22-S1	-2.99	118.61	122.37
5	F	259	BCO	C24-C23-C22	-2.90	118.26	123.68
5	F	259	BCO	O1-C3-C5	-2.56	100.17	109.32
5	F	259	BCO	C14-C9-C10	-2.55	104.68	109.34
4	C	258	COA	CDP-CBP-CCP	-2.49	105.28	108.50
4	C	258	COA	C4A-C5A-N7A	-2.15	107.50	109.48
5	F	259	BCO	O8-P3-O13	-2.10	101.46	109.62
5	F	259	BCO	O6-P1-O9	2.00	117.02	110.58
4	C	258	COA	CEP-CBP-CCP	2.06	111.17	108.50
5	F	259	BCO	O14-P3-O7	2.07	114.47	105.09
4	C	258	COA	O5P-C5P-N4P	2.10	127.09	122.94
4	C	258	COA	C2A-N1A-C6A	2.27	122.82	118.77
5	F	259	BCO	C20-N7-C19	2.31	125.86	122.41
5	F	259	BCO	O16-C19-N7	2.33	125.52	122.53
5	F	259	BCO	C17-N6-C16	2.58	128.40	123.80
4	C	258	COA	O2A-P1A-O5B	2.71	122.11	108.46
4	C	258	COA	O2A-P1A-O3A	2.79	117.77	105.09
5	F	259	BCO	C4-N1-C6	2.90	131.32	126.94
5	F	259	BCO	O12-P2-O7	3.17	119.48	105.09
4	C	258	COA	O9A-P3B-O8A	3.19	119.51	107.38
4	C	258	COA	P3B-O3B-C3B	3.42	129.76	121.56
4	C	258	COA	CEP-CBP-CAP	3.46	115.65	109.34
5	F	259	BCO	O4-P2-O10	3.46	123.03	109.62
5	F	259	BCO	O8-C11-C9	3.71	116.52	110.55
4	C	258	COA	O4B-C4B-C3B	3.98	114.04	104.86
5	F	259	BCO	C13-C9-C10	4.12	116.87	109.34
4	C	258	COA	O9A-P3B-O7A	4.16	123.97	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	259	BCO	O1-C3-C1	4.28	114.73	104.86
4	C	258	COA	O3B-C3B-C4B	4.28	126.80	109.99
4	C	258	COA	C2P-C3P-N4P	4.46	121.17	112.37
5	F	259	BCO	C21-S1-C22	4.48	105.29	99.59
4	C	258	COA	O4B-C1B-N9A	4.53	117.59	108.10
4	C	258	COA	C3P-N4P-C5P	4.69	132.01	122.79
5	F	259	BCO	C5-C3-C1	7.09	139.86	114.31
5	F	259	BCO	O4-C5-C3	8.19	139.30	109.12
4	C	258	COA	C5B-C4B-C3B	8.55	145.12	114.31
4	C	258	COA	O5B-C5B-C4B	9.05	142.49	109.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	259	BCO	C10

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	259	BCO	C22-C23-C24-C25

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	3	0
4	C	258	COA	8	0
5	F	259	BCO	7	0

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, 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	252/257 (98%)	0.68	15 (5%)	25	29	21, 42, 74, 102	0
1	B	253/257 (98%)	0.65	13 (5%)	32	36	20, 46, 86, 141	0
1	C	255/257 (99%)	0.63	19 (7%)	17	19	22, 42, 65, 79	0
1	D	250/257 (97%)	0.58	11 (4%)	38	43	22, 42, 67, 86	0
1	E	253/257 (98%)	0.72	21 (8%)	14	16	21, 47, 74, 96	0
1	F	254/257 (98%)	0.62	16 (6%)	23	27	23, 41, 65, 82	0
All	All	1517/1542 (98%)	0.65	95 (6%)	23	27	20, 43, 72, 141	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	THR	5.4
1	B	235	ALA	5.2
1	A	256	HIS	4.9
1	D	75	PHE	4.8
1	E	2	THR	4.7
1	A	67	ILE	4.7
1	D	22	PRO	4.4
1	D	67	ILE	4.1
1	C	2	THR	4.0
1	D	24	ALA	3.9
1	E	253	GLN	3.7
1	D	255	THR	3.7
1	F	255	THR	3.7
1	B	23	GLN	3.6
1	A	255	THR	3.6
1	E	234	PHE	3.6
1	A	78	ALA	3.5
1	F	54	ILE	3.4
1	E	24	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	247	ILE	3.3
1	E	237	GLU	3.3
1	E	233	ALA	3.3
1	E	235	ALA	3.3
1	A	2	THR	3.2
1	E	23	GLN	3.1
1	A	36	VAL	3.0
1	D	81	ALA	3.0
1	F	254	PHE	3.0
1	C	54	ILE	3.0
1	D	6	ILE	2.9
1	B	52	ILE	2.9
1	D	77	ASP	2.9
1	B	136	VAL	2.8
1	F	65	ALA	2.8
1	A	66	ASP	2.7
1	B	72	ASP	2.7
1	B	184	ASP	2.7
1	B	17	ILE	2.7
1	B	234	PHE	2.7
1	B	233	ALA	2.7
1	F	253	GLN	2.7
1	C	255	THR	2.7
1	A	28	LEU	2.7
1	C	19	LEU	2.7
1	C	67	ILE	2.7
1	E	240	SER	2.7
1	E	236	THR	2.7
1	B	232	SER	2.6
1	D	76	ALA	2.6
1	A	83	PHE	2.6
1	E	17	ILE	2.6
1	F	52	ILE	2.6
1	C	120	ILE	2.6
1	E	52	ILE	2.5
1	F	63	ALA	2.5
1	C	185	LEU	2.5
1	B	236	THR	2.5
1	E	137	LEU	2.5
1	C	249	LYS	2.4
1	E	51	ALA	2.4
1	E	238	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	17	ILE	2.4
1	F	67	ILE	2.4
1	C	1	MET	2.4
1	E	136	VAL	2.3
1	B	240	SER	2.3
1	F	11	ASP	2.3
1	A	119	LEU	2.3
1	F	17	ILE	2.3
1	F	4	GLU	2.3
1	F	12	GLN	2.3
1	E	183	ASP	2.3
1	D	254	PHE	2.3
1	A	77	ASP	2.3
1	C	51	ALA	2.3
1	C	251	ALA	2.2
1	C	53	ILE	2.2
1	C	11	ASP	2.2
1	F	72	ASP	2.2
1	A	81	ALA	2.2
1	C	124	THR	2.2
1	C	52	ILE	2.2
1	F	104	TYR	2.2
1	C	254	PHE	2.2
1	E	6	ILE	2.1
1	B	28	LEU	2.1
1	D	120	ILE	2.1
1	E	54	ILE	2.1
1	E	166	ASP	2.1
1	F	248	GLU	2.1
1	A	75	PHE	2.1
1	E	251	ALA	2.1
1	C	96	PRO	2.0
1	A	249	LYS	2.0
1	C	98	ILE	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 (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^{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	LLDF	B-factors(Å^2)	Q<0.9
4	COA	C	258	48/48	0.81	0.31	2.59	34,40,42,45	0
3	GOL	B	402	6/6	0.81	0.23	1.46	34,35,35,36	0
5	BCO	F	259	53/53	0.85	0.25	1.34	28,40,42,45	1
3	GOL	A	401	6/6	0.88	0.18	0.78	37,38,39,39	0
3	GOL	D	403	6/6	0.89	0.15	-0.52	28,31,32,32	0
2	MG	A	258	1/1	0.43	0.24	-	61,61,61,61	0
2	MG	F	258	1/1	0.42	0.21	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.