Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:01 PM GMT

PDB ID	:	4Z40
Title	:	Active site complex BamBC of Benzoyl Coenzyme A reductase as isolated
Authors	:	Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on	:	2015-04-01
Resolution	:	2.35 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 ⓘ symbol.

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

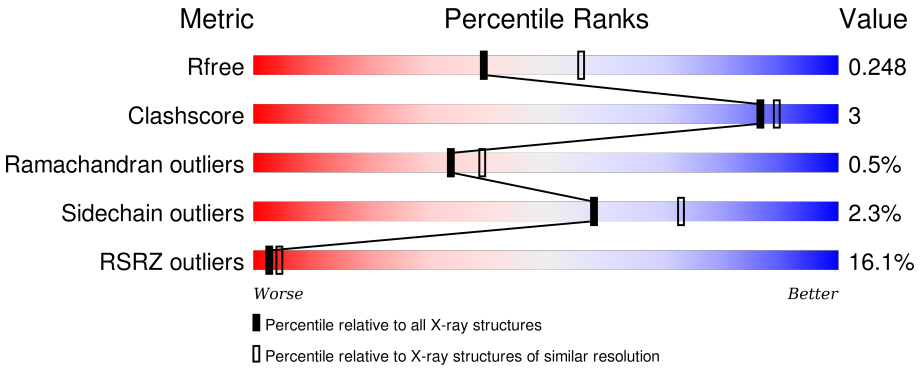
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	653	45% 92% 7% •
1	B	653	9% 93% 6% •
1	C	653	11% 93% 6%
1	D	653	5% 92% 8% •
2	E	179	12% 80% 12% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	179	14% 82% 12% • 5%
2	G	179	6% 83% 11% • 6%
2	H	179	6% 78% 12% 10%

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
3	UNL	A	701	-	-	X	-
3	UNL	D	701	-	-	X	-
4	SF4	F	1002	-	-	X	-
4	SF4	G	1002	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26313 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 Benzoyl-CoA reductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	0	0
			5180	3308	875	963	34			
1	B	652	Total	C	N	O	S	0	0	0
			5180	3308	875	963	34			
1	C	652	Total	C	N	O	S	0	0	0
			5185	3311	875	965	34			
1	D	652	Total	C	N	O	S	0	0	0
			5180	3308	875	963	34			

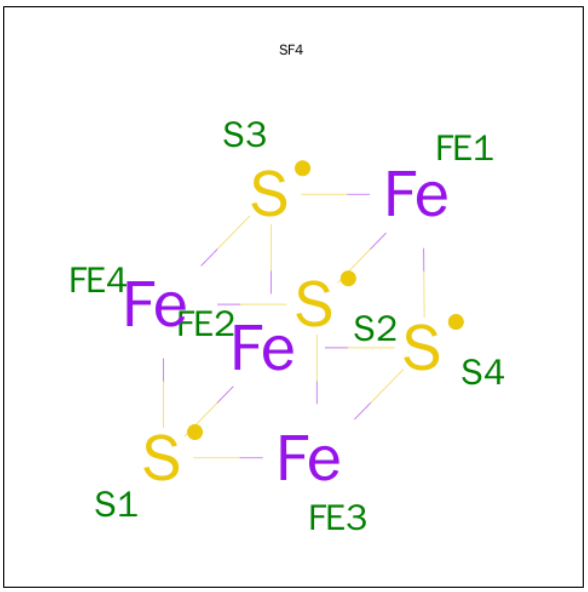
- Molecule 2 is a protein called Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	166	Total	C	N	O	S	0	0	0
			1260	784	223	239	14			
2	F	170	Total	C	N	O	S	0	1	0
			1317	816	226	261	14			
2	G	169	Total	C	N	O	S	0	2	0
			1315	814	228	259	14			
2	H	161	Total	C	N	O	S	0	0	0
			1221	758	213	236	14			

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



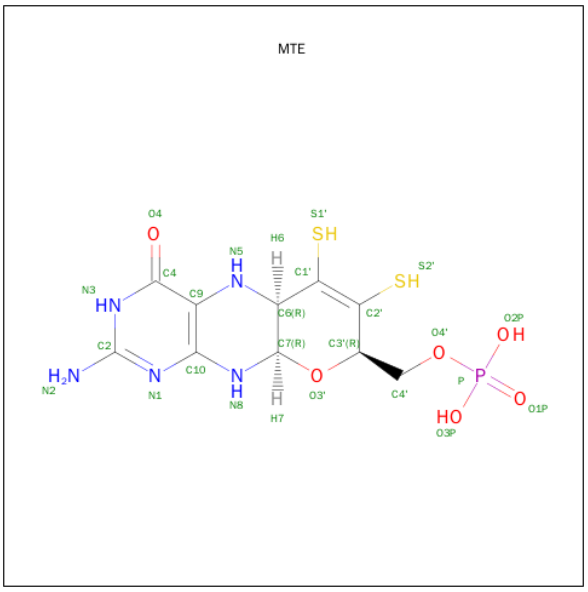
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	C	1	Total Fe S 8 4 4	0	0
4	D	1	Total Fe S 8 4 4	0	0
4	E	1	Total Fe S 8 4 4	0	0
4	E	1	Total Fe S 8 4 4	0	0
4	E	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	G	1	Total Fe S 8 4 4	0	0
4	G	1	Total Fe S 8 4 4	0	0
4	G	1	Total Fe S 8 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Fe S 8 4 4	0	0
4	H	1	Total Fe S 8 4 4	0	0
4	H	1	Total Fe S 8 4 4	0	0

- Molecule 5 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 24 10 5 6 1 2	0	0
5	A	1	Total C N O P S 24 10 5 6 1 2	0	0
5	B	1	Total C N O P S 24 10 5 6 1 2	0	0
5	B	1	Total C N O P S 24 10 5 6 1 2	0	0
5	C	1	Total C N O P S 24 10 5 6 1 2	0	0
5	C	1	Total C N O P S 24 10 5 6 1 2	0	0
5	D	1	Total C N O P S 24 10 5 6 1 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 6 is TUNGSTEN ION (three-letter code: W) (formula: W).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		
8	A	1	Total	Zn	0	0
			1	1		
8	D	1	Total	Zn	0	0
			1	1		
8	C	1	Total	Zn	0	0
			1	1		

- Molecule 9 is water.

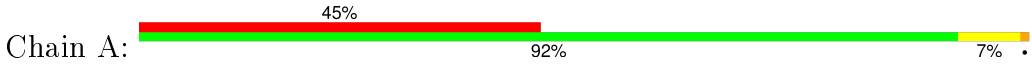
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	11	Total O 11 11	0	0
9	B	37	Total O 37 37	0	0
9	C	22	Total O 22 22	0	0
9	D	24	Total O 24 24	0	0
9	E	9	Total O 9 9	0	0
9	F	12	Total O 12 12	0	0
9	G	10	Total O 10 10	0	0
9	H	14	Total O 14 14	0	0

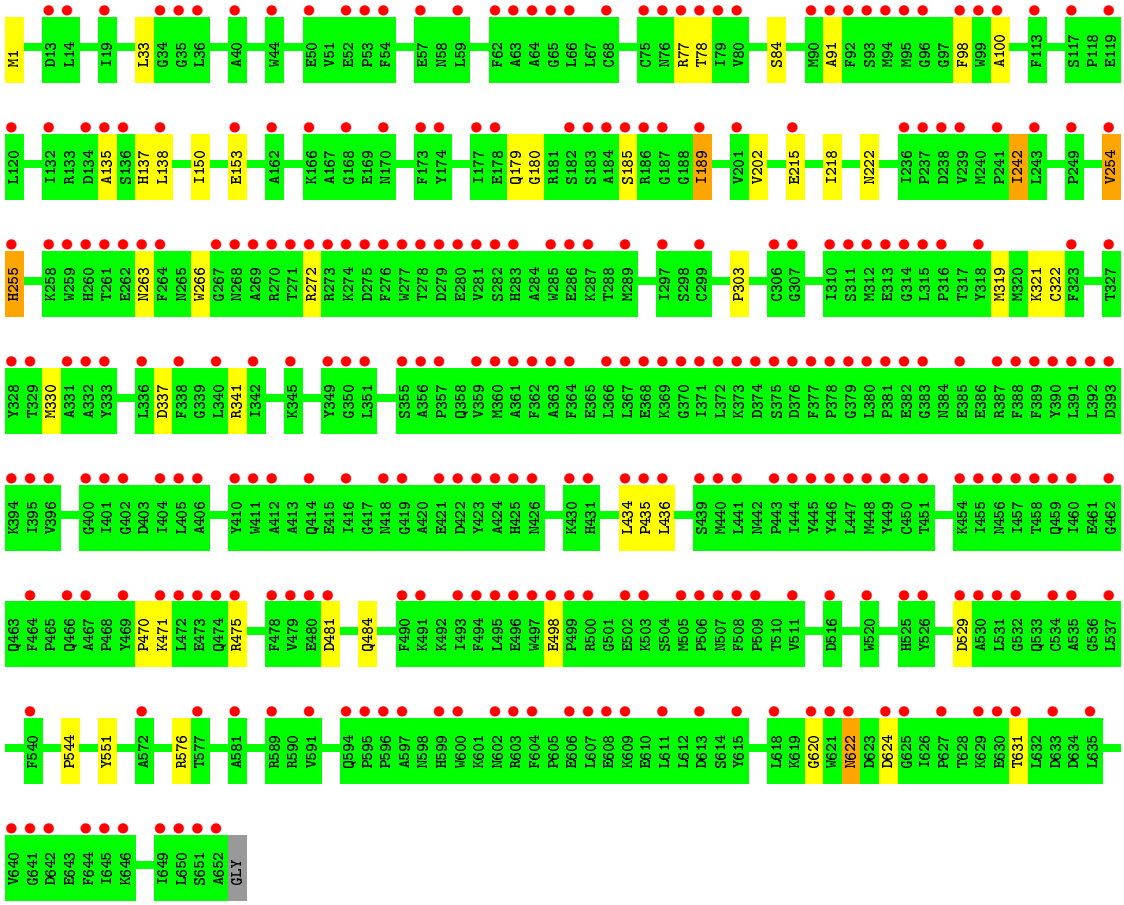
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Benzoyl-CoA reductase, putative

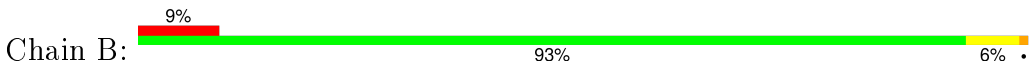
Chain A:

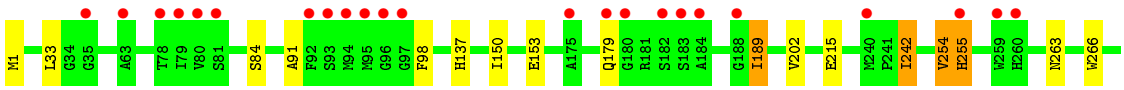


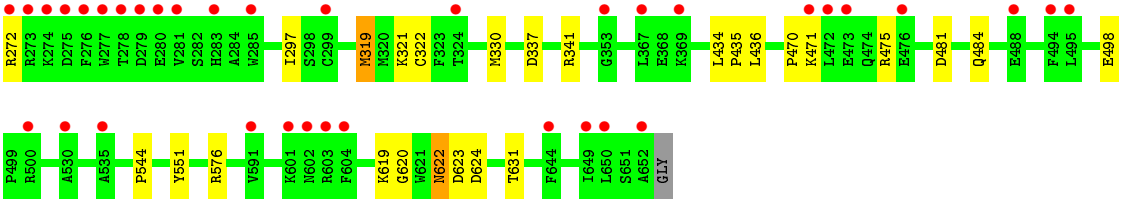


- Molecule 1: Benzoyl-CoA reductase, putative

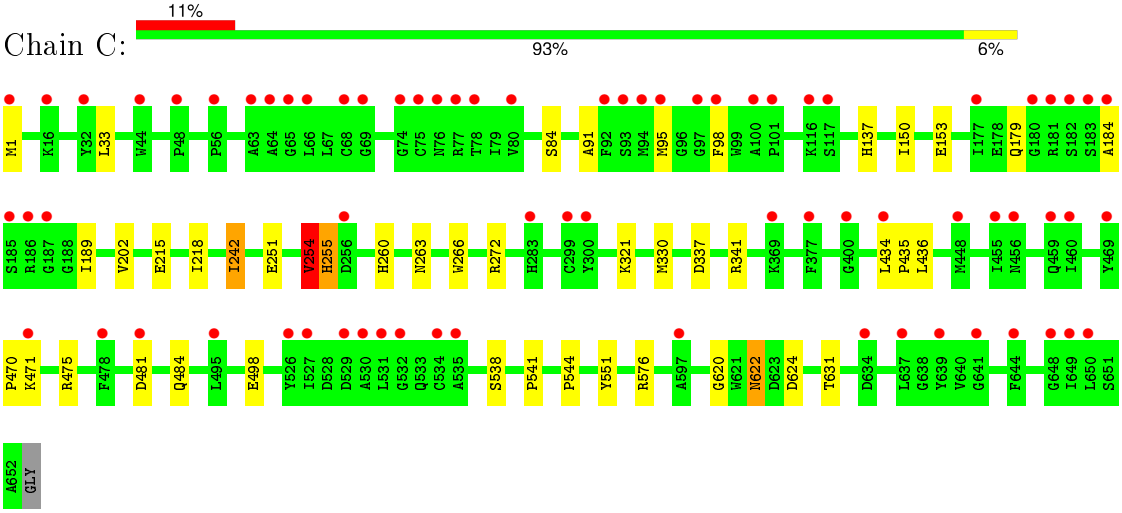
Chain B:



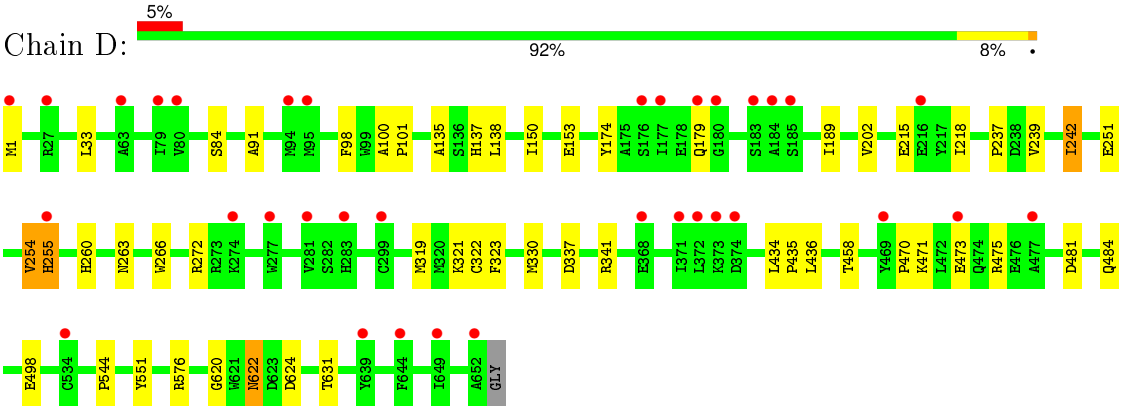




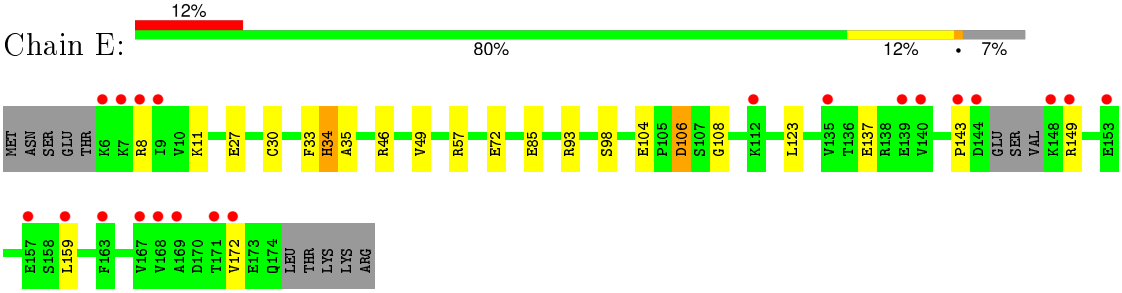
• Molecule 1: Benzoyl-CoA reductase, putative



• Molecule 1: Benzoyl-CoA reductase, putative

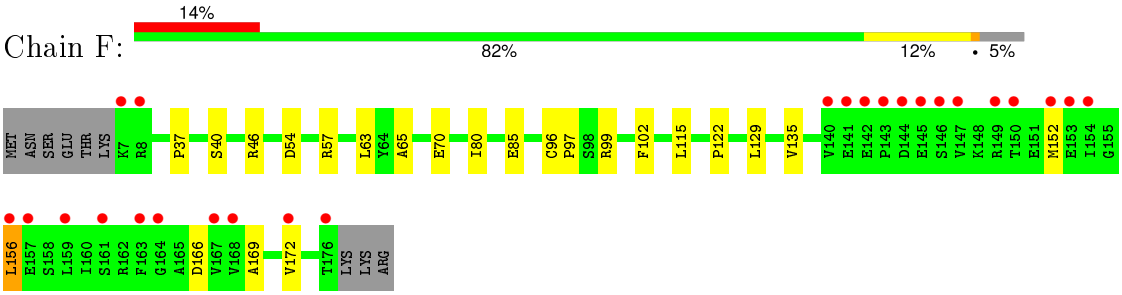


• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



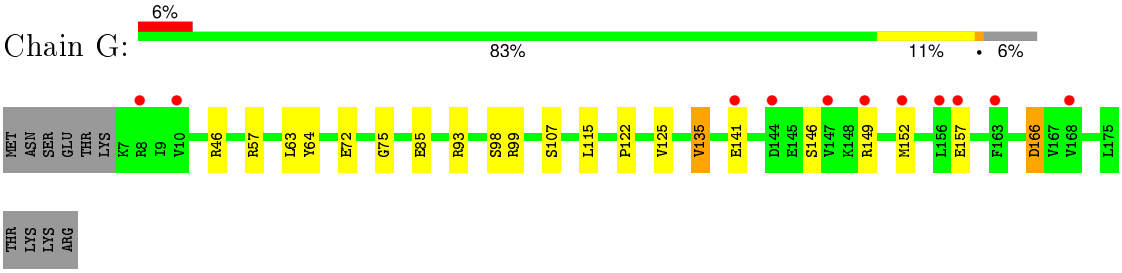
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain F:



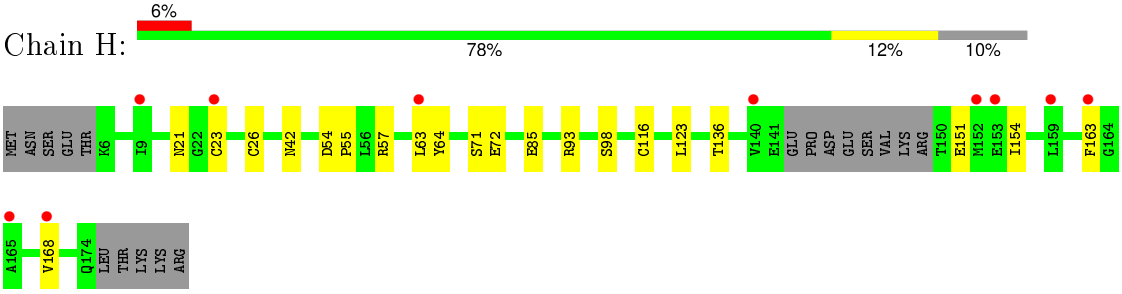
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain G:



• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.19Å 116.82Å 143.60Å 90.00° 110.39° 90.00°	Depositor
Resolution (Å)	49.50 – 2.35 49.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.50-2.35) 98.5 (49.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.212 , 0.238 0.226 , 0.248	Depositor DCC
R_{free} test set	1594 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 158836 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26313	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% 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, 0.375 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: MG, SF4, ZN, W, UNL, MTE

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	0.26	0/5306	0.41	0/7172
1	B	0.30	0/5306	0.43	0/7172
1	C	0.30	0/5311	0.43	0/7179
1	D	0.32	0/5306	0.43	0/7172
2	E	0.37	0/1282	0.50	0/1734
2	F	0.37	0/1343	0.51	0/1819
2	G	0.36	0/1344	0.51	0/1819
2	H	0.34	0/1242	0.50	0/1681
All	All	0.31	0/26440	0.44	0/35748

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	5180	0	5111	27	0
1	B	5180	0	5111	20	0
1	C	5185	0	5120	20	0
1	D	5180	0	5111	24	0
2	E	1260	0	1209	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1317	0	1266	13	0
2	G	1315	0	1263	16	0
2	H	1221	0	1158	12	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	2	0
4	A	8	0	0	1	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	24	0	0	1	0
4	F	24	0	0	2	0
4	G	24	0	0	2	0
4	H	24	0	0	0	0
5	A	48	0	22	3	0
5	B	48	0	23	0	0
5	C	48	0	20	0	0
5	D	48	0	20	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	11	0	0	2	0
9	B	37	0	0	0	0
9	C	22	0	0	0	0
9	D	24	0	0	0	0
9	E	9	0	0	0	0
9	F	12	0	0	0	0
9	G	10	0	0	1	0
9	H	14	0	0	0	0
All	All	26313	0	25434	139	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 3.

All (139) 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)
3:A:701:UNL:X	5:A:703:MTE:S1'	2.61	0.88
2:G:166:ASP:OD1	2:G:166:ASP:N	2.24	0.71
2:G:72:GLU:HG2	2:G:98:SER:HB3	1.71	0.71
2:E:30:CYS:SG	2:E:34:HIS:ND1	2.65	0.68
2:E:34:HIS:NE2	4:E:1002:SF4:S1	2.67	0.67
2:G:122:PRO:HG2	2:G:135:VAL:HG11	1.76	0.67
1:D:322:CYS:SG	5:D:704:MTE:S1'	2.93	0.66
1:D:434:LEU:HD22	1:D:435:PRO:HD2	1.79	0.64
1:B:434:LEU:HD22	1:B:435:PRO:HD2	1.79	0.64
1:A:185:SER:HB2	5:A:704:MTE:H4'1	1.81	0.63
2:F:80:ILE:HG12	2:F:85:GLU:HG2	1.81	0.62
1:A:434:LEU:HD22	1:A:435:PRO:HD2	1.80	0.62
1:B:254:VAL:O	1:B:255:HIS:ND1	2.33	0.61
2:E:159:LEU:HD13	2:F:156:LEU:HD22	1.81	0.61
1:C:254:VAL:O	1:C:255:HIS:ND1	2.34	0.60
1:D:254:VAL:O	1:D:255:HIS:ND1	2.34	0.60
1:C:434:LEU:HD22	1:C:435:PRO:HD2	1.84	0.60
1:A:254:VAL:O	1:A:255:HIS:ND1	2.35	0.59
2:H:57:ARG:NH1	2:H:85:GLU:O	2.36	0.59
2:E:172:VAL:HG21	2:F:172:VAL:HG21	1.86	0.57
2:G:149:ARG:NH1	2:G:157:GLU:OE1	2.38	0.56
2:F:37:PRO:HG2	2:F:40:SER:HB3	1.87	0.56
2:G:107:SER:HA	2:H:151:GLU:HB3	1.86	0.55
1:A:98:PHE:H	1:A:179:GLN:HE22	1.55	0.54
2:G:57:ARG:NH1	2:G:85:GLU:O	2.40	0.54
3:D:701:UNL:X	5:D:703:MTE:S1'	2.95	0.53
1:A:222:ASN:ND2	9:A:801:HOH:O	2.35	0.53
1:A:622:ASN:HD22	1:A:624:ASP:H	1.55	0.52
1:D:137:HIS:NE2	1:D:153:GLU:OE2	2.43	0.52
1:B:137:HIS:NE2	1:B:153:GLU:OE2	2.43	0.51
1:B:98:PHE:H	1:B:179:GLN:HE22	1.58	0.51
1:A:337:ASP:O	1:A:341:ARG:HG3	2.11	0.51
2:G:146:SER:HB3	2:H:71:SER:HB2	1.92	0.51
2:G:64:TYR:O	2:G:93:ARG:HD2	2.11	0.50
2:E:46:ARG:NH2	2:E:104:GLU:OE1	2.44	0.50
1:B:337:ASP:O	1:B:341:ARG:HG3	2.12	0.50
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.93	0.50
1:B:84:SER:HB2	1:B:91:ALA:HB2	1.93	0.50
1:D:98:PHE:H	1:D:179:GLN:HE22	1.59	0.50
1:C:622:ASN:HD22	1:C:624:ASP:H	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:SER:HB2	1:C:91:ALA:HB2	1.92	0.50
1:A:137:HIS:NE2	1:A:153:GLU:OE2	2.44	0.49
1:B:622:ASN:HD22	1:B:624:ASP:H	1.60	0.49
1:D:337:ASP:O	1:D:341:ARG:HG3	2.11	0.49
1:D:622:ASN:HD22	1:D:624:ASP:H	1.60	0.49
1:C:98:PHE:H	1:C:179:GLN:HE22	1.59	0.49
2:F:115:LEU:HA	4:F:1002:SF4:S2	2.53	0.49
1:C:337:ASP:O	1:C:341:ARG:HG3	2.13	0.49
2:G:46:ARG:HD3	9:G:1108:HOH:O	2.13	0.48
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.94	0.48
1:C:137:HIS:NE2	1:C:153:GLU:OE2	2.46	0.48
1:D:263:ASN:OD1	1:D:272:ARG:NH2	2.47	0.47
2:H:64:TYR:O	2:H:93:ARG:HD2	2.13	0.47
1:D:484:GLN:HG2	1:D:544:PRO:HD2	1.96	0.47
2:F:152:MET:HG2	2:F:156:LEU:HD23	1.95	0.47
2:E:11:LYS:HG2	2:E:137:GLU:HG2	1.98	0.46
2:F:122:PRO:HB3	4:F:1002:SF4:S2	2.55	0.46
1:A:484:GLN:HG2	1:A:544:PRO:HD2	1.97	0.46
1:C:263:ASN:OD1	1:C:272:ARG:NH2	2.49	0.46
1:C:254:VAL:HB	1:C:255:HIS:H	1.34	0.46
2:G:75:GLY:O	2:H:93:ARG:NH1	2.47	0.46
1:A:529:ASP:OD1	5:A:703:MTE:N2	2.49	0.46
2:F:166:ASP:OD1	2:F:166:ASP:N	2.47	0.45
1:D:242:ILE:H	1:D:242:ILE:HD13	1.81	0.45
2:E:33:PHE:C	2:E:35:ALA:H	2.20	0.45
1:D:251:GLU:OE1	1:D:260:HIS:HE1	1.92	0.45
1:B:263:ASN:OD1	1:B:272:ARG:NH2	2.49	0.45
1:B:242:ILE:HD13	1:B:242:ILE:H	1.82	0.45
1:B:619:LYS:HD3	1:B:619:LYS:HA	1.83	0.45
2:H:116:CYS:SG	2:H:123:LEU:HD12	2.56	0.45
2:H:154:ILE:HD12	2:H:154:ILE:H	1.81	0.45
2:E:172:VAL:HG11	2:F:169:ALA:HA	1.98	0.45
1:C:484:GLN:HG2	1:C:544:PRO:HD2	1.99	0.45
2:G:152:MET:HB2	2:H:163:PHE:CE1	2.52	0.45
1:C:251:GLU:OE1	1:C:260:HIS:HE1	1.93	0.45
1:A:180:GLY:N	9:A:802:HOH:O	2.49	0.44
1:C:620:GLY:HA3	1:C:631:THR:HG21	1.99	0.44
2:F:96:CYS:SG	2:F:97:PRO:HD2	2.57	0.44
1:D:322:CYS:SG	1:D:323:PHE:N	2.90	0.44
2:G:141:GLU:HG2	2:G:141:GLU:H	1.55	0.44
2:G:115:LEU:HA	4:G:1002:SF4:S2	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:122:PRO:HB3	4:G:1002:SF4:S2	2.58	0.44
1:A:263:ASN:OD1	1:A:272:ARG:NH2	2.51	0.44
1:D:100:ALA:HB3	1:D:101:PRO:HD3	2.00	0.44
1:C:242:ILE:H	1:C:242:ILE:HD13	1.83	0.43
1:B:484:GLN:HG2	1:B:544:PRO:HD2	2.00	0.43
1:B:266:TRP:CE3	1:B:330:MET:HA	2.53	0.43
1:C:266:TRP:CE3	1:C:330:MET:HA	2.54	0.43
2:G:125:VAL:HG21	2:G:135:VAL:HG12	2.00	0.43
1:B:189:ILE:HD13	1:B:189:ILE:H	1.83	0.43
1:D:135:ALA:HB1	1:D:138:LEU:HD12	1.99	0.43
1:D:473:GLU:N	1:D:473:GLU:OE2	2.52	0.43
1:A:242:ILE:HD13	1:A:242:ILE:H	1.84	0.43
1:C:481:ASP:OD1	1:C:481:ASP:N	2.51	0.43
1:A:620:GLY:HA3	1:A:631:THR:HG21	2.00	0.43
1:A:218:ILE:HD12	1:A:218:ILE:HA	1.87	0.43
1:A:189:ILE:H	1:A:189:ILE:HD13	1.84	0.43
1:A:266:TRP:CE3	1:A:330:MET:HA	2.53	0.43
2:F:65:ALA:HB2	2:F:102:PHE:CD1	2.53	0.43
1:D:266:TRP:CE3	1:D:330:MET:HA	2.54	0.43
1:A:135:ALA:HB1	1:A:138:LEU:HD12	2.01	0.42
1:A:150:ILE:HG21	1:A:202:VAL:HG21	2.02	0.42
1:A:322:CYS:SG	3:A:701:UNL:X	3.08	0.42
1:D:620:GLY:HA3	1:D:631:THR:HG21	2.01	0.42
1:C:475:ARG:NH2	1:C:498:GLU:HG2	2.35	0.42
1:C:150:ILE:HG21	1:C:202:VAL:HG21	2.02	0.42
2:E:72:GLU:HG2	2:E:98:SER:HB3	2.02	0.42
2:E:27:GLU:HG2	2:E:49:VAL:O	2.20	0.42
1:A:481:ASP:OD1	1:A:481:ASP:N	2.52	0.42
1:A:303:PRO:HG3	2:F:129:LEU:HD22	2.02	0.42
2:E:104:GLU:HB2	2:E:108:GLY:H	1.85	0.41
2:G:152:MET:HE2	2:H:168:VAL:HA	2.03	0.41
1:B:481:ASP:OD1	1:B:481:ASP:N	2.52	0.41
1:D:481:ASP:OD1	1:D:481:ASP:N	2.53	0.41
1:B:297:ILE:HD11	1:B:319:MET:HG2	2.02	0.41
2:H:72:GLU:HG2	2:H:98:SER:HB3	2.03	0.41
1:A:77:ARG:NH1	4:A:702:SF4:S3	2.93	0.41
2:H:21:ASN:OD1	2:H:23:CYS:HB3	2.20	0.41
1:B:475:ARG:NH2	1:B:498:GLU:HG2	2.35	0.41
1:D:458:THR:HB	3:D:701:UNL:X	2.50	0.41
2:E:106:ASP:N	2:E:106:ASP:OD1	2.34	0.41
2:E:8:ARG:HE	2:E:143:PRO:HD3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ARG:NH2	1:A:498:GLU:HG2	2.36	0.41
2:F:54:ASP:OD2	2:F:57:ARG:NE	2.53	0.41
1:B:620:GLY:HA3	1:B:631:THR:HG21	2.02	0.41
1:B:150:ILE:HG21	1:B:202:VAL:HG21	2.03	0.41
1:C:218:ILE:HD12	1:C:218:ILE:HA	1.91	0.41
1:D:218:ILE:HD12	1:D:218:ILE:HA	1.92	0.41
1:D:475:ARG:NH2	1:D:498:GLU:HG2	2.36	0.41
1:B:623:ASP:OD1	1:B:623:ASP:N	2.52	0.41
2:E:57:ARG:NH1	2:E:85:GLU:O	2.50	0.41
1:A:78:THR:OG1	1:A:100:ALA:HB2	2.21	0.41
2:H:54:ASP:HA	2:H:55:PRO:HD3	1.90	0.41
1:C:95:MET:HE3	1:C:184:ALA:H	1.85	0.41
1:A:622:ASN:ND2	1:A:624:ASP:H	2.19	0.40
1:D:150:ILE:HG21	1:D:202:VAL:HG21	2.02	0.40
1:C:538:SER:O	1:C:541:PRO:HD2	2.21	0.40
1:B:322:CYS:SG	3:B:701:UNL:X	3.10	0.40
1:D:237:PRO:O	1:D:239:VAL:HG23	2.21	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	650/653 (100%)	620 (95%)	26 (4%)	4 (1%)	30	34
1	B	650/653 (100%)	621 (96%)	25 (4%)	4 (1%)	30	34
1	C	650/653 (100%)	619 (95%)	27 (4%)	4 (1%)	30	34
1	D	650/653 (100%)	618 (95%)	28 (4%)	4 (1%)	30	34
2	E	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	30	34
2	F	169/179 (94%)	162 (96%)	7 (4%)	0	100	100
2	G	169/179 (94%)	163 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	157/179 (88%)	151 (96%)	6 (4%)	0	100 100
All	All	3257/3328 (98%)	3111 (96%)	129 (4%)	17 (0%)	34 39

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	VAL
1	B	254	VAL
1	C	254	VAL
1	D	254	VAL
1	A	255	HIS
1	B	33	LEU
1	B	255	HIS
1	C	255	HIS
1	D	255	HIS
2	E	34	HIS
1	A	33	LEU
1	C	33	LEU
1	D	33	LEU
1	C	470	PRO
1	D	470	PRO
1	A	470	PRO
1	B	470	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	546/548 (100%)	535 (98%)	11 (2%)	63 77
1	B	546/548 (100%)	535 (98%)	11 (2%)	63 77
1	C	548/548 (100%)	537 (98%)	11 (2%)	63 77
1	D	546/548 (100%)	534 (98%)	12 (2%)	60 75
2	E	136/159 (86%)	132 (97%)	4 (3%)	50 64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	148/159 (93%)	142 (96%)	6 (4%)	37 48
2	G	147/159 (92%)	143 (97%)	4 (3%)	52 67
2	H	132/159 (83%)	128 (97%)	4 (3%)	48 62
All	All	2749/2828 (97%)	2686 (98%)	63 (2%)	58 73

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	189	ILE
1	A	215	GLU
1	A	242	ILE
1	A	319	MET
1	A	321	LYS
1	A	436	LEU
1	A	471	LYS
1	A	551	TYR
1	A	576	ARG
1	A	622	ASN
1	B	1	MET
1	B	189	ILE
1	B	215	GLU
1	B	242	ILE
1	B	319	MET
1	B	321	LYS
1	B	436	LEU
1	B	471	LYS
1	B	551	TYR
1	B	576	ARG
1	B	622	ASN
1	C	1	MET
1	C	189	ILE
1	C	215	GLU
1	C	242	ILE
1	C	254	VAL
1	C	321	LYS
1	C	436	LEU
1	C	471	LYS
1	C	551	TYR
1	C	576	ARG
1	C	622	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1	MET
1	D	174	TYR
1	D	189	ILE
1	D	215	GLU
1	D	242	ILE
1	D	319	MET
1	D	321	LYS
1	D	436	LEU
1	D	471	LYS
1	D	551	TYR
1	D	576	ARG
1	D	622	ASN
2	E	93	ARG
2	E	106	ASP
2	E	123	LEU
2	E	149	ARG
2	F	46	ARG
2	F	63	LEU
2	F	70	GLU
2	F	99	ARG
2	F	135	VAL
2	F	156	LEU
2	G	63	LEU
2	G	99	ARG
2	G	135	VAL
2	G	166	ASP
2	H	26	CYS
2	H	42	ASN
2	H	63	LEU
2	H	136	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	463	GLN
1	A	622	ASN
1	B	179	GLN
1	B	463	GLN
1	B	622	ASN
1	C	179	GLN
1	C	463	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	622	ASN
1	D	179	GLN
1	D	463	GLN
1	D	622	ASN

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

Of 40 ligands modelled in this entry, 4 are unknown and 12 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
4	SF4	A	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	A	703	5,7,6	21,26,26	2.86	12 (57%)	18,40,40	1.84	3 (16%)
5	MTE	A	704	5,7,6	21,26,26	2.69	10 (47%)	18,40,40	2.93	5 (27%)
4	SF4	B	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	B	703	7,6	21,26,26	2.85	10 (47%)	18,40,40	2.15	5 (27%)
5	MTE	B	704	7,6	21,26,26	2.84	10 (47%)	18,40,40	2.57	4 (22%)
4	SF4	C	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	C	703	7,6	21,26,26	2.65	11 (52%)	18,40,40	2.15	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MTE	C	704	7,6	21,26,26	2.88	10 (47%)	18,40,40	2.02	3 (16%)
4	SF4	D	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	D	703	7,6	21,26,26	2.61	11 (52%)	18,40,40	2.00	5 (27%)
5	MTE	D	704	7,6	21,26,26	2.73	10 (47%)	18,40,40	2.03	3 (16%)
4	SF4	E	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	G	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	G	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	G	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	1003	2	0,12,12	0.00	-	0,24,24	0.00	-

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
4	SF4	A	702	1	-	0/0/48/48	0/6/5/5
5	MTE	A	703	5,7,6	-	0/6/34/34	0/3/3/3
5	MTE	A	704	5,7,6	-	0/6/34/34	0/3/3/3
4	SF4	B	702	1	-	0/0/48/48	0/6/5/5
5	MTE	B	703	7,6	-	0/6/34/34	0/3/3/3
5	MTE	B	704	7,6	-	0/6/34/34	0/3/3/3
4	SF4	C	702	1	-	0/0/48/48	0/6/5/5
5	MTE	C	703	7,6	-	0/6/34/34	0/3/3/3
5	MTE	C	704	7,6	-	0/6/34/34	0/3/3/3
4	SF4	D	702	1	-	0/0/48/48	0/6/5/5
5	MTE	D	703	7,6	-	0/6/34/34	0/3/3/3
5	MTE	D	704	7,6	-	0/6/34/34	0/3/3/3
4	SF4	E	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	E	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	E	1003	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1003	2	-	0/0/48/48	0/6/5/5
4	SF4	G	1001	2	-	0/0/48/48	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	G	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	G	1003	2	-	0/0/48/48	0/6/5/5
4	SF4	H	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	H	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	H	1003	2	-	0/0/48/48	0/6/5/5

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	MTE	C9-C10	-6.86	1.28	1.41
5	B	703	MTE	C9-C10	-6.39	1.29	1.41
5	C	704	MTE	C9-C10	-6.19	1.29	1.41
5	B	704	MTE	C9-C10	-6.16	1.29	1.41
5	B	704	MTE	C7-C6	-6.07	1.49	1.53
5	A	703	MTE	C9-C10	-6.06	1.30	1.41
5	C	703	MTE	C9-C10	-6.03	1.30	1.41
5	C	704	MTE	C7-C6	-6.00	1.49	1.53
5	D	704	MTE	C9-C10	-5.87	1.30	1.41
5	D	703	MTE	C9-C10	-5.78	1.30	1.41
5	B	703	MTE	C7-C6	-5.33	1.49	1.53
5	D	704	MTE	C7-C6	-5.09	1.49	1.53
5	A	703	MTE	C7-C6	-4.43	1.50	1.53
5	C	703	MTE	C7-C6	-3.94	1.50	1.53
5	A	703	MTE	O3'-C7	-3.33	1.38	1.43
5	B	704	MTE	O3'-C7	-3.25	1.39	1.43
5	B	703	MTE	O3'-C3'	-3.08	1.39	1.43
5	D	703	MTE	O3'-C7	-3.06	1.39	1.43
5	D	703	MTE	O3'-C3'	-2.98	1.39	1.43
5	C	703	MTE	O3'-C3'	-2.93	1.39	1.43
5	C	704	MTE	O3'-C3'	-2.91	1.39	1.43
5	B	703	MTE	O3'-C7	-2.89	1.39	1.43
5	C	704	MTE	O3'-C7	-2.86	1.39	1.43
5	B	704	MTE	O3'-C3'	-2.76	1.39	1.43
5	A	704	MTE	C7-C6	-2.69	1.51	1.53
5	A	703	MTE	O3'-C3'	-2.65	1.39	1.43
5	C	703	MTE	O3'-C7	-2.63	1.39	1.43
5	A	704	MTE	O3'-C7	-2.44	1.40	1.43
5	A	704	MTE	O3'-C3'	-2.43	1.40	1.43
5	D	703	MTE	C7-C6	-2.29	1.51	1.53
5	D	704	MTE	O3'-C7	-2.20	1.40	1.43
5	C	703	MTE	C2-N3	2.14	1.39	1.35
5	D	704	MTE	C9-N5	2.19	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	703	MTE	C9-N5	2.24	1.43	1.38
5	D	703	MTE	C9-N5	2.25	1.43	1.38
5	C	704	MTE	C2-N3	2.29	1.39	1.35
5	B	703	MTE	C2-N3	2.30	1.39	1.35
5	A	703	MTE	C2-N3	2.31	1.39	1.35
5	A	703	MTE	C9-N5	2.36	1.43	1.38
5	B	704	MTE	C2-N3	2.40	1.39	1.35
5	A	703	MTE	C2'-C1'	2.42	1.51	1.35
5	D	703	MTE	C10-N8	2.45	1.43	1.35
5	A	704	MTE	C2-N3	2.46	1.40	1.35
5	A	704	MTE	C10-N8	2.46	1.43	1.35
5	D	704	MTE	C2-N3	2.48	1.40	1.35
5	B	703	MTE	C10-N8	2.50	1.43	1.35
5	B	703	MTE	C10-N1	2.64	1.39	1.34
5	B	704	MTE	C10-N1	2.64	1.39	1.34
5	C	704	MTE	C10-N8	2.68	1.43	1.35
5	A	703	MTE	C10-N8	2.68	1.43	1.35
5	C	704	MTE	C10-N1	2.69	1.39	1.34
5	D	704	MTE	C10-N8	2.76	1.44	1.35
5	D	704	MTE	C10-N1	2.79	1.39	1.34
5	B	704	MTE	C10-N8	2.79	1.44	1.35
5	B	704	MTE	C4-N3	2.81	1.38	1.33
5	D	703	MTE	C10-N1	2.82	1.39	1.34
5	C	703	MTE	C10-N8	2.82	1.44	1.35
5	A	704	MTE	C10-N1	2.86	1.39	1.34
5	D	703	MTE	C2-N3	2.87	1.40	1.35
5	C	703	MTE	C10-N1	2.87	1.39	1.34
5	A	703	MTE	C10-N1	2.88	1.39	1.34
5	D	704	MTE	C4-N3	3.08	1.38	1.33
5	A	703	MTE	C4-N3	3.09	1.38	1.33
5	B	703	MTE	C4-N3	3.18	1.38	1.33
5	A	704	MTE	C4-N3	3.21	1.38	1.33
5	C	703	MTE	C4-N3	3.25	1.38	1.33
5	C	704	MTE	C4-N3	3.26	1.38	1.33
5	D	703	MTE	C4-N3	3.42	1.39	1.33
5	C	704	MTE	C2-N2	4.02	1.42	1.34
5	C	703	MTE	C2-N2	4.27	1.43	1.34
5	C	703	MTE	C4-C9	4.29	1.47	1.41
5	B	704	MTE	C2-N2	4.31	1.43	1.34
5	D	703	MTE	C4-C9	4.33	1.47	1.41
5	D	704	MTE	C2-N2	4.35	1.43	1.34
5	B	704	MTE	C4-C9	4.42	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	MTE	C2-N2	4.47	1.43	1.34
5	D	703	MTE	C2-N2	4.47	1.43	1.34
5	A	703	MTE	C2-N2	4.49	1.43	1.34
5	B	703	MTE	C2-N2	4.57	1.43	1.34
5	A	704	MTE	C4-C9	4.76	1.48	1.41
5	B	703	MTE	C4-C9	4.86	1.48	1.41
5	D	704	MTE	C4-C9	5.02	1.48	1.41
5	C	704	MTE	C4-C9	5.10	1.48	1.41
5	A	703	MTE	C4-C9	5.18	1.48	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	704	MTE	O3'-C7-C6	-6.11	104.78	108.96
5	C	703	MTE	O3'-C7-C6	-3.90	106.30	108.96
5	D	703	MTE	N3-C2-N1	-2.49	121.44	125.51
5	B	703	MTE	O3'-C7-C6	-2.27	107.41	108.96
5	B	703	MTE	N3-C2-N1	-2.17	121.97	125.51
5	D	704	MTE	N8-C10-N1	2.12	120.00	116.62
5	D	703	MTE	N2-C2-N3	2.19	120.81	117.20
5	A	704	MTE	C9-N5-C6	2.29	124.54	118.60
5	A	703	MTE	C9-C10-N8	2.34	120.42	118.19
5	C	703	MTE	C9-C10-N8	2.54	120.61	118.19
5	A	704	MTE	C9-C10-N8	2.61	120.67	118.19
5	B	704	MTE	C2-N1-C10	2.67	120.62	114.63
5	A	703	MTE	C2-N1-C10	2.67	120.63	114.63
5	D	704	MTE	C2-N1-C10	2.70	120.68	114.63
5	C	704	MTE	C2-N1-C10	2.71	120.72	114.63
5	D	703	MTE	C2-N1-C10	2.72	120.75	114.63
5	C	703	MTE	C2-N1-C10	2.73	120.77	114.63
5	B	704	MTE	C9-C10-N8	2.88	120.92	118.19
5	B	703	MTE	C9-C10-N8	2.91	120.95	118.19
5	A	704	MTE	C2-N1-C10	2.95	121.25	114.63
5	B	703	MTE	C2-N1-C10	2.96	121.27	114.63
5	C	704	MTE	C9-C10-N8	3.01	121.05	118.19
5	D	703	MTE	C9-C10-N8	3.88	121.88	118.19
5	D	703	MTE	C4-C9-C10	5.38	119.35	114.61
5	A	703	MTE	C4-C9-C10	5.77	119.69	114.61
5	C	703	MTE	C4-C9-C10	6.33	120.18	114.61
5	C	704	MTE	C4-C9-C10	6.53	120.36	114.61
5	B	703	MTE	C4-C9-C10	6.59	120.41	114.61
5	A	704	MTE	C4-C9-C10	6.90	120.68	114.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	704	MTE	C4-C9-C10	6.98	120.75	114.61
5	B	704	MTE	C4-C9-C10	7.30	121.03	114.61
5	A	704	MTE	O3'-C7-C6	8.26	114.61	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	SF4	1	0
5	A	703	MTE	2	0
5	A	704	MTE	1	0
5	D	703	MTE	1	0
5	D	704	MTE	1	0
4	E	1002	SF4	1	0
4	F	1002	SF4	2	0
4	G	1002	SF4	2	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	652/653 (99%)	2.25	295 (45%) 0 0	65, 151, 230, 286	0
1	B	652/653 (99%)	0.62	59 (9%) 12 18	53, 82, 134, 173	0
1	C	652/653 (99%)	0.75	72 (11%) 7 12	54, 89, 124, 145	0
1	D	652/653 (99%)	0.48	34 (5%) 31 46	54, 82, 118, 144	0
2	E	166/179 (92%)	0.69	21 (12%) 5 9	62, 85, 124, 219	0
2	F	170/179 (94%)	0.58	25 (14%) 3 6	55, 78, 121, 147	0
2	G	169/179 (94%)	0.38	11 (6%) 22 33	54, 72, 153, 188	0
2	H	161/179 (89%)	0.57	10 (6%) 24 36	57, 79, 140, 151	0
All	All	3274/3328 (98%)	0.93	527 (16%) 3 4	53, 89, 184, 286	0

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	TYR	13.3
1	A	366	LEU	11.8
1	A	255	HIS	11.1
1	A	405	LEU	10.8
1	A	364	PHE	10.2
1	A	401	ILE	9.5
1	A	277	TRP	9.1
1	A	285	TRP	9.0
1	A	359	VAL	8.9
1	A	416	ILE	8.8
1	A	377	PHE	8.7
1	A	625	GLY	8.6
1	A	607	LEU	8.4
1	A	421	GLU	8.2
1	A	281	VAL	7.9
1	A	440	MET	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	652	ALA	7.8
1	A	271	THR	7.6
2	E	144	ASP	7.3
1	A	471	LYS	7.1
1	A	372	LEU	6.9
1	A	267	GLY	6.7
1	A	394	LYS	6.6
1	A	500	ARG	6.5
1	A	396	VAL	6.4
1	C	68	CYS	6.4
1	A	260	HIS	6.4
1	A	390	TYR	6.3
1	A	503	LYS	6.3
1	A	370	GLY	6.3
1	A	263	ASN	6.3
1	A	135	ALA	6.2
1	A	499	PRO	6.1
1	A	289	MET	6.1
1	A	276	PHE	6.0
1	A	603	ARG	6.0
1	A	332	ALA	6.0
1	A	645	ILE	5.9
1	A	383	GLY	5.8
1	A	283	HIS	5.8
1	A	261	THR	5.8
1	A	173	PHE	5.7
1	A	392	LEU	5.7
1	A	494	PHE	5.7
1	A	473	GLU	5.6
1	A	495	LEU	5.5
1	A	506	PRO	5.5
1	A	329	THR	5.3
1	A	236	ILE	5.3
1	A	374	ASP	5.3
1	C	644	PHE	5.2
1	A	241	PRO	5.1
1	A	94	MET	5.1
1	A	371	ILE	5.1
1	A	378	PRO	5.1
1	A	369	LYS	5.1
1	A	299	CYS	5.1
1	A	391	LEU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	474	GLN	5.0
1	A	272	ARG	5.0
1	A	238	ASP	5.0
1	A	360	MET	5.0
1	A	362	PHE	5.0
1	A	419	GLY	5.0
1	A	387	ARG	5.0
1	B	652	ALA	5.0
1	A	264	PHE	5.0
1	A	615	TYR	4.9
1	A	184	ALA	4.9
1	A	650	LEU	4.9
1	A	280	GLU	4.9
1	A	450	CYS	4.8
1	A	379	GLY	4.8
1	A	185	SER	4.8
2	H	163	PHE	4.7
1	A	651	SER	4.6
1	A	258	LYS	4.6
2	F	168	VAL	4.6
1	A	508	PHE	4.6
1	A	166	LYS	4.6
1	A	259	TRP	4.6
1	A	454	LYS	4.6
1	A	641	GLY	4.6
1	A	414	GLN	4.5
1	A	496	GLU	4.5
1	A	275	ASP	4.5
1	A	187	GLY	4.5
1	A	402	GLY	4.5
2	E	148	LYS	4.5
1	A	367	LEU	4.5
1	A	472	LEU	4.5
1	A	600	TRP	4.5
1	C	530	ALA	4.5
1	B	277	TRP	4.5
1	A	455	ILE	4.5
1	A	182	SER	4.4
2	G	168	VAL	4.4
1	B	473	GLU	4.4
1	A	249	PRO	4.4
1	A	357	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	145	GLU	4.4
2	F	7	LYS	4.4
1	A	604	PHE	4.4
2	E	143	PRO	4.4
2	G	149	ARG	4.3
1	C	377	PHE	4.3
1	A	611	LEU	4.3
2	E	159	LEU	4.3
1	A	475	ARG	4.3
1	A	491	LYS	4.3
1	A	373	LYS	4.3
1	A	183	SER	4.2
1	A	389	PHE	4.2
1	A	331	ALA	4.2
2	F	144	ASP	4.2
2	G	152	MET	4.2
1	A	509	PRO	4.1
1	A	132	ILE	4.1
1	A	381	PRO	4.1
1	B	280	GLU	4.1
1	A	95	MET	4.1
1	A	411	TRP	4.1
1	D	1	MET	4.1
1	C	75	CYS	4.1
1	A	376	ASP	4.1
1	A	526	TYR	4.1
1	D	277	TRP	4.0
2	H	140	VAL	4.0
1	A	57	GLU	4.0
1	A	591	VAL	4.0
1	B	94	MET	4.0
1	C	1	MET	4.0
1	A	457	ILE	4.0
1	A	412	ALA	4.0
1	A	445	TYR	4.0
1	A	59	LEU	4.0
1	B	472	LEU	4.0
2	H	159	LEU	4.0
1	A	418	ASN	3.9
2	F	147	VAL	3.9
1	A	363	ALA	3.9
1	A	502	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	644	PHE	3.9
1	A	168	GLY	3.9
1	A	327	THR	3.9
1	A	439	SER	3.9
1	A	54	PHE	3.8
1	A	375	SER	3.8
1	A	382	GLU	3.8
1	A	162	ALA	3.8
1	A	93	SER	3.8
1	A	597	ALA	3.8
1	A	446	TYR	3.8
1	A	78	THR	3.8
1	A	380	LEU	3.7
1	B	274	LYS	3.7
1	A	313	GLU	3.7
1	C	534	CYS	3.7
1	A	460	ILE	3.7
1	A	441	LEU	3.7
1	A	447	LEU	3.7
1	A	262	GLU	3.7
1	A	174	TYR	3.7
1	A	90	MET	3.7
1	A	237	PRO	3.7
1	B	650	LEU	3.7
1	A	268	ASN	3.7
1	A	385	GLU	3.7
1	A	52	GLU	3.6
1	A	602	ASN	3.6
1	B	275	ASP	3.6
1	A	609	LYS	3.6
1	B	602	ASN	3.6
1	A	589	ARG	3.6
1	A	435	PRO	3.6
1	B	79	ILE	3.6
1	B	500	ARG	3.6
1	D	469	TYR	3.6
1	A	278	THR	3.6
1	A	186	ARG	3.5
1	A	640	VAL	3.5
2	F	154	ILE	3.5
2	F	156	LEU	3.5
1	C	92	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	448	MET	3.5
1	A	458	THR	3.5
2	G	163	PHE	3.5
2	F	159	LEU	3.5
1	A	269	ALA	3.5
1	A	273	ARG	3.5
1	A	633	ASP	3.5
1	B	278	THR	3.5
1	A	340	LEU	3.4
1	A	342	ILE	3.4
1	A	355	SER	3.4
1	A	464	PHE	3.4
1	A	356	ALA	3.4
1	D	184	ALA	3.4
1	A	120	LEU	3.4
1	A	621	TRP	3.4
2	E	168	VAL	3.4
1	A	279	ASP	3.4
1	D	652	ALA	3.4
1	A	520	TRP	3.4
1	A	599	HIS	3.4
1	B	471	LYS	3.4
1	A	456	ASN	3.4
1	C	471	LYS	3.4
1	A	449	TYR	3.4
2	H	168	VAL	3.3
1	C	94	MET	3.3
2	E	172	VAL	3.3
1	C	32	TYR	3.3
1	C	535	ALA	3.3
1	A	312	MET	3.3
1	A	336	LEU	3.3
1	A	314	GLY	3.3
1	B	494	PHE	3.3
1	C	649	ILE	3.3
1	A	530	ALA	3.3
2	F	152	MET	3.3
1	A	393	ASP	3.3
1	A	76	ASN	3.2
1	B	283	HIS	3.2
1	A	62	PHE	3.2
1	A	505	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	369	LYS	3.2
1	A	535	ALA	3.2
1	C	44	TRP	3.2
1	A	79	ILE	3.2
2	E	139	GLU	3.2
1	A	287	LYS	3.2
1	C	650	LEU	3.2
1	D	177	ILE	3.1
2	E	171	THR	3.1
1	A	469	TYR	3.1
1	A	189	ILE	3.1
1	A	136	SER	3.1
1	A	270	ARG	3.1
1	A	479	VAL	3.1
1	A	529	ASP	3.1
1	A	75	CYS	3.1
1	D	283	HIS	3.1
1	C	300	TYR	3.1
1	A	630	GLU	3.1
1	B	182	SER	3.1
1	A	80	VAL	3.1
1	B	183	SER	3.1
1	A	608	GLU	3.0
1	B	272	ARG	3.0
1	C	76	ASN	3.0
1	C	183	SER	3.0
1	A	511	VAL	3.0
2	E	140	VAL	3.0
1	A	631	THR	3.0
1	A	351	LEU	3.0
1	A	430	LYS	3.0
1	A	646	LYS	3.0
1	C	526	TYR	3.0
2	F	143	PRO	3.0
1	A	65	GLY	3.0
2	F	140	VAL	3.0
1	B	63	ALA	3.0
1	A	649	ILE	3.0
1	A	481	ASP	3.0
1	B	80	VAL	3.0
1	A	507	ASN	3.0
1	A	629	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	181	ARG	3.0
1	A	406	ALA	2.9
1	C	93	SER	2.9
1	A	99	TRP	2.9
1	A	92	PHE	2.9
1	C	77	ARG	2.9
1	A	254	VAL	2.9
1	A	282	SER	2.9
1	B	93	SER	2.9
1	C	97	GLY	2.9
1	B	649	ILE	2.9
1	A	239	VAL	2.9
1	C	400	GLY	2.9
1	B	240	MET	2.9
1	D	216	GLU	2.9
1	C	455	ILE	2.9
1	A	91	ALA	2.9
1	B	95	MET	2.9
1	A	315	LEU	2.8
1	A	328	TYR	2.8
1	A	19	ILE	2.8
1	A	77	ARG	2.8
1	B	603	ARG	2.8
1	A	134	ASP	2.8
1	A	274	LYS	2.8
1	A	410	TYR	2.8
2	E	6	LYS	2.8
1	A	459	GLN	2.8
1	A	618	LEU	2.8
1	C	187	GLY	2.8
2	G	144	ASP	2.8
1	C	460	ILE	2.8
1	A	63	ALA	2.8
1	A	424	ALA	2.8
1	A	434	LEU	2.8
1	B	180	GLY	2.8
1	B	476	GLU	2.8
1	A	577	THR	2.8
1	A	286	GLU	2.7
1	B	273	ARG	2.7
1	A	595	PRO	2.7
1	A	596	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	74	GLY	2.7
2	F	176	THR	2.7
1	C	64	ALA	2.7
1	A	388	PHE	2.7
1	A	478	PHE	2.7
1	A	498	GLU	2.7
2	E	149	ARG	2.7
1	D	183	SER	2.7
1	A	338	PHE	2.7
2	F	149	ARG	2.7
2	G	8	ARG	2.7
1	C	78	THR	2.7
1	C	634	ASP	2.7
1	A	119	GLU	2.7
1	C	184	ALA	2.7
1	D	281	VAL	2.7
1	A	345	LYS	2.7
2	F	142	GLU	2.7
1	A	323	PHE	2.7
2	F	161	SER	2.6
1	A	201	VAL	2.6
1	A	531	LEU	2.6
1	D	644	PHE	2.6
1	A	422	ASP	2.6
1	D	274	LYS	2.6
1	B	184	ALA	2.6
1	B	78	THR	2.6
1	A	318	TYR	2.6
1	B	604	PHE	2.6
1	C	531	LEU	2.6
1	A	68	CYS	2.6
1	A	177	ILE	2.6
1	D	63	ALA	2.6
1	D	649	ILE	2.6
1	D	368	GLU	2.6
1	A	620	GLY	2.6
1	B	35	GLY	2.6
2	G	156	LEU	2.6
1	D	94	MET	2.6
1	C	283	HIS	2.6
2	E	9	ILE	2.6
1	A	594	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	490	PHE	2.6
1	A	307	GLY	2.6
1	B	530	ALA	2.6
1	B	259	TRP	2.6
1	A	537	LEU	2.6
2	F	172	VAL	2.6
1	A	349	TYR	2.6
1	B	96	GLY	2.6
1	B	535	ALA	2.6
1	C	80	VAL	2.5
2	E	163	PHE	2.5
1	A	606	GLU	2.5
1	D	179	GLN	2.5
1	C	95	MET	2.5
1	A	35	GLY	2.5
1	C	100	ALA	2.5
1	A	316	PRO	2.5
2	E	167	VAL	2.5
1	D	534	CYS	2.5
2	E	7	LYS	2.5
1	A	622	ASN	2.5
1	A	243	LEU	2.5
1	A	480	GLU	2.5
1	B	285	TRP	2.5
1	A	425	HIS	2.5
2	E	157	GLU	2.5
1	A	613	ASP	2.5
1	B	644	PHE	2.5
1	A	44	TRP	2.5
1	C	597	ALA	2.5
1	C	69	GLY	2.5
1	C	66	LEU	2.5
1	A	395	ILE	2.4
1	A	444	ILE	2.4
1	A	117	SER	2.4
1	A	153	GLU	2.4
1	B	92	PHE	2.4
1	B	276	PHE	2.4
1	C	478	PHE	2.4
1	A	350	GLY	2.4
1	B	255	HIS	2.4
1	A	635	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	443	PRO	2.4
1	C	101	PRO	2.4
2	F	150	THR	2.4
1	A	333	TYR	2.4
1	D	79	ILE	2.4
2	F	157	GLU	2.4
1	A	53	PRO	2.4
1	A	451	THR	2.4
1	C	529	ASP	2.4
1	D	473	GLU	2.4
1	B	495	LEU	2.4
1	C	637	LEU	2.4
1	B	601	LYS	2.4
1	C	180	GLY	2.4
1	A	466	GLN	2.4
1	D	639	TYR	2.4
1	D	374	ASP	2.4
2	H	152	MET	2.4
1	A	534	CYS	2.4
2	H	9	ILE	2.3
1	D	255	HIS	2.3
1	A	178	GLU	2.3
1	B	367	LEU	2.3
1	A	98	PHE	2.3
1	A	540	PHE	2.3
1	B	281	VAL	2.3
1	A	462	GLY	2.3
2	G	141	GLU	2.3
1	A	467	ALA	2.3
1	A	581	ALA	2.3
1	D	27	ARG	2.3
1	B	591	VAL	2.3
1	C	481	ASP	2.3
1	B	353	GLY	2.3
1	C	641	GLY	2.3
1	D	180	GLY	2.3
1	C	369	LYS	2.3
1	A	310	ILE	2.3
1	C	299	CYS	2.3
1	A	66	LEU	2.3
1	B	175	ALA	2.3
1	A	13	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	185	SER	2.3
2	E	112	LYS	2.3
1	A	297	ILE	2.3
1	D	372	LEU	2.3
1	D	176	SER	2.3
1	C	456	ASN	2.3
1	B	179	GLN	2.3
1	C	469	TYR	2.3
1	D	299	CYS	2.3
1	A	34	GLY	2.3
1	A	525	HIS	2.3
1	C	527	ILE	2.3
1	A	516	ASP	2.2
1	A	64	ALA	2.2
1	A	404	ILE	2.2
1	A	493	ILE	2.2
1	A	400	GLY	2.2
1	D	80	VAL	2.2
2	F	167	VAL	2.2
2	F	163	PHE	2.2
1	A	311	SER	2.2
1	C	117	SER	2.2
1	C	182	SER	2.2
1	B	324	THR	2.2
1	A	426	ASN	2.2
1	A	642	ASP	2.2
2	H	63	LEU	2.2
1	C	116	LYS	2.2
1	C	63	ALA	2.2
1	B	488	GLU	2.2
2	E	135	VAL	2.2
1	A	113	PHE	2.2
1	B	279	ASP	2.2
1	C	98	PHE	2.2
2	E	153	GLU	2.2
2	E	169	ALA	2.2
1	D	371	ILE	2.2
2	F	8	ARG	2.2
2	F	141	GLU	2.2
1	A	100	ALA	2.2
1	A	138	LEU	2.2
1	A	497	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	50	GLU	2.2
2	G	157	GLU	2.2
1	A	624	ASP	2.2
1	D	373	LYS	2.1
1	C	177	ILE	2.1
1	A	36	LEU	2.1
2	E	8	ARG	2.1
2	H	153	GLU	2.1
1	A	361	ALA	2.1
1	A	572	ALA	2.1
1	C	48	PRO	2.1
1	C	532	GLY	2.1
1	D	95	MET	2.1
1	B	260	HIS	2.1
1	C	639	TYR	2.1
1	A	170	ASN	2.1
1	A	215	GLU	2.1
1	C	185	SER	2.1
2	F	146	SER	2.1
1	C	434	LEU	2.1
1	C	459	GLN	2.1
2	G	147	VAL	2.1
1	B	97	GLY	2.1
1	C	495	LEU	2.1
1	B	299	CYS	2.1
1	C	186	ARG	2.1
2	F	153	GLU	2.1
2	H	23	CYS	2.1
1	A	96	GLY	2.1
1	A	532	GLY	2.1
2	F	164	GLY	2.1
1	A	436	LEU	2.1
2	G	10	VAL	2.1
1	A	627	PRO	2.1
1	C	56	PRO	2.1
1	C	648	GLY	2.0
1	D	477	ALA	2.0
2	H	165	ALA	2.0
1	C	256	ASP	2.0
1	A	431	HIS	2.0
1	A	14	LEU	2.0
1	B	188	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	2.0
1	B	81	SER	2.0
1	C	16	LYS	2.0
1	A	306	CYS	2.0
1	A	368	GLU	2.0
1	C	65	GLY	2.0
1	C	448	MET	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
5	MTE	C	704	24/24	0.93	0.24	0.19	45,61,112,116	0
5	MTE	C	703	24/24	0.96	0.27	0.11	45,58,60,67	0
5	MTE	D	703	24/24	0.96	0.22	-0.02	34,54,66,66	0
5	MTE	B	704	24/24	0.95	0.25	-0.06	56,63,67,69	0
5	MTE	B	703	24/24	0.96	0.23	-0.28	41,54,59,65	0
4	SF4	H	1002	8/8	0.98	0.13	-0.33	64,66,76,82	0
4	SF4	F	1002	8/8	0.98	0.12	-0.36	46,49,51,51	0
4	SF4	H	1001	8/8	0.99	0.15	-0.38	53,57,63,67	0
5	MTE	A	704	24/24	0.91	0.25	-0.73	81,101,118,296	0
5	MTE	A	703	24/24	0.86	0.24	-0.92	89,101,106,269	0
4	SF4	G	1001	8/8	0.99	0.12	-0.94	50,53,55,65	0
5	MTE	D	704	24/24	0.96	0.18	-1.01	44,53,63,97	0
4	SF4	H	1003	8/8	0.99	0.11	-1.03	59,61,66,67	0
4	SF4	E	1003	8/8	0.99	0.09	-1.04	54,57,62,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SF4	E	1002	8/8	0.98	0.12	-1.18	61,65,70,80	0
4	SF4	A	702	8/8	0.97	0.15	-1.24	85,98,123,150	0
4	SF4	G	1002	8/8	0.99	0.09	-1.27	53,57,59,59	0
4	SF4	E	1001	8/8	0.98	0.13	-1.29	56,60,65,66	0
4	SF4	B	702	8/8	0.98	0.13	-1.38	43,54,60,68	0
8	ZN	A	707	1/1	0.86	0.07	-1.43	65,65,65,65	1
4	SF4	G	1003	8/8	0.98	0.10	-1.53	56,62,64,73	0
4	SF4	F	1001	8/8	0.99	0.12	-1.71	49,53,54,60	0
4	SF4	C	702	8/8	0.98	0.12	-1.72	52,59,65,72	0
8	ZN	D	707	1/1	0.95	0.07	-1.72	60,60,60,60	1
8	ZN	B	707	1/1	0.93	0.10	-1.74	57,57,57,57	1
4	SF4	F	1003	8/8	0.99	0.09	-1.83	50,59,62,70	0
8	ZN	C	707	1/1	0.93	0.06	-2.46	58,58,58,58	1
4	SF4	D	702	8/8	0.98	0.12	-2.71	53,57,66,71	0
7	MG	A	706	1/1	0.54	0.16	-9.33	86,86,86,86	0
3	UNL	B	701	1/-	0.99	0.52	-	62,62,62,62	0
7	MG	B	706	1/1	0.96	0.41	-	59,59,59,59	0
3	UNL	A	701	1/-	0.97	0.43	-	56,56,56,56	0
7	MG	D	706	1/1	0.86	0.31	-	47,47,47,47	0
6	W	D	705	1/1	0.99	0.17	-	71,71,71,71	0
6	W	B	705	1/1	0.99	0.21	-	77,77,77,77	0
7	MG	C	706	1/1	0.93	0.34	-	49,49,49,49	0
3	UNL	D	701	1/-	0.99	0.33	-	94,94,94,94	0
6	W	C	705	1/1	0.99	0.17	-	68,68,68,68	0
3	UNL	C	701	1/-	0.91	0.51	-	67,67,67,67	0
6	W	A	705	1/1	0.88	0.18	-	131,131,131,131	0

6.5 Other polymers (i)

There are no such residues in this entry.