Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2016 – 11:31 AM GMT

PDB ID	:	4Z3Y
Title	:	Active site complex BamBC of Benzoyl Coenzyme A reductase in complex with Benzoyl-CoA
Authors	:	Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on	:	2015-04-01
Resolution	:	2.36 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:

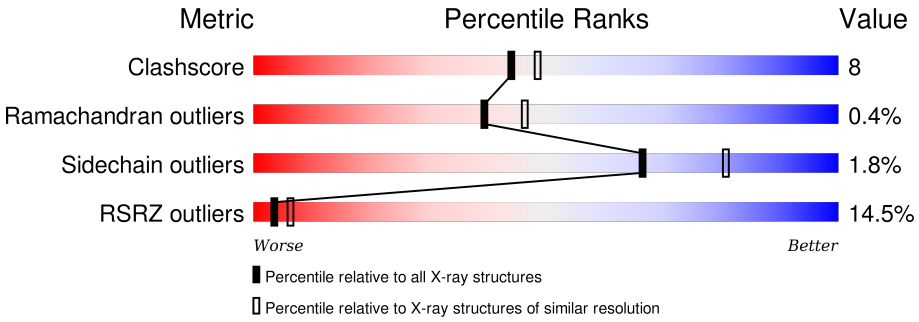
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.36 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))
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	7% 80% 19% •
1	B	653	40% 81% 18% •
1	C	653	9% 77% 22% •
1	D	653	9% 78% 21% •
2	E	179	8% 78% 12% 9%
2	F	179	10% 73% 21% • 5%
2	G	179	4% 79% 15% • 6%

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Mol	Chain	Length	Quality of chain
2	H	179	3% 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
7	UNL	B	705	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26541 atoms, of which 160 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.

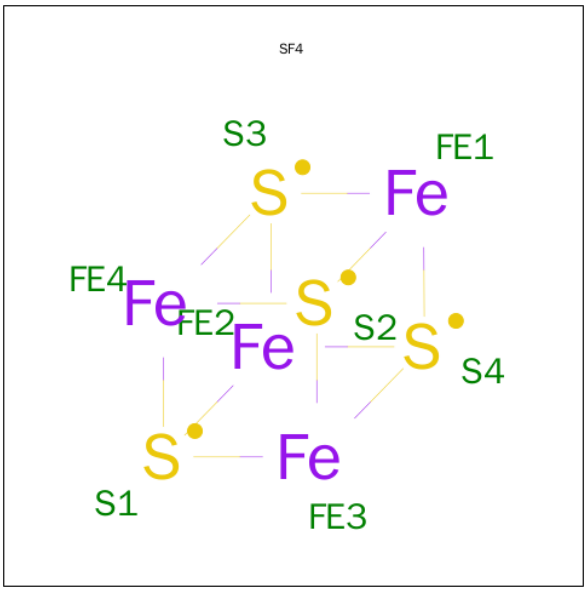
- Molecule 1 is a protein called Benzoyl-CoA reductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	653	Total	C	N	O	S	0	0	0
			5186	3311	876	966	33			
1	B	653	Total	C	N	O	S	0	0	0
			5189	3313	876	966	34			
1	C	653	Total	C	N	O	S	0	0	0
			5189	3313	876	966	34			
1	D	652	Total	C	N	O	S	0	0	0
			5178	3306	874	965	33			

- 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	162	Total	C	N	O	S	0	0	0
			1230	764	217	235	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 IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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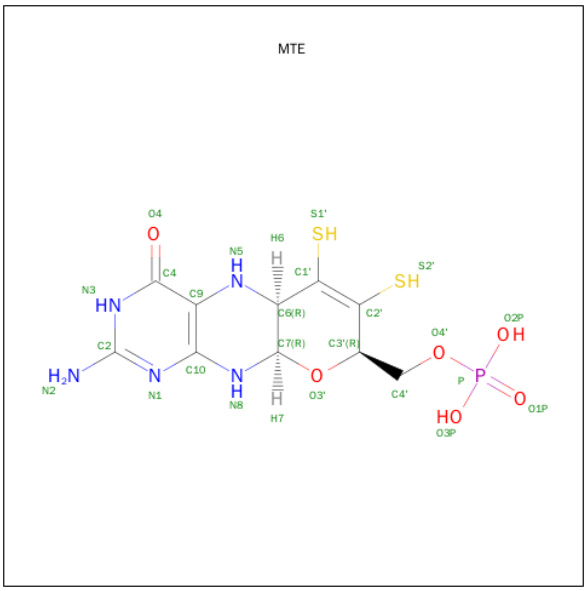
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Fe S 8 4 4	0	0
3	H	1	Total Fe S 8 4 4	0	0

- Molecule 4 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
4	A	1	Total C N O P S 24 10 5 6 1 2	0	0
4	A	1	Total C N O P S 24 10 5 6 1 2	0	0
4	B	1	Total C N O P S 24 10 5 6 1 2	0	0
4	B	1	Total C N O P S 24 10 5 6 1 2	0	0
4	C	1	Total C N O P S 24 10 5 6 1 2	0	0
4	C	1	Total C N O P S 24 10 5 6 1 2	0	0
4	D	1	Total C N O P S 24 10 5 6 1 2	0	0
4	D	1	Total C N O P S 24 10 5 6 1 2	0	0

- Molecule 5 is TUNGSTEN ION (three-letter code: W) (formula: W).

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

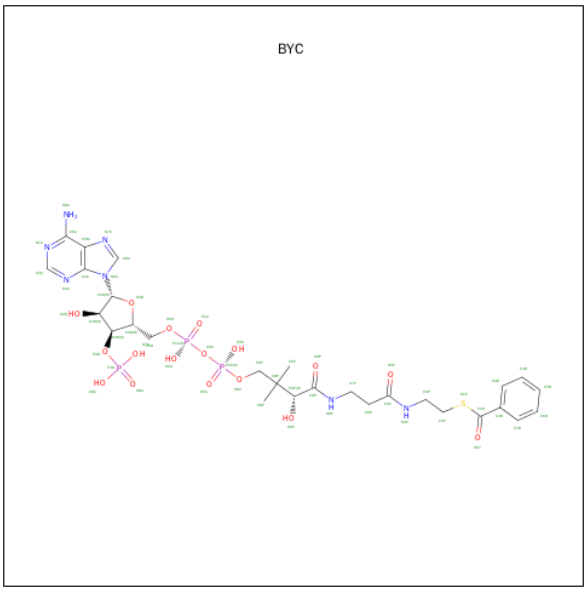
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 8 is benzoyl coenzyme A (three-letter code: BYC) (formula: $C_{28}H_{40}N_7O_{17}P_3S$).



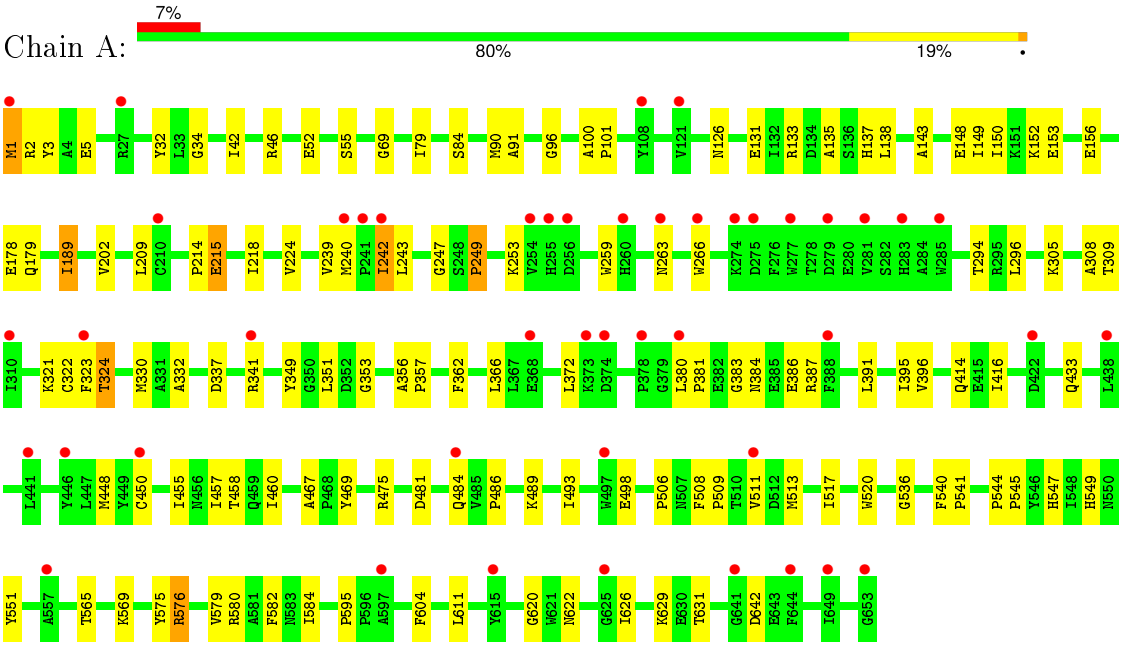
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	P	S	0	0
			96	28	40	7	17	3	1		
8	B	1	Total	C	H	N	O	P	S	0	0
			96	28	40	7	17	3	1		
8	C	1	Total	C	H	N	O	P	S	0	0
			96	28	40	7	17	3	1		
8	D	1	Total	C	H	N	O	P	S	0	0
			96	28	40	7	17	3	1		

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.

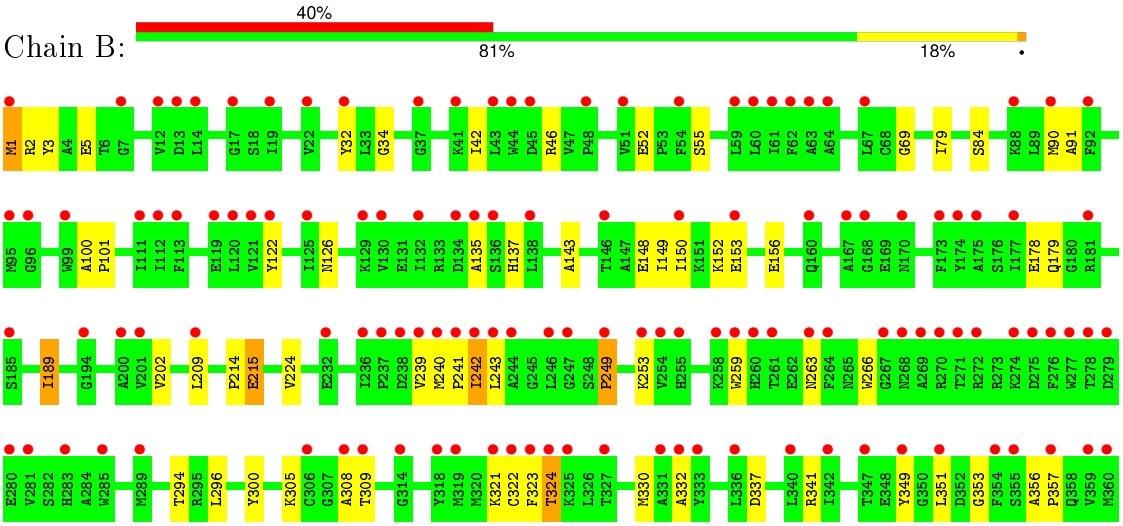
- Molecule 1: Benzoyl-CoA reductase, putative

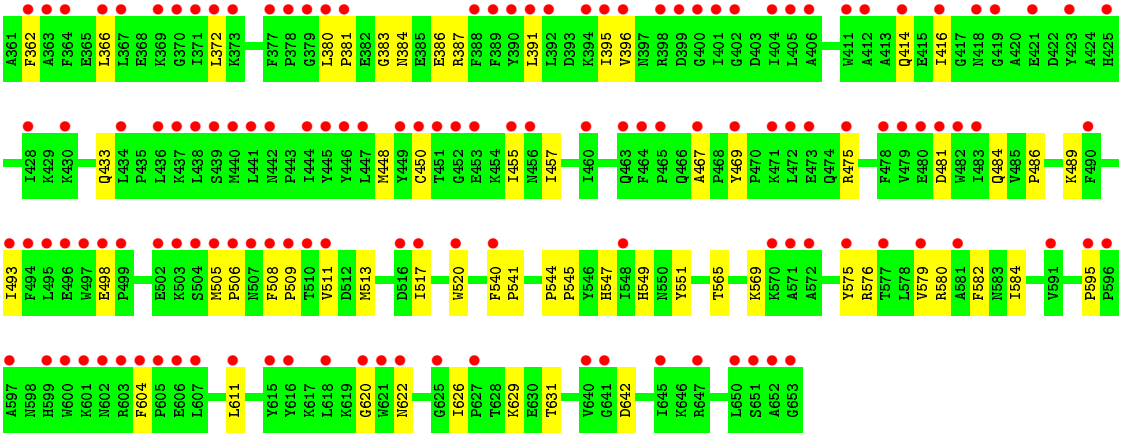
Chain A:



- Molecule 1: Benzoyl-CoA reductase, putative

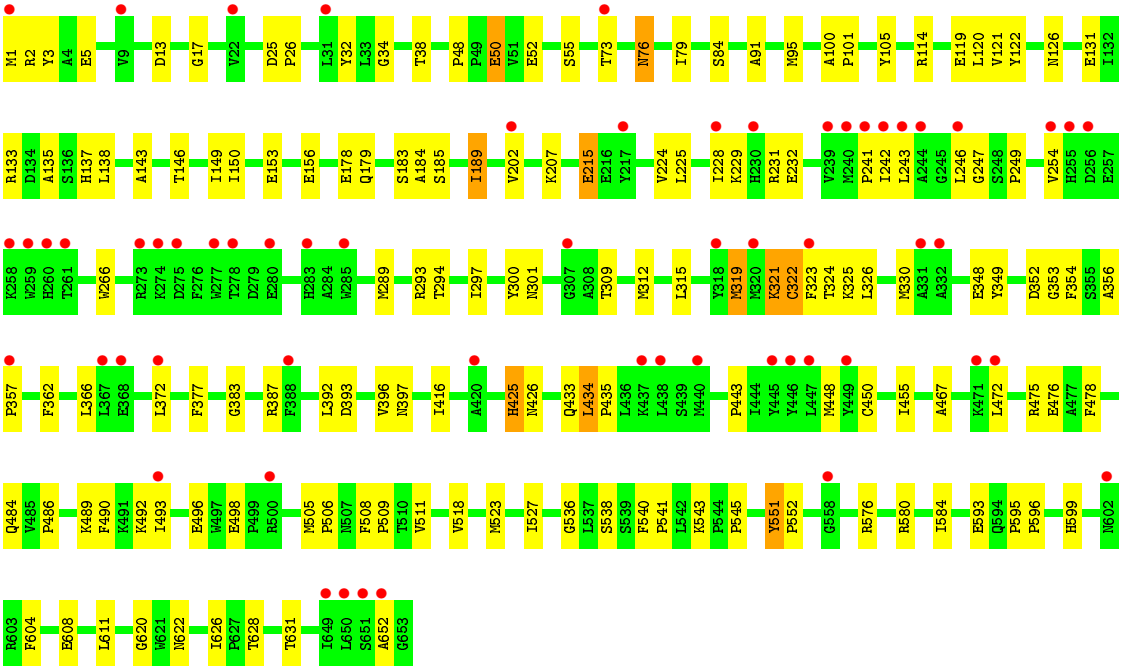
Chain B:

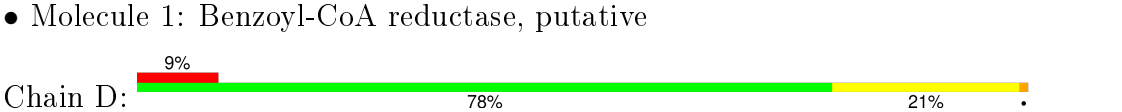


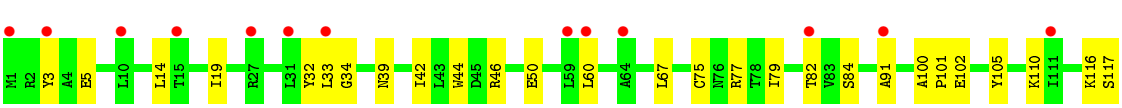


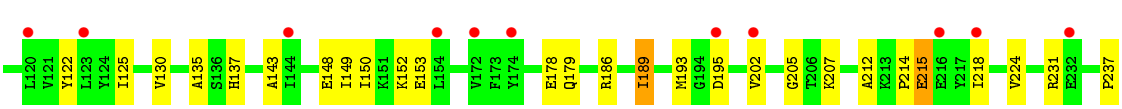
• Molecule 1: Benzoyl-CoA reductase, putative

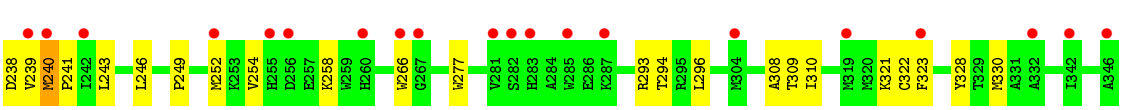
Chain C:





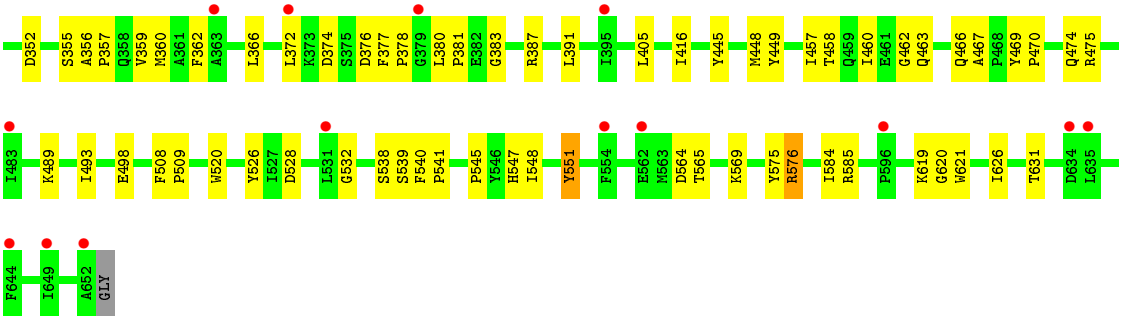






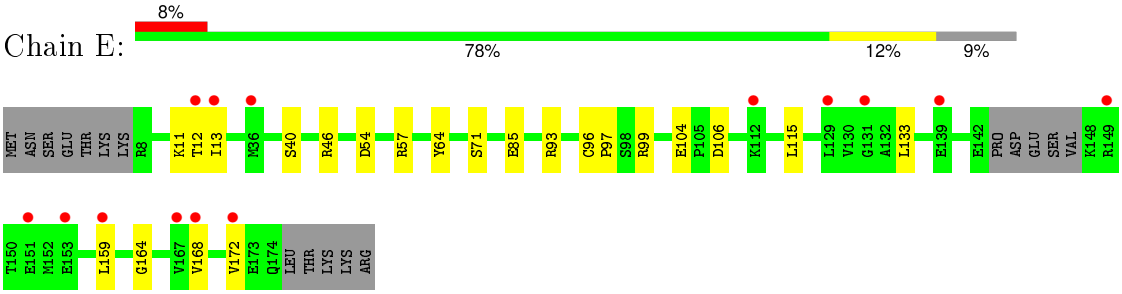
• Molecule 1: Benzoyl-CoA reductase, putative

Chain D:



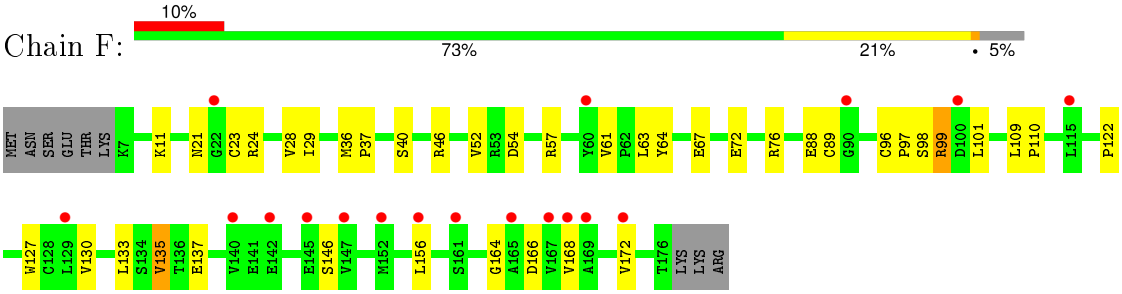
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain E:



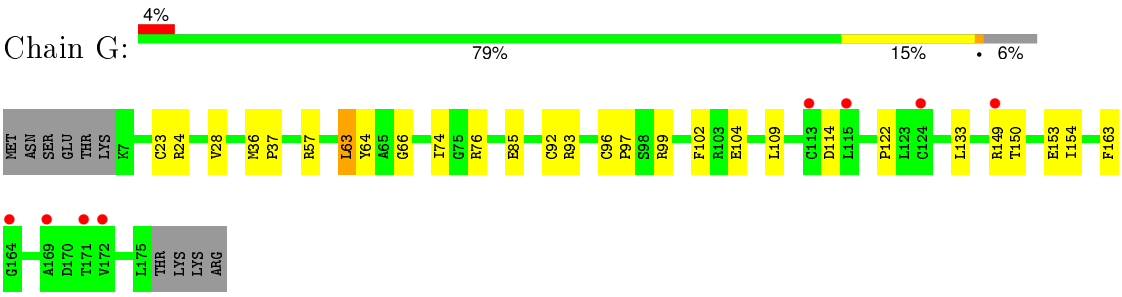
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain F:



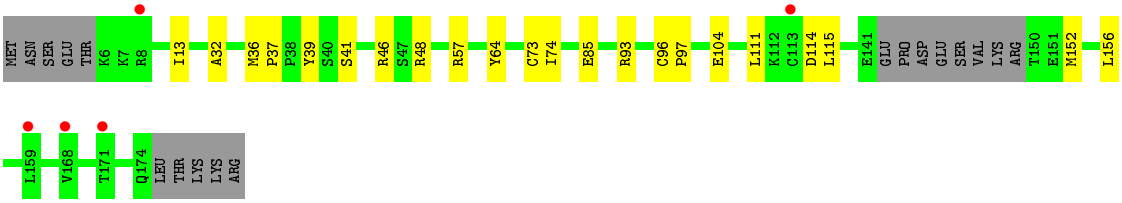
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain G:



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

Chain H:


MET ASN SER GLU THR K6 K7 R8 I13 A32 M36 P37 P38 Y39 S40 S41 R46 S47 R48 R57 Y64 C73 I74 E85 R93 C96 P97 E104 L111 K112 C113 D114 L115 E141 GLU PRO ASP GLU SER VAL LYS ARG T150 E151 M152 L156
L159 V168 T171 Q174 LEU THR LYS LYS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.77Å 116.26Å 143.97Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	79.80 – 2.36 88.07 – 2.36	Depositor EDS
% Data completeness (in resolution range)	94.3 (79.80-2.36) 94.4 (88.07-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.241 , 0.275 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 150838 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26541	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% 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, W, UNL, BYC, 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	0.21	0/5312	0.37	0/7181
1	B	0.20	0/5315	0.37	0/7184
1	C	0.21	0/5315	0.38	0/7184
1	D	0.21	0/5304	0.38	0/7172
2	E	0.20	0/1251	0.40	0/1693
2	F	0.21	0/1343	0.41	0/1819
2	G	0.20	0/1344	0.39	0/1819
2	H	0.20	0/1242	0.40	0/1681
All	All	0.21	0/26426	0.38	0/35733

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	5186	0	5115	79	0
1	B	5189	0	5122	79	0
1	C	5189	0	5122	98	0
1	D	5178	0	5101	88	0
2	E	1230	0	1174	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1317	0	1266	25	0
2	G	1315	0	1263	21	0
2	H	1221	0	1158	16	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	8	0	0	1	0
3	D	8	0	0	0	0
3	E	24	0	0	0	0
3	F	24	0	0	0	0
3	G	24	0	0	1	0
3	H	24	0	0	0	0
4	A	48	0	20	4	0
4	B	48	0	20	7	0
4	C	48	0	20	1	0
4	D	48	0	20	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	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	1	0
7	B	1	0	0	2	0
7	C	1	0	0	0	0
7	D	1	0	0	1	0
8	A	56	40	36	5	0
8	B	56	40	36	6	0
8	C	56	40	36	7	0
8	D	56	40	36	3	0
All	All	26381	160	25545	416	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 (416) 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:380:LEU:HD12	1:B:381:PRO:HD2	1.37	1.06
1:A:380:LEU:HD12	1:A:381:PRO:HD2	1.37	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.54	0.89
1:C:356:ALA:HB3	1:C:357:PRO:HD3	1.65	0.79
1:C:242:ILE:HG13	1:C:243:LEU:HG	1.66	0.78
1:D:356:ALA:HB3	1:D:357:PRO:HD3	1.65	0.77
1:D:240:MET:HB2	1:D:243:LEU:HD12	1.67	0.77
1:B:322:CYS:HB3	4:B:703:MTE:S1'	2.24	0.76
4:B:702:MTE:C2'	4:B:703:MTE:S2'	2.75	0.74
4:B:702:MTE:C1'	4:B:703:MTE:S2'	2.71	0.73
1:A:356:ALA:HB3	1:A:357:PRO:HD3	1.72	0.72
1:D:565:THR:HG22	1:D:569:LYS:HE3	1.69	0.72
1:B:356:ALA:HB3	1:B:357:PRO:HD3	1.71	0.71
4:B:702:MTE:S1'	7:B:705:UNL:X	2.79	0.70
1:B:100:ALA:HB3	1:B:101:PRO:HD3	1.75	0.69
1:A:100:ALA:HB3	1:A:101:PRO:HD3	1.75	0.68
2:E:159:LEU:HD13	2:F:156:LEU:HD22	1.74	0.68
1:B:475:ARG:NH2	1:B:498:GLU:HG2	2.10	0.67
1:C:100:ALA:HB3	1:C:101:PRO:HD3	1.76	0.67
1:A:475:ARG:NH2	1:A:498:GLU:HG2	2.10	0.67
1:D:372:LEU:HD11	1:D:416:ILE:HD13	1.76	0.67
1:C:266:TRP:CE3	1:C:330:MET:HA	2.29	0.67
1:C:467:ALA:HB2	8:C:707:BYC:HDPB	1.77	0.66
1:A:620:GLY:HA3	1:A:631:THR:HG21	1.78	0.66
2:E:57:ARG:NH1	2:E:85:GLU:O	2.28	0.66
1:D:294:THR:HB	1:D:309:THR:OG1	1.96	0.66
1:C:189:ILE:HD13	1:C:189:ILE:H	1.61	0.65
1:B:620:GLY:HA3	1:B:631:THR:HG21	1.78	0.64
1:C:297:ILE:HD11	1:C:319:MET:HG2	1.79	0.64
1:A:266:TRP:CE3	1:A:330:MET:HA	2.33	0.63
1:D:620:GLY:HA3	1:D:631:THR:HG21	1.80	0.63
1:B:266:TRP:CE3	1:B:330:MET:HA	2.33	0.63
1:C:540:PHE:HB3	1:C:541:PRO:HD3	1.79	0.63
1:C:366:LEU:HB3	1:C:372:LEU:HD13	1.79	0.62
1:B:484:GLN:HG2	1:B:544:PRO:HD2	1.82	0.62
2:F:29:ILE:HD13	2:F:127:TRP:CZ2	2.33	0.62
1:A:322:CYS:HB2	4:A:702:MTE:S2'	2.38	0.62
1:A:484:GLN:HG2	1:A:544:PRO:HD2	1.81	0.62
1:A:372:LEU:HD11	1:A:416:ILE:HD13	1.82	0.61
2:F:122:PRO:HG2	2:F:135:VAL:HG11	1.82	0.61
1:A:540:PHE:HB3	1:A:541:PRO:HD3	1.83	0.61
1:B:372:LEU:HD11	1:B:416:ILE:HD13	1.82	0.61
1:B:150:ILE:HG21	1:B:202:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:163:PHE:CE2	2:H:152:MET:HB3	2.35	0.61
2:E:172:VAL:HG21	2:F:172:VAL:HG21	1.81	0.61
1:D:238:ASP:OD2	1:D:474:GLN:NE2	2.33	0.61
1:B:540:PHE:HB3	1:B:541:PRO:HD3	1.83	0.61
1:A:322:CYS:CB	4:A:702:MTE:S2'	2.88	0.61
1:D:540:PHE:HB3	1:D:541:PRO:HD3	1.82	0.61
1:A:150:ILE:HG21	1:A:202:VAL:HG21	1.82	0.60
1:C:584:ILE:HG21	1:C:626:ILE:HG23	1.82	0.60
1:D:3:TYR:O	1:D:5:GLU:N	2.34	0.60
2:H:96:CYS:SG	2:H:97:PRO:HD2	2.42	0.60
2:G:149:ARG:NH1	2:G:153:GLU:OE1	2.35	0.60
1:C:224:VAL:HG13	1:C:545:PRO:HB2	1.83	0.59
1:B:240:MET:HE2	1:B:241:PRO:HD2	1.83	0.59
1:A:450:CYS:SG	1:A:595:PRO:HD3	2.43	0.59
2:F:96:CYS:SG	2:F:97:PRO:HD2	2.43	0.59
1:C:354:PHE:CE2	1:C:434:LEU:HD21	2.38	0.58
1:B:450:CYS:SG	1:B:595:PRO:HD3	2.43	0.58
1:C:84:SER:HB2	1:C:91:ALA:HB2	1.83	0.58
1:C:228:ILE:O	1:C:232:GLU:HG2	2.04	0.58
1:D:224:VAL:HG13	1:D:545:PRO:HB2	1.86	0.58
1:B:322:CYS:CB	4:B:703:MTE:S1'	2.86	0.57
1:C:443:PRO:HD2	1:C:505:MET:SD	2.44	0.57
1:C:372:LEU:HD11	1:C:416:ILE:HD13	1.85	0.57
1:A:508:PHE:HA	1:A:509:PRO:C	2.25	0.57
1:D:266:TRP:CE3	1:D:330:MET:HA	2.40	0.57
1:D:355:SER:O	1:D:359:VAL:HG23	2.05	0.57
1:D:322:CYS:HB2	4:D:703:MTE:S2'	2.45	0.57
1:C:383:GLY:O	1:C:387:ARG:HG3	2.05	0.57
1:C:448:MET:HG2	1:C:518:VAL:HG13	1.87	0.57
1:B:508:PHE:HA	1:B:509:PRO:C	2.25	0.56
1:D:14:LEU:HB3	1:D:117:SER:HB2	1.87	0.56
1:C:215:GLU:H	1:C:215:GLU:CD	2.07	0.56
1:B:189:ILE:HD13	1:B:189:ILE:H	1.70	0.56
1:D:293:ARG:HD2	1:D:296:LEU:HD21	1.87	0.56
1:D:448:MET:HB3	1:D:460:ILE:HG21	1.87	0.56
1:A:189:ILE:H	1:A:189:ILE:HD13	1.70	0.56
1:C:95:MET:HE2	1:C:184:ALA:H	1.71	0.56
1:B:323:PHE:CG	8:B:707:BYC:H4B	2.40	0.56
1:C:620:GLY:HA3	1:C:631:THR:HG21	1.88	0.56
1:D:189:ILE:HD13	1:D:189:ILE:H	1.71	0.55
1:C:231:ARG:HG2	1:C:246:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ILE:O	1:B:243:LEU:HD23	2.07	0.55
1:B:126:ASN:ND2	1:B:156:GLU:OE2	2.39	0.55
1:A:126:ASN:ND2	1:A:156:GLU:OE2	2.39	0.55
1:D:143:ALA:HB1	1:D:178:GLU:HB2	1.90	0.54
1:D:100:ALA:HB3	1:D:101:PRO:HD3	1.89	0.54
2:E:54:ASP:OD2	2:E:57:ARG:NE	2.30	0.54
2:F:54:ASP:OD2	2:F:57:ARG:NE	2.35	0.54
1:B:351:LEU:O	4:B:703:MTE:N2	2.26	0.54
1:A:467:ALA:HB2	8:A:707:BYC:HDPB	1.90	0.54
1:C:241:PRO:HB2	1:C:254:VAL:HG21	1.89	0.54
1:A:242:ILE:O	1:A:243:LEU:HD23	2.07	0.54
1:B:137:HIS:NE2	1:B:153:GLU:OE2	2.39	0.54
1:C:475:ARG:HH22	1:C:498:GLU:HG2	1.73	0.54
1:D:528:ASP:OD2	1:D:538:SER:HB3	2.08	0.53
1:A:143:ALA:HB1	1:A:178:GLU:HB2	1.91	0.53
1:D:296:LEU:HD23	1:D:308:ALA:HB2	1.90	0.53
1:D:186:ARG:HD2	1:D:352:ASP:OD2	2.08	0.53
1:D:538:SER:O	1:D:541:PRO:HD2	2.09	0.53
1:C:580:ARG:HH22	1:C:593:GLU:CD	2.12	0.53
1:B:622:ASN:N	1:B:626:ILE:O	2.40	0.53
1:B:224:VAL:HG13	1:B:545:PRO:HB2	1.90	0.53
1:C:312:MET:HB2	1:C:315:LEU:HD12	1.91	0.53
1:C:580:ARG:O	1:C:584:ILE:HG12	2.09	0.53
1:A:332:ALA:O	1:A:384:ASN:ND2	2.42	0.53
1:D:252:MET:CE	1:D:310:ILE:HD11	2.39	0.52
2:F:52:VAL:HB	2:F:61:VAL:HB	1.92	0.52
1:B:332:ALA:O	1:B:384:ASN:ND2	2.42	0.52
1:D:137:HIS:NE2	1:D:153:GLU:OE2	2.36	0.52
1:C:362:PHE:CZ	1:C:366:LEU:HD11	2.45	0.52
1:D:526:TYR:O	1:D:575:TYR:OH	2.17	0.52
1:A:224:VAL:HG13	1:A:545:PRO:HB2	1.90	0.52
1:B:249:PRO:CG	8:B:707:BYC:H6B	2.39	0.52
1:B:337:ASP:O	1:B:341:ARG:HG3	2.09	0.52
1:A:137:HIS:NE2	1:A:153:GLU:OE2	2.39	0.52
2:E:96:CYS:SG	2:E:97:PRO:HD2	2.50	0.52
2:F:64:TYR:OH	2:F:133:LEU:HD13	2.10	0.52
1:B:84:SER:HB2	1:B:91:ALA:HB2	1.92	0.52
1:A:362:PHE:CZ	1:A:366:LEU:HD11	2.45	0.52
2:G:104:GLU:HG3	2:G:109:LEU:HB2	1.92	0.52
1:C:392:LEU:O	1:C:396:VAL:HG22	2.09	0.52
1:D:548:ILE:HG13	1:D:565:THR:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ALA:HB1	1:B:178:GLU:HB2	1.91	0.51
1:A:337:ASP:O	1:A:341:ARG:HG3	2.10	0.51
1:C:1:MET:SD	1:C:2:ARG:N	2.82	0.51
1:C:323:PHE:CG	8:C:707:BYC:H4B	2.44	0.51
1:D:150:ILE:HG21	1:D:202:VAL:HG21	1.91	0.51
1:D:508:PHE:HA	1:D:509:PRO:C	2.29	0.51
1:A:249:PRO:CG	8:A:707:BYC:H6B	2.39	0.51
1:B:322:CYS:CB	4:B:702:MTE:S2'	2.98	0.51
1:B:240:MET:CE	1:B:241:PRO:HD2	2.40	0.51
2:E:46:ARG:NH2	2:E:104:GLU:OE1	2.43	0.51
1:C:604:PHE:O	1:C:608:GLU:HG3	2.11	0.51
1:A:383:GLY:O	1:A:387:ARG:HG3	2.11	0.51
1:B:52:GLU:O	1:B:55:SER:HB3	2.11	0.51
1:C:372:LEU:HD23	1:C:377:PHE:CZ	2.45	0.51
1:D:362:PHE:CZ	1:D:366:LEU:HD11	2.46	0.51
1:D:116:LYS:HE2	1:D:195:ASP:OD2	2.11	0.51
2:E:64:TYR:O	2:E:93:ARG:HD2	2.10	0.51
1:C:143:ALA:HB1	1:C:178:GLU:HB2	1.92	0.51
1:D:377:PHE:HB3	1:D:380:LEU:HB2	1.93	0.51
1:C:628:THR:OG1	1:C:631:THR:HG23	2.10	0.50
1:B:383:GLY:O	1:B:387:ARG:HG3	2.11	0.50
1:C:126:ASN:ND2	1:C:156:GLU:OE2	2.44	0.50
1:C:131:GLU:OE2	1:C:133:ARG:NE	2.37	0.50
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.92	0.50
1:B:489:LYS:O	1:B:493:ILE:HG13	2.11	0.50
8:C:707:BYC:N8P	8:C:707:BYC:HDPA	2.27	0.50
1:D:148:GLU:O	1:D:152:LYS:HG3	2.11	0.50
1:B:362:PHE:CZ	1:B:366:LEU:HD11	2.46	0.50
1:D:619:LYS:HB3	1:D:621:TRP:CE2	2.47	0.50
1:D:366:LEU:HB3	1:D:372:LEU:HD13	1.92	0.50
1:C:13:ASP:O	1:C:17:GLY:N	2.44	0.50
1:C:324:THR:HG22	1:C:353:GLY:HA3	1.94	0.50
8:B:707:BYC:HDPA	8:B:707:BYC:N8P	2.27	0.50
1:A:52:GLU:O	1:A:55:SER:HB3	2.11	0.50
1:A:489:LYS:O	1:A:493:ILE:HG13	2.11	0.50
2:G:64:TYR:OH	2:G:133:LEU:HD13	2.12	0.50
1:C:323:PHE:CD1	8:C:707:BYC:H4B	2.47	0.49
1:B:239:VAL:HG12	1:B:240:MET:N	2.27	0.49
1:B:296:LEU:HD23	1:B:308:ALA:HB2	1.94	0.49
2:E:71:SER:HB2	2:F:146:SER:HB3	1.93	0.49
2:G:64:TYR:O	2:G:93:ARG:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ASN:N	1:A:626:ILE:O	2.40	0.49
1:A:296:LEU:HD23	1:A:308:ALA:HB2	1.94	0.49
2:G:74:ILE:HD12	2:H:114:ASP:HA	1.94	0.49
1:D:32:TYR:O	1:D:34:GLY:N	2.46	0.49
1:B:90:MET:HB2	1:B:582:PHE:CD2	2.47	0.49
8:A:707:BYC:N8P	8:A:707:BYC:HDPA	2.27	0.49
8:D:707:BYC:HDPA	8:D:707:BYC:N8P	2.28	0.49
1:A:90:MET:HB2	1:A:582:PHE:CD2	2.47	0.49
1:A:239:VAL:HG12	1:A:240:MET:N	2.28	0.49
1:D:149:ILE:O	1:D:153:GLU:HG3	2.13	0.48
1:D:77:ARG:HB2	1:D:532:GLY:O	2.13	0.48
2:G:76:ARG:O	2:H:13:ILE:N	2.39	0.48
1:D:79:ILE:N	1:D:79:ILE:HD12	2.28	0.48
1:A:323:PHE:CG	8:A:707:BYC:H4B	2.48	0.48
1:C:505:MET:O	8:C:707:BYC:N6A	2.47	0.48
8:A:707:BYC:HDPA	8:A:707:BYC:HN8P	1.78	0.48
2:F:168:VAL:O	2:F:172:VAL:HG23	2.13	0.48
1:A:214:PRO:HG3	2:E:40:SER:HA	1.95	0.48
1:D:565:THR:O	1:D:569:LYS:HG3	2.13	0.48
1:B:511:VAL:HG13	1:B:611:LEU:HD23	1.95	0.48
2:G:66:GLY:N	2:G:93:ARG:O	2.39	0.48
1:D:467:ALA:HB2	8:D:707:BYC:HDPB	1.96	0.48
1:C:189:ILE:HD13	1:C:189:ILE:N	2.28	0.48
1:C:425:HIS:O	1:C:596:PRO:HB3	2.14	0.48
1:D:445:TYR:OH	1:D:466:GLN:HG2	2.13	0.47
1:A:565:THR:CG2	1:A:569:LYS:HE3	2.44	0.47
2:H:32:ALA:HA	2:H:41:SER:O	2.14	0.47
2:E:164:GLY:O	2:E:168:VAL:HG23	2.14	0.47
1:D:360:MET:HG2	1:D:391:LEU:HD23	1.96	0.47
2:G:122:PRO:HB3	3:G:1002:SF4:S2	2.54	0.47
1:C:105:TYR:O	1:C:207:LYS:HB2	2.15	0.47
1:C:511:VAL:HG13	1:C:611:LEU:HD23	1.96	0.47
1:A:79:ILE:N	1:A:79:ILE:HD12	2.30	0.47
1:A:511:VAL:HG13	1:A:611:LEU:HD23	1.96	0.47
1:C:138:LEU:HD13	1:C:146:THR:HG23	1.97	0.47
1:B:79:ILE:N	1:B:79:ILE:HD12	2.29	0.47
1:C:508:PHE:CG	1:C:509:PRO:HA	2.50	0.47
1:C:3:TYR:O	1:C:5:GLU:N	2.45	0.47
1:C:393:ASP:O	1:C:397:ASN:ND2	2.42	0.47
1:B:1:MET:HG3	1:B:2:ARG:N	2.30	0.47
1:C:489:LYS:O	1:C:493:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:N	1:A:189:ILE:HD13	2.30	0.47
1:C:425:HIS:H	1:C:425:HIS:CD2	2.32	0.47
1:A:508:PHE:CG	1:A:509:PRO:HA	2.50	0.46
1:A:547:HIS:CE1	1:A:549:HIS:HB2	2.50	0.46
1:D:44:TRP:O	1:D:585:ARG:NH2	2.34	0.46
1:C:486:PRO:HD2	1:C:490:PHE:CE2	2.51	0.46
8:B:707:BYC:HDPA	8:B:707:BYC:HN8P	1.80	0.46
8:C:707:BYC:HN8P	8:C:707:BYC:HDPA	1.80	0.46
1:B:189:ILE:N	1:B:189:ILE:HD13	2.30	0.46
1:D:445:TYR:HA	1:D:448:MET:HE2	1.97	0.46
1:D:122:TYR:HD2	1:D:135:ALA:HB2	1.81	0.46
1:A:575:TYR:O	1:A:579:VAL:HG23	2.16	0.46
1:D:189:ILE:HD13	1:D:189:ILE:N	2.29	0.46
1:B:148:GLU:O	1:B:152:LYS:HG3	2.16	0.46
1:B:506:PRO:HG3	1:B:604:PHE:CE1	2.51	0.46
1:B:565:THR:CG2	1:B:569:LYS:HE3	2.44	0.46
1:D:547:HIS:O	1:D:551:TYR:HB2	2.14	0.46
1:B:547:HIS:CE1	1:B:549:HIS:HB2	2.50	0.46
2:F:23:CYS:O	2:F:24:ARG:HB2	2.15	0.46
1:B:493:ILE:HD13	1:B:513:MET:HB3	1.97	0.46
8:D:707:BYC:HN8P	8:D:707:BYC:HDPA	1.78	0.46
1:D:102:GLU:OE1	1:D:205:GLY:N	2.30	0.46
1:C:326:LEU:O	1:C:330:MET:HG3	2.15	0.46
1:C:249:PRO:CG	8:C:707:BYC:H6B	2.46	0.46
1:A:322:CYS:SG	1:A:323:PHE:N	2.89	0.46
1:B:575:TYR:O	1:B:579:VAL:HG23	2.16	0.46
1:A:1:MET:HG3	1:A:2:ARG:N	2.29	0.46
1:B:300:TYR:OH	2:F:28:VAL:HG22	2.16	0.46
1:B:508:PHE:CG	1:B:509:PRO:HA	2.50	0.46
1:D:212:ALA:O	1:D:214:PRO:HD3	2.15	0.46
1:C:478:PHE:CE1	1:C:543:LYS:HE3	2.51	0.46
1:D:584:ILE:HD12	1:D:626:ILE:HG12	1.98	0.46
1:D:489:LYS:O	1:D:493:ILE:HG13	2.15	0.46
2:G:23:CYS:O	2:G:24:ARG:HB2	2.16	0.46
1:C:150:ILE:HG21	1:C:202:VAL:HG21	1.97	0.46
1:C:372:LEU:HD23	1:C:377:PHE:HZ	1.81	0.46
1:D:391:LEU:HD11	1:D:405:LEU:HD12	1.98	0.46
1:B:214:PRO:HG3	2:F:40:SER:HA	1.98	0.46
1:A:32:TYR:O	1:A:34:GLY:N	2.49	0.46
1:C:79:ILE:N	1:C:79:ILE:HD12	2.30	0.46
1:A:481:ASP:OD1	1:A:481:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ARG:HD2	1:D:296:LEU:CD2	2.45	0.45
1:C:475:ARG:NH2	1:C:498:GLU:HG2	2.31	0.45
1:A:493:ILE:HD13	1:A:513:MET:HB3	1.97	0.45
1:A:247:GLY:N	1:A:536:GLY:O	2.45	0.45
1:C:450:CYS:SG	1:C:595:PRO:HD3	2.57	0.45
2:E:13:ILE:N	2:F:76:ARG:O	2.40	0.45
1:D:458:THR:HB	7:D:701:UNL:X	2.46	0.45
1:C:122:TYR:HD2	1:C:135:ALA:HB2	1.82	0.45
1:C:321:LYS:HG2	1:C:322:CYS:HB2	1.98	0.45
1:B:149:ILE:O	1:B:153:GLU:HG3	2.17	0.45
1:A:486:PRO:HD3	1:A:520:TRP:CE2	2.52	0.45
1:B:467:ALA:HB2	8:B:707:BYC:HDPB	1.99	0.45
1:B:486:PRO:HD3	1:B:520:TRP:CE2	2.52	0.45
1:B:32:TYR:O	1:B:34:GLY:N	2.49	0.45
1:D:576:ARG:HD3	1:D:576:ARG:O	2.15	0.45
1:A:148:GLU:O	1:A:152:LYS:HG3	2.16	0.45
2:G:93:ARG:NH1	2:H:73:CYS:SG	2.90	0.45
1:A:349:TYR:CD2	1:A:396:VAL:HG11	2.51	0.45
1:B:349:TYR:CD2	1:B:396:VAL:HG11	2.51	0.45
1:D:462:GLY:HA3	1:D:539:SER:O	2.17	0.45
1:A:506:PRO:HG3	1:A:604:PHE:CE1	2.51	0.45
1:D:237:PRO:O	1:D:239:VAL:HG23	2.17	0.45
1:A:149:ILE:O	1:A:153:GLU:HG3	2.17	0.45
1:C:506:PRO:HG3	1:C:604:PHE:CE1	2.51	0.45
1:B:383:GLY:HA3	1:B:386:GLU:OE1	2.17	0.45
1:C:508:PHE:HA	1:C:509:PRO:C	2.37	0.45
2:F:88:GLU:O	2:F:89:CYS:HB2	2.17	0.45
2:F:11:LYS:HG2	2:F:137:GLU:HG2	1.99	0.45
1:C:349:TYR:CD2	1:C:396:VAL:HG11	2.52	0.45
1:D:241:PRO:HB2	1:D:254:VAL:HG11	1.99	0.45
2:E:46:ARG:HH12	2:E:106:ASP:CG	2.20	0.44
1:C:300:TYR:OH	2:G:28:VAL:HG22	2.17	0.44
1:C:137:HIS:NE2	1:C:153:GLU:OE2	2.48	0.44
1:A:629:LYS:NZ	1:A:642:ASP:OD1	2.50	0.44
1:D:125:ILE:HG23	1:D:130:VAL:HG22	1.98	0.44
1:D:19:ILE:HD13	1:D:130:VAL:HG12	1.99	0.44
2:F:72:GLU:HG2	2:F:98:SER:HB3	1.99	0.44
1:B:481:ASP:N	1:B:481:ASP:OD1	2.48	0.44
1:C:538:SER:O	1:C:541:PRO:HD2	2.17	0.44
1:A:383:GLY:HA3	1:A:386:GLU:OE1	2.17	0.44
1:D:576:ARG:HD3	1:D:576:ARG:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LYS:NZ	1:B:642:ASP:OD1	2.51	0.44
1:C:120:LEU:HD23	1:C:135:ALA:O	2.17	0.44
2:F:36:MET:HA	2:F:37:PRO:HA	1.91	0.44
1:A:3:TYR:O	1:A:5:GLU:N	2.49	0.44
1:A:215:GLU:H	1:A:215:GLU:CD	2.21	0.44
1:B:580:ARG:O	1:B:584:ILE:HG12	2.17	0.44
1:D:475:ARG:NH2	1:D:498:GLU:HG2	2.33	0.44
1:A:69:GLY:HA3	1:A:209:LEU:HD22	2.00	0.44
1:A:580:ARG:O	1:A:584:ILE:HG12	2.17	0.44
1:B:69:GLY:HA3	1:B:209:LEU:HD22	2.00	0.44
1:D:238:ASP:HB2	1:D:469:TYR:HE1	1.82	0.44
1:C:486:PRO:HD2	1:C:490:PHE:CD2	2.53	0.44
1:B:215:GLU:CD	1:B:215:GLU:H	2.21	0.44
1:C:247:GLY:HA2	3:C:701:SF4:S1	2.58	0.44
2:G:96:CYS:SG	2:G:97:PRO:HD2	2.58	0.44
2:G:63:LEU:HD11	2:G:92:CYS:O	2.18	0.43
2:G:63:LEU:HD12	2:G:102:PHE:CE2	2.53	0.43
1:A:294:THR:HB	1:A:309:THR:OG1	2.19	0.43
1:B:433:GLN:HE22	1:B:455:ILE:HG22	1.83	0.43
1:C:325:LYS:HG2	1:C:325:LYS:O	2.17	0.43
1:D:322:CYS:CB	4:D:703:MTE:S2'	3.03	0.43
1:A:448:MET:HE3	1:A:457:ILE:HD11	2.00	0.43
2:G:57:ARG:NH1	2:G:85:GLU:O	2.51	0.43
1:D:328:TYR:CE1	1:D:357:PRO:HG3	2.53	0.43
1:B:249:PRO:HG2	7:B:705:UNL:X	2.47	0.43
1:A:458:THR:HB	7:A:706:UNL:X	2.48	0.43
1:A:433:GLN:HE22	1:A:455:ILE:HG22	1.83	0.43
1:B:469:TYR:HB2	1:B:475:ARG:HG2	2.01	0.43
2:E:12:THR:OG1	2:F:88:GLU:OE2	2.34	0.43
1:D:67:LEU:HB2	1:D:75:CYS:SG	2.59	0.43
2:F:99:ARG:HG3	2:F:101:LEU:HB2	2.00	0.43
1:D:463:GLN:HB3	1:D:520:TRP:CH2	2.53	0.43
1:A:96:GLY:N	4:A:702:MTE:O2P	2.42	0.43
1:C:434:LEU:HD13	1:C:435:PRO:HD2	2.01	0.43
1:D:508:PHE:CG	1:D:509:PRO:HA	2.54	0.43
1:A:131:GLU:OE2	1:A:133:ARG:NE	2.39	0.43
2:H:57:ARG:NH1	2:H:85:GLU:O	2.49	0.43
1:A:469:TYR:HB2	1:A:475:ARG:HG2	2.01	0.43
1:B:253:LYS:HG2	1:B:296:LEU:HD13	2.00	0.43
1:A:253:LYS:HG2	1:A:296:LEU:HD13	2.00	0.43
2:F:166:ASP:N	2:F:166:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:HB	1:C:309:THR:OG1	2.19	0.43
2:G:114:ASP:HA	2:H:74:ILE:HD12	2.01	0.43
1:B:322:CYS:SG	1:B:323:PHE:N	2.89	0.42
1:C:247:GLY:N	1:C:536:GLY:O	2.43	0.42
1:D:39:ASN:OD1	1:D:110:LYS:NZ	2.38	0.42
1:C:189:ILE:H	1:C:189:ILE:CD1	2.29	0.42
2:F:109:LEU:HA	2:F:110:PRO:HD3	1.84	0.42
1:B:294:THR:HB	1:B:309:THR:OG1	2.19	0.42
1:D:82:THR:HG22	1:D:189:ILE:HG22	2.02	0.42
2:G:36:MET:HA	2:G:37:PRO:HA	1.91	0.42
1:B:505:MET:O	8:B:707:BYC:N6A	2.53	0.42
1:D:105:TYR:O	1:D:207:LYS:HB2	2.18	0.42
1:B:259:TRP:O	1:B:263:ASN:HB2	2.20	0.42
1:B:448:MET:HE3	1:B:457:ILE:HD11	2.01	0.42
1:C:48:PRO:HB2	1:C:50:GLU:OE1	2.19	0.42
2:H:36:MET:HA	2:H:37:PRO:HA	1.88	0.42
1:C:95:MET:CE	1:C:184:ALA:H	2.33	0.42
1:C:322:CYS:HB3	4:C:703:MTE:S1'	2.58	0.42
1:D:218:ILE:HG12	2:H:39:TYR:CD1	2.55	0.42
2:E:11:LYS:HD3	2:E:115:LEU:CD1	2.50	0.42
1:C:32:TYR:O	1:C:34:GLY:N	2.53	0.42
1:C:492:LYS:O	1:C:496:GLU:HG3	2.20	0.42
1:C:551:TYR:N	1:C:552:PRO:CD	2.83	0.42
1:C:76:ASN:ND2	1:C:300:TYR:O	2.52	0.42
1:C:289:MET:HG3	1:C:293:ARG:NH1	2.35	0.42
1:A:391:LEU:O	1:A:395:ILE:HG13	2.20	0.42
1:B:324:THR:CG2	1:B:353:GLY:HA3	2.49	0.41
1:B:42:ILE:O	1:B:46:ARG:HB2	2.20	0.41
1:B:3:TYR:O	1:B:5:GLU:N	2.50	0.41
2:G:150:THR:O	2:G:154:ILE:HG13	2.20	0.41
1:C:149:ILE:O	1:C:153:GLU:HG3	2.20	0.41
1:C:119:GLU:O	1:C:121:VAL:HG13	2.20	0.41
1:D:215:GLU:CD	1:D:215:GLU:H	2.22	0.41
1:C:73:THR:HG23	1:C:301:ASN:O	2.20	0.41
1:A:351:LEU:O	4:A:703:MTE:N2	2.36	0.41
1:A:324:THR:CG2	1:A:353:GLY:HA3	2.50	0.41
1:B:391:LEU:O	1:B:395:ILE:HG13	2.20	0.41
1:D:328:TYR:CD1	1:D:357:PRO:HG3	2.54	0.41
1:A:259:TRP:O	1:A:263:ASN:HB2	2.20	0.41
1:C:348:GLU:HA	1:C:348:GLU:OE2	2.20	0.41
1:D:383:GLY:O	1:D:387:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:64:TYR:OH	2:E:133:LEU:HD13	2.19	0.41
1:A:513:MET:O	1:A:517:ILE:HG13	2.20	0.41
1:C:426:ASN:ND2	1:C:433:GLN:O	2.53	0.41
1:D:376:ASP:C	1:D:378:PRO:HD3	2.40	0.41
1:D:449:TYR:CE1	1:D:457:ILE:HB	2.56	0.41
2:H:13:ILE:HD11	2:H:115:LEU:HD21	2.03	0.41
1:A:42:ILE:HG23	1:A:46:ARG:HD3	2.03	0.41
2:H:64:TYR:O	2:H:93:ARG:HD2	2.20	0.41
1:D:239:VAL:CG1	1:D:243:LEU:HB3	2.51	0.41
1:D:380:LEU:HD12	1:D:381:PRO:HD2	2.02	0.41
1:A:42:ILE:O	1:A:46:ARG:HB2	2.20	0.41
1:C:52:GLU:O	1:C:55:SER:HB3	2.20	0.41
1:B:366:LEU:HB3	1:B:372:LEU:HD13	2.03	0.41
2:G:163:PHE:CD2	2:H:152:MET:HB3	2.56	0.41
2:H:152:MET:O	2:H:156:LEU:HG	2.20	0.41
1:C:349:TYR:CG	1:C:396:VAL:HG11	2.55	0.41
1:B:513:MET:O	1:B:517:ILE:HG13	2.20	0.41
2:F:21:ASN:ND2	2:F:130:VAL:HG11	2.36	0.41
1:C:484:GLN:OE1	1:C:484:GLN:N	2.52	0.41
1:D:42:ILE:HG23	1:D:46:ARG:HD3	2.03	0.41
2:F:164:GLY:O	2:F:168:VAL:HG23	2.21	0.41
2:H:48:ARG:CZ	2:H:111:LEU:HD22	2.50	0.41
1:B:240:MET:SD	1:B:242:ILE:HG12	2.62	0.40
1:D:322:CYS:SG	1:D:323:PHE:N	2.94	0.40
1:D:60:LEU:HD22	1:D:193:MET:HA	2.03	0.40
1:C:143:ALA:CB	1:C:178:GLU:HB2	2.52	0.40
2:G:63:LEU:HD12	2:G:102:PHE:CZ	2.56	0.40
1:B:42:ILE:HG23	1:B:46:ARG:HD3	2.03	0.40
1:C:225:LEU:O	1:C:229:LYS:HG3	2.21	0.40
1:C:523:MET:O	1:C:527:ILE:HG13	2.21	0.40
1:D:258:LYS:HB2	1:D:277:TRP:CD1	2.56	0.40
1:C:472:LEU:O	1:C:476:GLU:HG3	2.21	0.40
1:A:576:ARG:O	1:A:576:ARG:HD3	2.22	0.40
2:H:46:ARG:NH1	2:H:104:GLU:OE1	2.53	0.40
1:D:469:TYR:HA	1:D:470:PRO:HD3	1.93	0.40
1:A:448:MET:HB3	1:A:460:ILE:HG21	2.02	0.40
1:B:122:TYR:HD2	1:B:135:ALA:HB2	1.86	0.40
1:D:239:VAL:CG1	1:D:243:LEU:CB	2.99	0.40
1:A:366:LEU:HB3	1:A:372:LEU:HD13	2.03	0.40
1:A:135:ALA:HB1	1:A:138:LEU:HD12	2.03	0.40
1:D:231:ARG:HG2	1:D:246:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:SER:O	1:C:352:ASP:HB2	2.21	0.40
1:C:25:ASP:HA	1:C:26:PRO:HD2	1.92	0.40
1:A:218:ILE:HD12	1:A:218:ILE:HA	1.91	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	651/653 (100%)	624 (96%)	24 (4%)	3 (0%)	34	39
1	B	651/653 (100%)	624 (96%)	24 (4%)	3 (0%)	34	39
1	C	651/653 (100%)	623 (96%)	24 (4%)	4 (1%)	30	34
1	D	650/653 (100%)	626 (96%)	22 (3%)	2 (0%)	46	55
2	E	158/179 (88%)	154 (98%)	4 (2%)	0	100	100
2	F	169/179 (94%)	168 (99%)	1 (1%)	0	100	100
2	G	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
2	H	157/179 (88%)	156 (99%)	1 (1%)	0	100	100
All	All	3256/3328 (98%)	3140 (96%)	104 (3%)	12 (0%)	39	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	652	ALA
1	D	33	LEU
1	C	622	ASN
1	A	249	PRO
1	A	305	LYS
1	B	249	PRO
1	B	305	LYS

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Mol	Chain	Res	Type
1	C	76	ASN
1	C	455	ILE
1	A	242	ILE
1	B	242	ILE
1	D	249	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	547/548 (100%)	538 (98%)	9 (2%)	70	83
1	B	548/548 (100%)	539 (98%)	9 (2%)	70	83
1	C	548/548 (100%)	533 (97%)	15 (3%)	52	67
1	D	546/548 (100%)	536 (98%)	10 (2%)	66	81
2	E	133/159 (84%)	132 (99%)	1 (1%)	86	94
2	F	148/159 (93%)	144 (97%)	4 (3%)	52	67
2	G	147/159 (92%)	145 (99%)	2 (1%)	74	86
2	H	132/159 (83%)	132 (100%)	0	100	100
All	All	2749/2828 (97%)	2699 (98%)	50 (2%)	66	81

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	179	GLN
1	A	189	ILE
1	A	215	GLU
1	A	321	LYS
1	A	324	THR
1	A	414	GLN
1	A	551	TYR
1	A	576	ARG
1	B	1	MET

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Mol	Chain	Res	Type
1	B	179	GLN
1	B	189	ILE
1	B	215	GLU
1	B	321	LYS
1	B	324	THR
1	B	414	GLN
1	B	551	TYR
1	B	576	ARG
1	C	38	THR
1	C	50	GLU
1	C	114	ARG
1	C	179	GLN
1	C	183	SER
1	C	189	ILE
1	C	215	GLU
1	C	319	MET
1	C	321	LYS
1	C	322	CYS
1	C	425	HIS
1	C	434	LEU
1	C	551	TYR
1	C	576	ARG
1	C	599	HIS
1	D	50	GLU
1	D	179	GLN
1	D	189	ILE
1	D	215	GLU
1	D	240	MET
1	D	321	LYS
1	D	374	ASP
1	D	551	TYR
1	D	564	ASP
1	D	576	ARG
2	E	99	ARG
2	F	46	ARG
2	F	63	LEU
2	F	99	ARG
2	F	135	VAL
2	G	63	LEU
2	G	99	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	433	GLN
1	B	179	GLN
1	B	433	GLN

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 8 are monoatomic - leaving 28 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	SF4	A	701	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MTE	A	702	5,6	21,26,26	2.91	10 (47%)	18,40,40	2.17	4 (22%)
4	MTE	A	703	5,6	21,26,26	2.94	10 (47%)	18,40,40	2.20	4 (22%)
8	BYC	A	707	-	50,59,59	0.42	0	62,87,87	0.61	1 (1%)
3	SF4	B	701	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MTE	B	702	5,6	21,26,26	2.88	10 (47%)	18,40,40	2.07	4 (22%)
4	MTE	B	703	5,6	21,26,26	2.81	10 (47%)	18,40,40	2.15	4 (22%)
8	BYC	B	707	-	50,59,59	0.43	0	62,87,87	0.60	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SF4	C	701	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MTE	C	702	5,6	21,26,26	2.85	10 (47%)	18,40,40	2.21	3 (16%)
4	MTE	C	703	5,6	21,26,26	2.86	10 (47%)	18,40,40	2.19	4 (22%)
8	BYC	C	707	-	50,59,59	0.42	0	62,87,87	0.57	0
3	SF4	D	702	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MTE	D	703	5,6	21,26,26	2.89	10 (47%)	18,40,40	2.38	5 (27%)
4	MTE	D	704	5,6	21,26,26	2.93	10 (47%)	18,40,40	2.24	4 (22%)
8	BYC	D	707	-	50,59,59	0.42	0	62,87,87	0.60	1 (1%)
3	SF4	E	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	E	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	E	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	G	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	G	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	G	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	H	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	H	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
3	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
3	SF4	A	701	1	-	0/0/48/48	0/6/5/5
4	MTE	A	702	5,6	-	0/6/34/34	0/3/3/3
4	MTE	A	703	5,6	-	0/6/34/34	0/3/3/3
8	BYC	A	707	-	-	1/50/71/71	0/4/4/4
3	SF4	B	701	1	-	0/0/48/48	0/6/5/5
4	MTE	B	702	5,6	-	0/6/34/34	0/3/3/3
4	MTE	B	703	5,6	-	0/6/34/34	0/3/3/3
8	BYC	B	707	-	-	1/50/71/71	0/4/4/4
3	SF4	C	701	1	-	0/0/48/48	0/6/5/5
4	MTE	C	702	5,6	-	0/6/34/34	0/3/3/3
4	MTE	C	703	5,6	-	0/6/34/34	0/3/3/3
8	BYC	C	707	-	-	1/50/71/71	0/4/4/4
3	SF4	D	702	1	-	0/0/48/48	0/6/5/5
4	MTE	D	703	5,6	-	0/6/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MTE	D	704	5,6	-	0/6/34/34	0/3/3/3
8	BYC	D	707	-	-	1/50/71/71	0/4/4/4
3	SF4	E	1001	2	-	0/0/48/48	0/6/5/5
3	SF4	E	1002	2	-	0/0/48/48	0/6/5/5
3	SF4	E	1003	2	-	0/0/48/48	0/6/5/5
3	SF4	F	1001	2	-	0/0/48/48	0/6/5/5
3	SF4	F	1002	2	-	0/0/48/48	0/6/5/5
3	SF4	F	1003	2	-	0/0/48/48	0/6/5/5
3	SF4	G	1001	2	-	0/0/48/48	0/6/5/5
3	SF4	G	1002	2	-	0/0/48/48	0/6/5/5
3	SF4	G	1003	2	-	0/0/48/48	0/6/5/5
3	SF4	H	1001	2	-	0/0/48/48	0/6/5/5
3	SF4	H	1002	2	-	0/0/48/48	0/6/5/5
3	SF4	H	1003	2	-	0/0/48/48	0/6/5/5

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	MTE	C9-C10	-6.55	1.29	1.41
4	A	703	MTE	C9-C10	-6.42	1.29	1.41
4	D	704	MTE	C9-C10	-6.41	1.29	1.41
4	D	703	MTE	C9-C10	-6.40	1.29	1.41
4	B	702	MTE	C9-C10	-6.39	1.29	1.41
4	C	702	MTE	C9-C10	-6.37	1.29	1.41
4	C	703	MTE	C9-C10	-6.27	1.29	1.41
4	A	702	MTE	C9-C10	-6.27	1.29	1.41
4	D	704	MTE	C7-C6	-5.99	1.49	1.53
4	A	703	MTE	C7-C6	-5.84	1.49	1.53
4	D	703	MTE	C7-C6	-5.73	1.49	1.53
4	A	702	MTE	C7-C6	-5.45	1.49	1.53
4	C	702	MTE	C7-C6	-5.36	1.49	1.53
4	C	703	MTE	C7-C6	-5.28	1.49	1.53
4	B	702	MTE	C7-C6	-4.75	1.50	1.53
4	B	703	MTE	C7-C6	-4.06	1.50	1.53
4	B	702	MTE	O3'-C7	-3.92	1.38	1.43
4	C	703	MTE	O3'-C7	-3.88	1.38	1.43
4	A	702	MTE	O3'-C7	-3.79	1.38	1.43
4	D	703	MTE	O3'-C7	-3.78	1.38	1.43
4	A	703	MTE	O3'-C7	-3.78	1.38	1.43
4	B	703	MTE	O3'-C7	-3.76	1.38	1.43
4	D	704	MTE	O3'-C7	-3.74	1.38	1.43
4	C	702	MTE	O3'-C7	-3.72	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	MTE	O3'-C3'	-3.20	1.39	1.43
4	C	702	MTE	O3'-C3'	-3.20	1.39	1.43
4	B	702	MTE	O3'-C3'	-3.19	1.39	1.43
4	A	702	MTE	O3'-C3'	-3.14	1.39	1.43
4	C	703	MTE	O3'-C3'	-3.13	1.39	1.43
4	D	703	MTE	O3'-C3'	-2.94	1.39	1.43
4	A	703	MTE	O3'-C3'	-2.77	1.39	1.43
4	D	704	MTE	O3'-C3'	-2.50	1.40	1.43
4	A	702	MTE	C2-N3	2.33	1.39	1.35
4	C	702	MTE	C2-N3	2.33	1.39	1.35
4	D	703	MTE	C2-N3	2.33	1.39	1.35
4	B	702	MTE	C2-N3	2.38	1.39	1.35
4	A	703	MTE	C2-N3	2.39	1.39	1.35
4	B	703	MTE	C2-N3	2.44	1.40	1.35
4	C	703	MTE	C2-N3	2.50	1.40	1.35
4	D	704	MTE	C2-N3	2.54	1.40	1.35
4	C	702	MTE	C10-N8	2.58	1.43	1.35
4	C	703	MTE	C10-N8	2.59	1.43	1.35
4	A	702	MTE	C10-N8	2.66	1.43	1.35
4	B	703	MTE	C10-N8	2.66	1.43	1.35
4	B	702	MTE	C10-N8	2.70	1.43	1.35
4	C	702	MTE	C10-N1	2.72	1.39	1.34
4	D	703	MTE	C10-N8	2.73	1.43	1.35
4	D	704	MTE	C10-N8	2.73	1.43	1.35
4	B	703	MTE	C10-N1	2.80	1.39	1.34
4	A	703	MTE	C10-N8	2.81	1.44	1.35
4	A	702	MTE	C10-N1	2.84	1.39	1.34
4	C	703	MTE	C10-N1	2.84	1.39	1.34
4	B	703	MTE	C4-N3	2.91	1.38	1.33
4	A	703	MTE	C10-N1	2.94	1.39	1.34
4	D	704	MTE	C10-N1	2.94	1.39	1.34
4	B	702	MTE	C10-N1	2.97	1.39	1.34
4	D	703	MTE	C10-N1	3.00	1.40	1.34
4	D	703	MTE	C4-N3	3.04	1.38	1.33
4	A	703	MTE	C4-N3	3.05	1.38	1.33
4	C	703	MTE	C4-N3	3.06	1.38	1.33
4	B	702	MTE	C4-N3	3.10	1.38	1.33
4	C	702	MTE	C4-N3	3.15	1.38	1.33
4	A	702	MTE	C4-N3	3.19	1.38	1.33
4	D	704	MTE	C4-N3	3.21	1.38	1.33
4	D	703	MTE	C4-C9	4.20	1.47	1.41
4	C	702	MTE	C2-N2	4.31	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	MTE	C4-C9	4.39	1.47	1.41
4	B	703	MTE	C2-N2	4.39	1.43	1.34
4	D	704	MTE	C2-N2	4.43	1.43	1.34
4	A	703	MTE	C2-N2	4.43	1.43	1.34
4	A	702	MTE	C2-N2	4.43	1.43	1.34
4	B	702	MTE	C2-N2	4.44	1.43	1.34
4	C	703	MTE	C4-C9	4.45	1.47	1.41
4	B	703	MTE	C4-C9	4.46	1.47	1.41
4	D	703	MTE	C2-N2	4.47	1.43	1.34
4	C	703	MTE	C2-N2	4.48	1.43	1.34
4	D	704	MTE	C4-C9	4.61	1.48	1.41
4	A	702	MTE	C4-C9	4.67	1.48	1.41
4	B	702	MTE	C4-C9	4.72	1.48	1.41
4	A	703	MTE	C4-C9	4.81	1.48	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	703	MTE	O3'-C7-C6	-5.21	105.40	108.96
4	C	702	MTE	O3'-C7-C6	-4.34	106.00	108.96
4	A	702	MTE	O3'-C7-C6	-3.87	106.31	108.96
4	C	703	MTE	O3'-C7-C6	-3.66	106.46	108.96
4	D	704	MTE	O3'-C7-C6	-3.57	106.52	108.96
4	B	702	MTE	O3'-C7-C6	-2.71	107.11	108.96
4	A	703	MTE	O3'-C7-C6	-2.62	107.17	108.96
4	D	703	MTE	N3-C2-N1	-2.01	122.23	125.51
4	C	703	MTE	C9-C10-N8	2.02	120.11	118.19
4	B	703	MTE	N8-C10-N1	2.10	119.96	116.62
4	B	702	MTE	N8-C10-N1	2.14	120.03	116.62
8	A	707	BYC	C2P-S1P-C1B	2.19	102.42	99.61
4	A	702	MTE	C9-C10-N8	2.25	120.33	118.19
4	D	703	MTE	N8-C10-N1	2.27	120.24	116.62
8	B	707	BYC	C2P-S1P-C1B	2.33	102.61	99.61
8	D	707	BYC	C2P-S1P-C1B	2.41	102.71	99.61
4	B	703	MTE	C9-C10-N8	2.43	120.50	118.19
4	A	703	MTE	N8-C10-N1	2.48	120.58	116.62
4	D	704	MTE	N8-C10-N1	2.64	120.83	116.62
4	C	702	MTE	C2-N1-C10	2.65	120.58	114.63
4	C	703	MTE	C2-N1-C10	2.67	120.62	114.63
4	D	704	MTE	C2-N1-C10	2.68	120.65	114.63
4	A	702	MTE	C2-N1-C10	2.69	120.67	114.63
4	B	703	MTE	C2-N1-C10	2.77	120.84	114.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	703	MTE	C2-N1-C10	2.78	120.87	114.63
4	B	702	MTE	C2-N1-C10	2.78	120.88	114.63
4	A	703	MTE	C2-N1-C10	2.81	120.95	114.63
4	A	702	MTE	C4-C9-C10	6.59	120.41	114.61
4	C	702	MTE	C4-C9-C10	6.66	120.47	114.61
4	B	702	MTE	C4-C9-C10	6.68	120.49	114.61
4	C	703	MTE	C4-C9-C10	6.92	120.70	114.61
4	D	703	MTE	C4-C9-C10	6.96	120.73	114.61
4	D	704	MTE	C4-C9-C10	7.24	120.98	114.61
4	A	703	MTE	C4-C9-C10	7.25	121.00	114.61
4	B	703	MTE	C4-C9-C10	7.48	121.19	114.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	707	BYC	O9P-C9P-CAP-CBP
8	D	707	BYC	O9P-C9P-CAP-CBP
8	B	707	BYC	O9P-C9P-CAP-CBP
8	C	707	BYC	O9P-C9P-CAP-CBP

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	MTE	3	0
4	A	703	MTE	1	0
8	A	707	BYC	5	0
4	B	702	MTE	4	0
4	B	703	MTE	5	0
8	B	707	BYC	6	0
3	C	701	SF4	1	0
4	C	703	MTE	1	0
8	C	707	BYC	7	0
4	D	703	MTE	2	0
8	D	707	BYC	3	0
3	G	1002	SF4	1	0

5.7 Other polymers (i)

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	653/653 (100%)	0.90	46 (7%) 19 29	42, 63, 96, 145	0
1	B	653/653 (100%)	2.12	264 (40%) 0 0	46, 116, 167, 195	0
1	C	653/653 (100%)	0.89	60 (9%) 11 18	37, 61, 111, 157	0
1	D	652/653 (99%)	0.82	58 (8%) 12 19	42, 65, 93, 132	0
2	E	162/179 (90%)	0.81	14 (8%) 13 21	38, 59, 95, 127	0
2	F	170/179 (94%)	0.91	18 (10%) 8 14	39, 58, 86, 110	0
2	G	169/179 (94%)	0.76	8 (4%) 35 50	40, 57, 132, 146	0
2	H	161/179 (89%)	0.56	5 (3%) 52 65	44, 63, 125, 149	0
All	All	3273/3328 (98%)	1.10	473 (14%) 3 6	37, 66, 135, 195	0

All (473) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	LEU	13.1
1	B	259	TRP	11.5
1	B	440	MET	11.0
1	C	602	ASN	10.0
1	B	264	PHE	9.7
1	B	394	LYS	9.5
1	B	416	ILE	9.2
1	B	357	PRO	9.0
1	C	259	TRP	8.7
1	B	366	LEU	8.7
1	B	405	LEU	8.7
1	A	242	ILE	8.7
1	B	434	LEU	8.5
1	B	173	PHE	8.1
1	B	418	ASN	7.9
1	B	404	ILE	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	641	GLY	7.7
1	B	607	LEU	7.6
1	B	369	LYS	7.6
1	B	392	LEU	7.3
1	B	274	LYS	7.2
1	B	323	PHE	7.1
1	B	241	PRO	7.0
1	C	243	LEU	6.9
1	B	260	HIS	6.9
1	B	285	TRP	6.8
1	B	601	LYS	6.7
1	B	506	PRO	6.5
1	B	455	ILE	6.4
1	B	625	GLY	6.4
1	B	354	PHE	6.4
1	C	274	LYS	6.3
1	B	439	SER	6.3
1	B	611	LEU	6.3
1	C	241	PRO	6.3
1	B	277	TRP	6.2
1	B	597	ALA	6.2
1	B	355	SER	6.2
1	C	277	TRP	6.1
1	B	247	GLY	6.1
1	B	258	LYS	6.0
1	B	54	PHE	5.9
1	B	600	TRP	5.9
1	A	644	PHE	5.8
1	B	62	PHE	5.7
1	B	377	PHE	5.7
1	C	242	ILE	5.7
1	B	577	THR	5.7
1	B	579	VAL	5.6
1	B	236	ILE	5.6
1	B	595	PRO	5.5
1	B	136	SER	5.5
1	B	240	MET	5.5
1	B	120	LEU	5.5
1	B	421	GLU	5.5
1	B	511	VAL	5.4
1	B	1	MET	5.4
1	B	239	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	446	TYR	5.4
1	B	396	VAL	5.4
1	B	599	HIS	5.3
1	B	509	PRO	5.3
1	B	132	ILE	5.3
1	B	604	PHE	5.2
1	B	414	GLN	5.2
1	B	618	LEU	5.2
1	B	254	VAL	5.2
1	B	379	GLY	5.2
1	C	255	HIS	5.2
1	B	508	PHE	5.2
1	C	260	HIS	5.1
1	C	239	VAL	5.0
1	B	438	LEU	5.0
1	B	465	PRO	4.9
2	G	164	GLY	4.9
1	B	14	LEU	4.9
1	C	280	GLU	4.9
1	B	174	TYR	4.9
1	B	575	TYR	4.9
1	B	402	GLY	4.8
1	B	505	MET	4.8
1	B	43	LEU	4.8
1	B	498	GLU	4.7
1	B	138	LEU	4.6
1	B	581	ALA	4.6
1	B	41	LYS	4.6
1	B	167	ALA	4.5
1	B	650	LEU	4.5
1	B	61	ILE	4.5
1	B	423	TYR	4.4
2	E	131	GLY	4.4
1	B	279	ASP	4.4
1	B	388	PHE	4.4
2	F	167	VAL	4.3
1	C	652	ALA	4.3
1	B	255	HIS	4.3
1	B	359	VAL	4.3
1	C	438	LEU	4.2
1	B	12	VAL	4.2
1	B	351	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	100	ASP	4.2
1	B	401	ILE	4.2
1	B	428	ILE	4.2
1	B	412	ALA	4.2
1	B	419	GLY	4.2
1	D	323	PHE	4.1
1	A	380	LEU	4.1
1	B	490	PHE	4.0
1	B	200	ALA	4.0
1	B	90	MET	4.0
1	B	362	PHE	4.0
1	B	482	TRP	4.0
1	B	276	PHE	3.9
1	A	256	ASP	3.9
1	B	447	LEU	3.9
1	B	450	CYS	3.9
1	B	602	ASN	3.9
1	B	281	VAL	3.9
1	B	289	MET	3.9
1	B	507	ASN	3.8
1	A	260	HIS	3.8
1	B	111	ILE	3.8
1	C	500	ARG	3.8
1	B	37	GLY	3.8
1	A	323	PHE	3.7
1	B	390	TYR	3.7
1	B	269	ALA	3.7
1	B	497	TRP	3.7
1	B	170	ASN	3.7
1	B	389	PHE	3.7
1	D	33	LEU	3.7
1	D	283	HIS	3.7
1	B	653	GLY	3.7
1	B	63	ALA	3.6
1	B	378	PRO	3.6
1	B	364	PHE	3.6
1	B	464	PHE	3.6
1	B	122	TYR	3.6
1	B	441	LEU	3.6
1	B	17	GLY	3.6
2	G	172	VAL	3.6
1	D	260	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	281	VAL	3.6
1	A	27	ARG	3.6
1	B	271	THR	3.6
1	B	520	TRP	3.6
1	B	372	LEU	3.5
1	B	596	PRO	3.5
1	B	483	ILE	3.5
1	C	273	ARG	3.5
2	E	129	LEU	3.5
1	B	283	HIS	3.5
1	B	333	TYR	3.5
1	B	606	GLU	3.5
1	C	285	TRP	3.5
1	D	634	ASP	3.4
1	C	447	LEU	3.4
1	B	32	TYR	3.4
1	D	267	GLY	3.4
1	B	360	MET	3.4
1	B	591	VAL	3.4
2	E	153	GLU	3.4
1	B	572	ALA	3.4
1	B	242	ILE	3.4
1	A	241	PRO	3.3
1	B	615	TYR	3.3
1	C	31	LEU	3.3
2	F	129	LEU	3.3
1	A	240	MET	3.3
1	B	325	LYS	3.3
1	D	31	LEU	3.3
1	B	135	ALA	3.3
2	H	8	ARG	3.3
1	B	496	GLU	3.3
2	H	159	LEU	3.3
2	F	168	VAL	3.3
2	F	142	GLU	3.3
1	B	249	PRO	3.2
1	B	406	ALA	3.2
1	B	19	ILE	3.2
1	B	194	GLY	3.2
1	C	217	TYR	3.2
1	A	279	ASP	3.2
1	B	499	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	475	ARG	3.2
1	C	254	VAL	3.2
1	B	321	LYS	3.2
1	B	278	THR	3.2
1	C	22	VAL	3.2
1	D	239	VAL	3.1
1	B	371	ILE	3.1
1	B	651	SER	3.1
1	C	275	ASP	3.1
1	B	472	LEU	3.1
1	D	649	ILE	3.1
1	B	603	ARG	3.1
2	F	115	LEU	3.1
1	C	331	ALA	3.1
1	B	60	LEU	3.1
1	B	253	LYS	3.1
1	B	280	GLU	3.1
1	B	456	ASN	3.1
1	C	440	MET	3.1
1	A	255	HIS	3.0
1	B	548	ILE	3.0
1	B	616	TYR	3.0
1	A	450	CYS	3.0
1	B	324	THR	3.0
1	A	1	MET	3.0
1	B	246	LEU	3.0
1	A	388	PHE	3.0
1	C	437	LYS	3.0
1	B	160	GLN	3.0
1	B	232	GLU	3.0
1	B	640	VAL	3.0
1	D	635	LEU	3.0
1	B	119	GLU	3.0
1	B	444	ILE	3.0
1	D	242	ILE	3.0
1	B	22	VAL	3.0
1	A	254	VAL	2.9
1	A	653	GLY	2.9
1	B	473	GLU	2.9
2	F	145	GLU	2.9
1	B	51	VAL	2.9
1	D	266	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	240	MET	2.9
1	B	308	ALA	2.9
1	D	256	ASP	2.9
1	B	503	LYS	2.9
1	D	216	GLU	2.9
1	B	67	LEU	2.9
1	A	511	VAL	2.9
1	B	181	ARG	2.9
2	E	172	VAL	2.9
2	E	159	LEU	2.9
1	B	363	ALA	2.9
1	D	27	ARG	2.9
1	B	621	TRP	2.9
1	B	244	ALA	2.8
1	B	275	ASP	2.8
1	B	467	ALA	2.8
1	B	112	ILE	2.8
2	E	167	VAL	2.8
2	F	156	LEU	2.8
2	F	169	ALA	2.8
1	C	283	HIS	2.8
1	B	314	GLY	2.8
1	B	318	TYR	2.8
1	B	113	PHE	2.8
2	F	22	GLY	2.8
1	A	274	LYS	2.8
1	B	95	MET	2.8
1	B	349	TYR	2.8
1	A	557	ALA	2.7
2	G	169	ALA	2.7
1	B	270	ARG	2.7
1	C	445	TYR	2.7
1	A	597	ALA	2.7
1	B	130	VAL	2.7
1	B	261	THR	2.7
1	B	605	PRO	2.7
1	C	446	TYR	2.7
1	D	363	ALA	2.7
1	B	398	ARG	2.7
1	A	368	GLU	2.7
1	D	285	TRP	2.7
1	B	370	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	380	LEU	2.7
1	B	267	GLY	2.7
1	C	420	ALA	2.7
1	B	263	ASN	2.7
1	A	615	TYR	2.7
2	H	171	THR	2.7
1	D	379	GLY	2.7
1	B	504	SER	2.6
1	A	374	ASP	2.6
1	D	287	LYS	2.6
1	C	9	VAL	2.6
2	F	140	VAL	2.6
2	E	36	MET	2.6
1	A	277	TRP	2.6
1	B	622	ASN	2.6
1	A	283	HIS	2.6
1	B	430	LYS	2.6
1	B	494	PHE	2.6
1	D	319	MET	2.6
1	B	331	ALA	2.6
2	G	115	LEU	2.6
1	B	150	ILE	2.6
2	F	161	SER	2.6
1	C	472	LEU	2.6
1	D	120	LEU	2.6
1	B	445	TYR	2.6
1	B	469	TYR	2.6
1	B	373	LYS	2.6
2	E	112	LYS	2.6
1	B	493	ILE	2.6
1	D	218	ILE	2.6
1	B	327	THR	2.6
1	B	340	LEU	2.6
1	B	88	LYS	2.5
1	B	64	ALA	2.5
1	B	48	PRO	2.5
1	D	172	VAL	2.5
2	F	172	VAL	2.5
1	B	460	ILE	2.5
1	D	395	ILE	2.5
1	B	570	LYS	2.5
1	D	255	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	304	MET	2.5
2	F	147	VAL	2.5
1	B	332	ALA	2.5
1	D	59	LEU	2.5
1	C	244	ALA	2.5
2	F	165	ALA	2.5
1	C	261	THR	2.5
1	D	483	ILE	2.5
1	D	232	GLU	2.4
1	D	15	THR	2.4
1	B	168	GLY	2.4
1	D	3	TYR	2.4
1	B	175	ALA	2.4
1	A	378	PRO	2.4
1	B	502	GLU	2.4
1	C	323	PHE	2.4
2	G	171	THR	2.4
1	B	510	THR	2.4
1	C	318	TYR	2.4
1	B	652	ALA	2.4
1	B	201	VAL	2.4
1	B	322	CYS	2.4
1	C	651	SER	2.4
1	B	400	GLY	2.4
1	B	237	PRO	2.4
1	B	463	GLN	2.4
1	B	306	CYS	2.4
1	B	437	LYS	2.3
1	D	144	ILE	2.3
1	D	342	ILE	2.3
1	B	153	GLU	2.3
2	E	13	ILE	2.3
1	C	73	THR	2.3
1	B	399	ASP	2.3
1	A	649	ILE	2.3
1	C	240	MET	2.3
1	B	121	VAL	2.3
1	D	202	VAL	2.3
1	D	562	GLU	2.3
1	B	449	TYR	2.3
1	C	1	MET	2.3
1	B	540	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	268	ASN	2.3
1	B	381	PRO	2.3
1	B	442	ASN	2.3
1	B	645	ILE	2.3
1	A	441	LEU	2.3
1	B	59	LEU	2.3
1	A	484	GLN	2.3
2	G	124	CYS	2.3
1	B	96	GLY	2.3
2	F	152	MET	2.3
1	A	266	TRP	2.3
1	C	471	LYS	2.3
1	A	641	GLY	2.2
1	B	7	GLY	2.2
1	B	620	GLY	2.2
2	F	60	TYR	2.2
1	B	129	LYS	2.2
1	A	121	VAL	2.2
1	B	479	VAL	2.2
2	E	168	VAL	2.2
1	B	99	TRP	2.2
1	B	125	ILE	2.2
1	C	307	GLY	2.2
1	A	373	LYS	2.2
1	C	449	TYR	2.2
1	B	92	PHE	2.2
1	B	478	PHE	2.2
1	B	44	TRP	2.2
1	D	282	SER	2.2
1	C	558	GLY	2.2
1	A	275	ASP	2.2
1	B	425	HIS	2.2
1	C	246	LEU	2.2
1	D	554	PHE	2.2
1	D	82	THR	2.2
1	D	91	ALA	2.2
1	D	652	ALA	2.2
1	A	438	LEU	2.2
1	B	367	LEU	2.2
1	B	391	LEU	2.2
1	C	372	LEU	2.2
2	E	149	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	627	PRO	2.2
1	B	13	ASP	2.2
1	B	134	ASP	2.2
1	C	388	PHE	2.2
1	D	644	PHE	2.2
1	B	309	THR	2.2
1	B	395	ILE	2.2
1	B	45	ASP	2.2
1	B	146	THR	2.2
1	D	346	ALA	2.2
2	E	12	THR	2.2
1	A	497	TRP	2.2
1	B	436	LEU	2.2
1	B	185	SER	2.2
2	F	90	GLY	2.2
1	A	108	TYR	2.1
1	B	453	GLU	2.1
1	C	228	ILE	2.1
1	B	336	LEU	2.1
1	B	495	LEU	2.1
1	C	258	LYS	2.1
1	C	320	MET	2.1
1	C	230	HIS	2.1
1	B	347	THR	2.1
1	C	367	LEU	2.1
1	C	650	LEU	2.1
1	D	1	MET	2.1
1	B	571	ALA	2.1
1	C	332	ALA	2.1
1	D	64	ALA	2.1
1	C	256	ASP	2.1
1	B	452	GLY	2.1
1	D	154	LEU	2.1
1	B	471	LYS	2.1
1	A	422	ASP	2.1
1	B	238	ASP	2.1
1	B	481	ASP	2.1
1	D	195	ASP	2.1
1	A	281	VAL	2.1
1	B	272	ARG	2.1
1	B	177	ILE	2.1
1	B	342	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	372	LEU	2.1
1	B	480	GLU	2.1
2	E	151	GLU	2.1
1	C	278	THR	2.1
1	C	649	ILE	2.1
1	D	60	LEU	2.1
1	D	123	LEU	2.1
1	D	252	MET	2.1
1	A	285	TRP	2.1
1	C	202	VAL	2.1
2	G	113	CYS	2.1
1	C	357	PRO	2.1
1	C	368	GLU	2.0
1	C	493	ILE	2.0
1	D	531	LEU	2.0
1	B	319	MET	2.0
2	E	139	GLU	2.0
1	D	596	PRO	2.0
1	A	210	CYS	2.0
1	B	411	TRP	2.0
2	H	168	VAL	2.0
1	D	174	TYR	2.0
2	H	113	CYS	2.0
1	B	209	LEU	2.0
1	B	517	ILE	2.0
1	D	10	LEU	2.0
1	A	263	ASN	2.0
1	A	625	GLY	2.0
1	A	341	ARG	2.0
1	B	516	ASP	2.0
1	B	647	ARG	2.0
1	A	446	TYR	2.0
1	A	310	ILE	2.0
1	D	111	ILE	2.0
1	B	451	THR	2.0
2	G	149	ARG	2.0
1	D	332	ALA	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
8	BYC	A	707	56/56	0.73	0.32	1.92	40,56,86,89	96
6	MG	A	705	1/1	0.88	0.23	1.23	42,42,42,42	0
6	MG	C	704	1/1	0.86	0.22	1.00	47,47,47,47	0
8	BYC	C	707	56/56	0.62	0.38	0.68	47,64,86,100	96
8	BYC	D	707	56/56	0.84	0.24	0.62	32,56,98,103	96
4	MTE	D	704	24/24	0.94	0.20	0.15	41,49,58,62	0
4	MTE	C	702	24/24	0.95	0.18	-0.07	24,37,48,57	0
8	BYC	B	707	56/56	0.59	0.36	-0.19	39,60,78,94	96
4	MTE	C	703	24/24	0.85	0.18	-0.26	41,50,55,60	0
4	MTE	B	702	24/24	0.88	0.21	-0.28	35,82,90,124	0
4	MTE	A	703	24/24	0.94	0.18	-0.34	41,43,56,61	0
4	MTE	A	702	24/24	0.96	0.18	-0.37	39,46,53,56	0
4	MTE	D	703	24/24	0.95	0.17	-0.44	26,40,49,68	0
3	SF4	F	1002	8/8	0.94	0.18	-0.58	36,50,70,91	0
3	SF4	E	1001	8/8	0.97	0.15	-0.60	52,55,56,57	0
3	SF4	E	1003	8/8	0.95	0.14	-0.68	49,52,55,55	0
3	SF4	E	1002	8/8	0.97	0.15	-0.71	52,59,61,66	0
3	SF4	G	1002	8/8	0.95	0.15	-0.76	42,46,57,60	0
3	SF4	H	1003	8/8	0.97	0.13	-0.83	49,57,70,72	0
4	MTE	B	703	24/24	0.93	0.18	-0.92	97,106,113,164	0
6	MG	D	706	1/1	0.77	0.13	-1.15	44,44,44,44	0
3	SF4	F	1001	8/8	0.96	0.12	-1.17	41,52,54,61	0
3	SF4	H	1001	8/8	0.96	0.14	-1.25	33,46,49,52	0
3	SF4	H	1002	8/8	0.94	0.12	-1.26	50,60,67,69	0
3	SF4	G	1001	8/8	0.93	0.14	-1.43	36,41,59,60	0
3	SF4	B	701	8/8	0.96	0.07	-1.58	79,94,134,153	0
3	SF4	D	702	8/8	0.93	0.09	-1.81	53,60,87,104	0
3	SF4	G	1003	8/8	0.97	0.11	-1.94	45,53,63,68	0
3	SF4	C	701	8/8	0.96	0.08	-2.42	49,52,79,137	0
6	MG	B	706	1/1	0.74	0.12	-2.50	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SF4	F	1003	8/8	0.97	0.11	-2.73	52,56,60,66	0
3	SF4	A	701	8/8	0.94	0.10	-2.85	46,56,87,133	0
5	W	C	706	1/1	0.99	0.16	-	44,44,44,44	0
5	W	A	704	1/1	0.99	0.20	-	51,51,51,51	0
7	UNL	A	706	1/-	0.89	0.54	-	55,55,55,55	0
5	W	D	705	1/1	0.98	0.18	-	43,43,43,43	0
7	UNL	B	705	1/-	0.97	0.43	-	95,95,95,95	0
5	W	B	704	1/1	0.71	0.40	-	286,286,286,286	0
7	UNL	C	705	1/-	0.89	0.65	-	63,63,63,63	0
7	UNL	D	701	1/-	0.97	0.26	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.