



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:35 pm 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

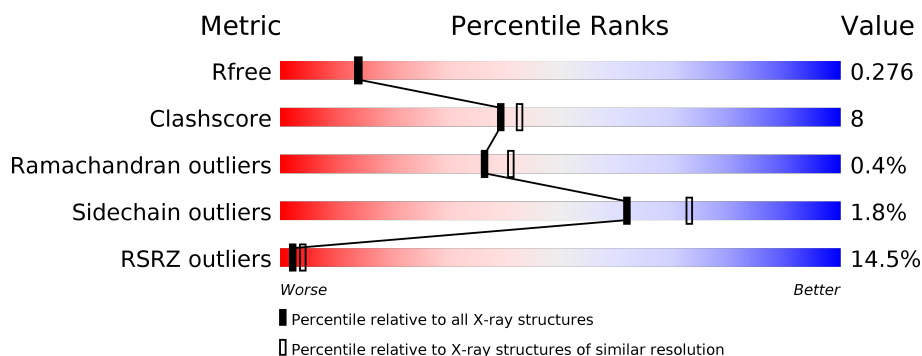
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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))
R_{free}	111664	1015 (2.36-2.36)
Clashscore	122126	1081 (2.36-2.36)
Ramachandran outliers	120053	1066 (2.36-2.36)
Sidechain outliers	120020	1067 (2.36-2.36)
RSRZ outliers	108989	1002 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	653	<div> <div>7%</div> <div>80% 19% .</div> </div>
1	B	653	<div> <div>41%</div> <div>81% 18% .</div> </div>
1	C	653	<div> <div>9%</div> <div>77% 22% .</div> </div>
1	D	653	<div> <div>9%</div> <div>78% 21% .</div> </div>
2	E	179	<div> <div>8%</div> <div>78% 12% 9%</div> </div>
2	F	179	<div> <div>10%</div> <div>73% 21% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	179	
2	H	179	

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
5	W	B	704	-	-	-	X
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.

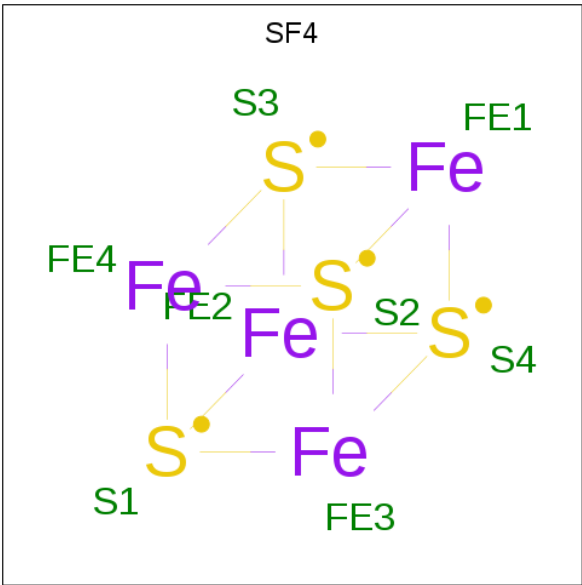
- Molecule 1 is a protein called Benzoyl-CoA reductase, putative.

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: Fe₄S₄).



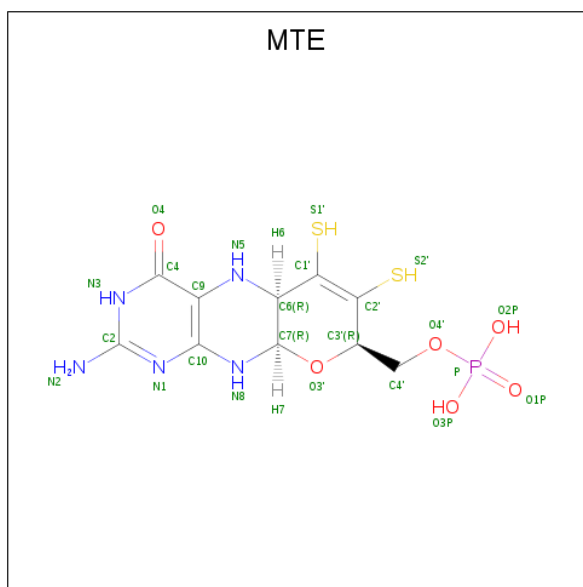
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3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

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

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

- 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

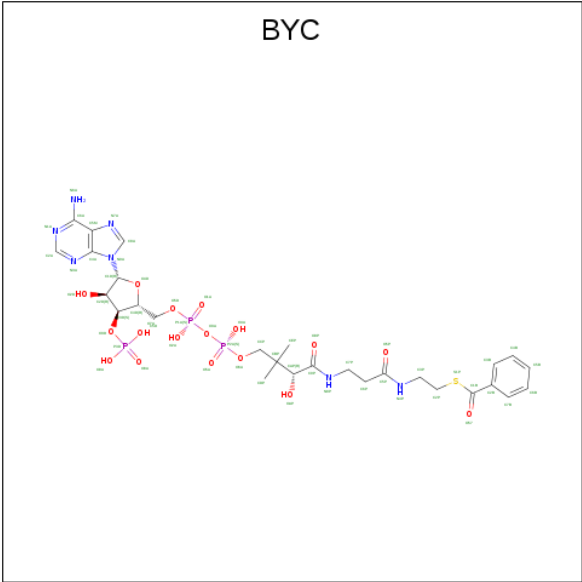
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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: C₂₈H₄₀N₇O₁₇P₃S).



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		

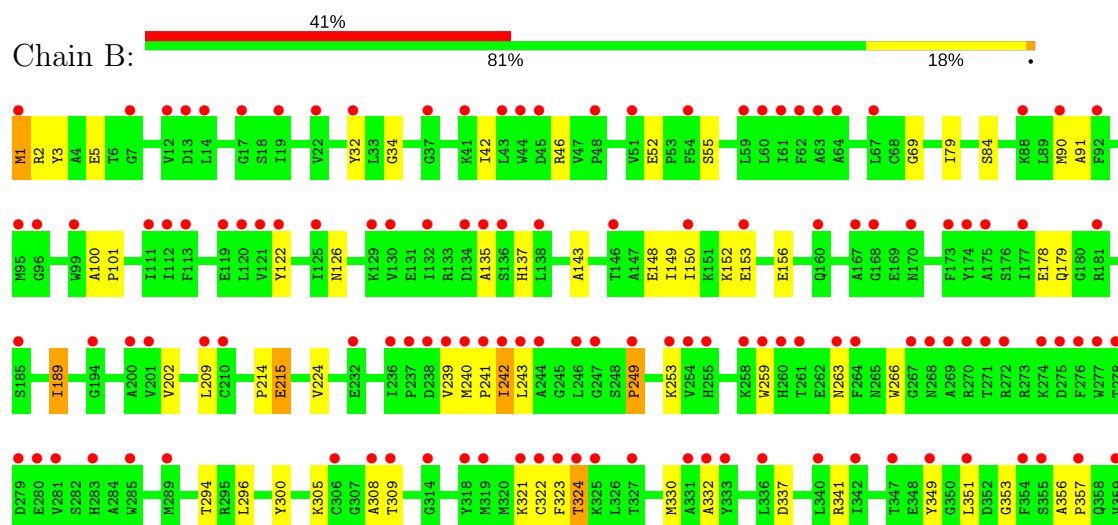
3 Residue-property plots

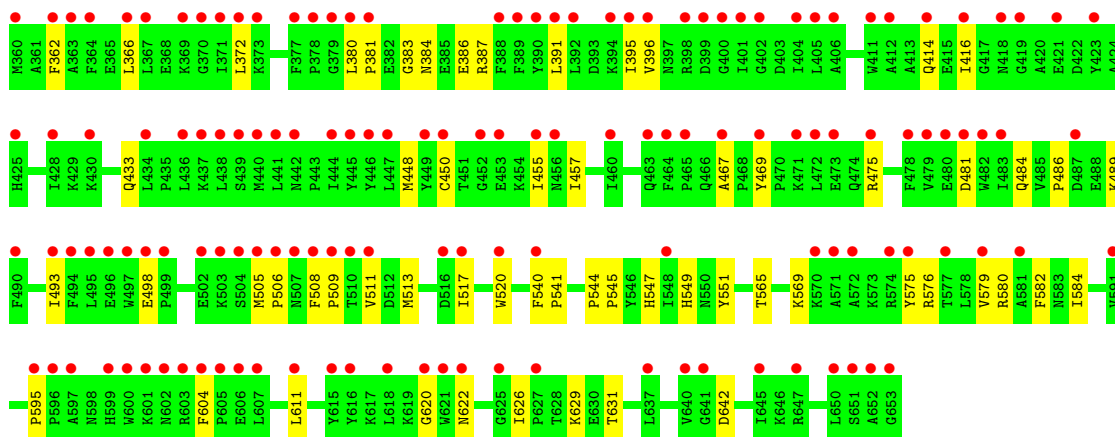
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Benzoyl-CoA reductase, putative

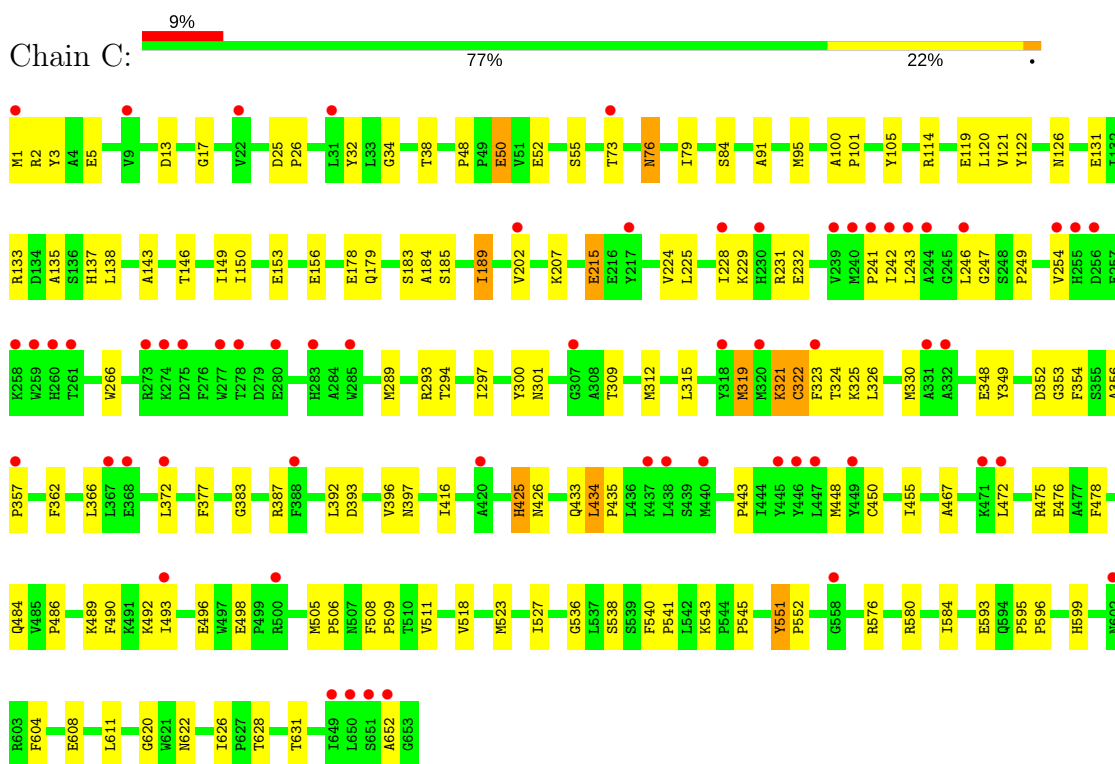


• Molecule 1: Benzoyl-CoA reductase, putative

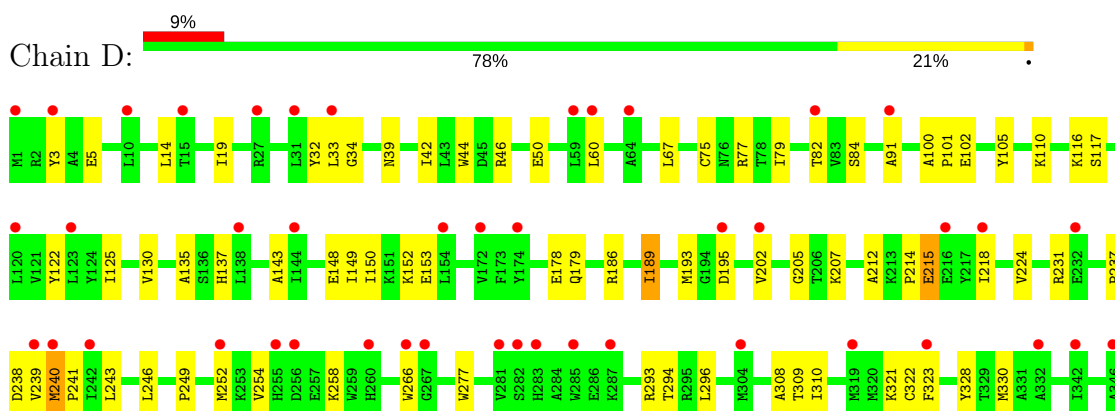


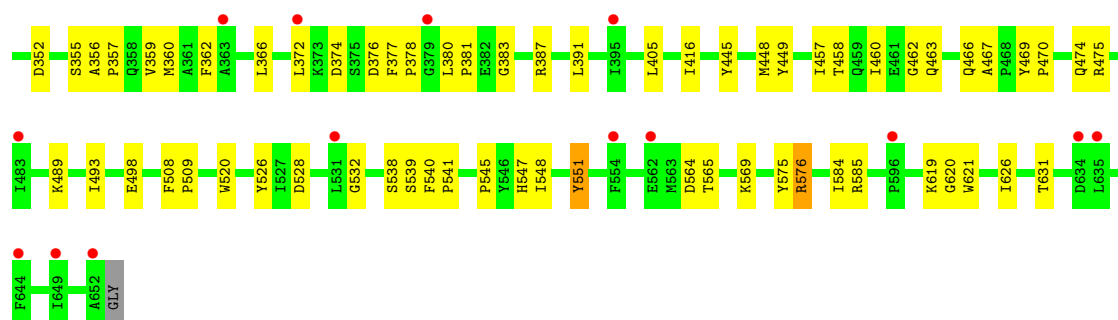


- Molecule 1: Benzoyl-CoA reductase, putative

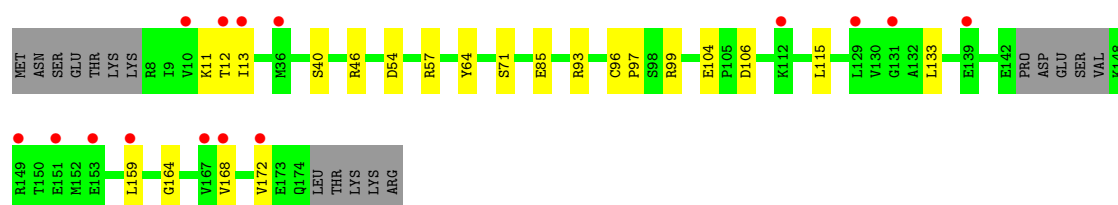
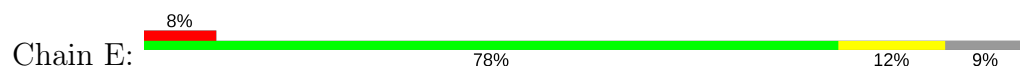


- Molecule 1: Benzoyl-CoA reductase, putative

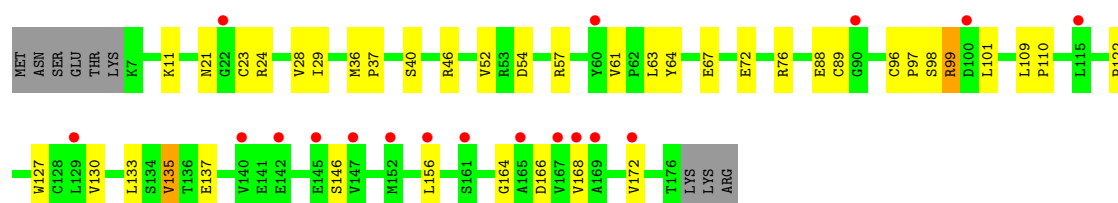
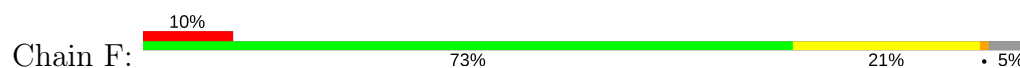




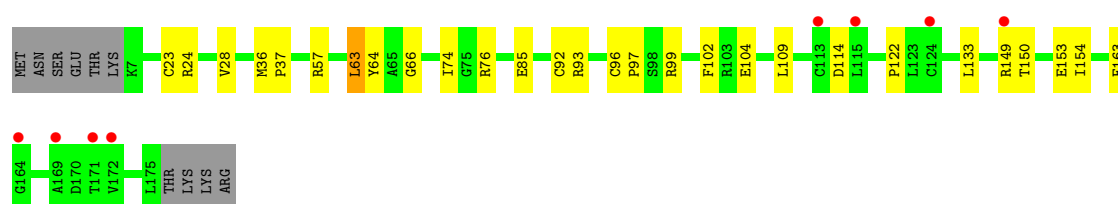
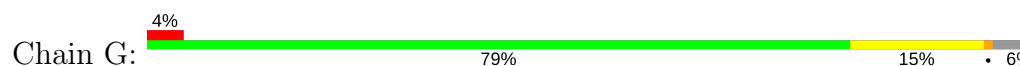
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



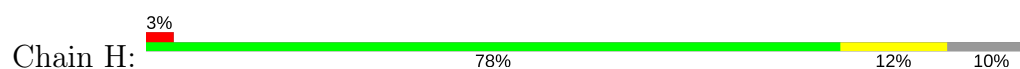
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

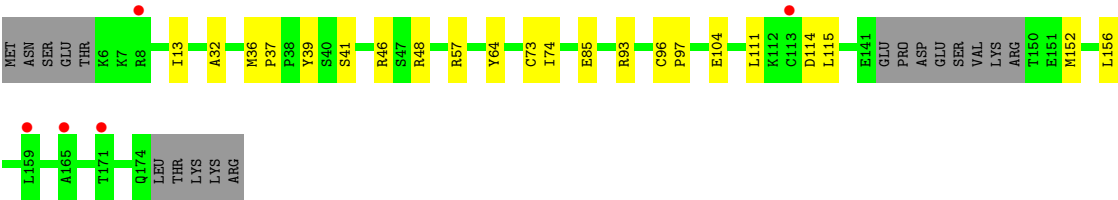


- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.241 , 0.275 0.244 , 0.276	Depositor DCC
R_{free} test set	1980 reflections (1.31%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
1:D:294:THR:HB	1:D:309:THR:OG1	1.96	0.66
2:E:57:ARG:NH1	2:E:85:GLU:O	2.28	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:150:ILE:HG21	1:B:202:VAL:HG21	1.82	0.61
1:B:372:LEU:HD11	1:B:416:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:VAL:HG21	2:F:172:VAL:HG21	1.81	0.61
2:G:163:PHE:CE2	2:H:152:MET:HB3	2.35	0.61
1:B:540:PHE:HB3	1:B:541:PRO:HD3	1.83	0.61
1:D:238:ASP:OD2	1:D:474:GLN:NE2	2.33	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:B:240:MET:HE2	1:B:241:PRO:HD2	1.83	0.59
1:C:224:VAL:HG13	1:C:545:PRO:HB2	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:B:450:CYS:SG	1:B:595:PRO:HD3	2.43	0.58
1:C:354:PHE:CE2	1:C:434:LEU:HD21	2.38	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:372:LEU:HD11	1:C:416:ILE:HD13	1.85	0.57
1:C:443:PRO:HD2	1:C:505:MET:SD	2.44	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:C:383:GLY:O	1:C:387:ARG:HG3	2.05	0.57
1:D:322:CYS:HB2	4:D:703:MTE:S2'	2.45	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:C:215:GLU:H	1:C:215:GLU:CD	2.07	0.56
1:D:14:LEU:HB3	1:D:117:SER:HB2	1.87	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:A:189:ILE:H	1:A:189:ILE:HD13	1.70	0.56
1:D:448:MET:HB3	1:D:460:ILE:HG21	1.87	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:A:126:ASN:ND2	1:A:156:GLU:OE2	2.39	0.55
1:B:126:ASN:ND2	1:B:156:GLU:OE2	2.39	0.55
1:B:242:ILE:O	1:B:243:LEU:HD23	2.07	0.55
1:D:100:ALA:HB3	1:D:101:PRO:HD3	1.89	0.54
1:D:143:ALA:HB1	1:D:178:GLU:HB2	1.90	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:A:467:ALA:HB2	8:A:707:BYC:HDPB	1.90	0.54
1:B:351:LEU:O	4:B:703:MTE:N2	2.26	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:B:224:VAL:HG13	1:B:545:PRO:HB2	1.90	0.53
1:B:622:ASN:N	1:B:626:ILE:O	2.40	0.53
1:C:580:ARG:HH22	1:C:593:GLU:CD	2.12	0.53
1:C:312:MET:HB2	1:C:315:LEU:HD12	1.91	0.53
1:A:332:ALA:O	1:A:384:ASN:ND2	2.42	0.53
1:C:580:ARG:O	1:C:584:ILE:HG12	2.09	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:A:224:VAL:HG13	1:A:545:PRO:HB2	1.90	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:137:HIS:NE2	1:A:153:GLU:OE2	2.39	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:B:84:SER:HB2	1:B:91:ALA:HB2	1.92	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: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:A:337:ASP:O	1:A:341:ARG:HG3	2.10	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:C:1:MET:SD	1:C:2:ARG:N	2.82	0.51
1:D:548:ILE:HG13	1:D:565:THR:HG23	1.91	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:240:MET:CE	1:B:241:PRO:HD2	2.40	0.51
1:B:322:CYS:CB	4:B:702:MTE:S2'	2.98	0.51
2:E:46:ARG:NH2	2:E:104:GLU:OE1	2.43	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:604:PHE:O	1:C:608:GLU:HG3	2.11	0.51
1:C:372:LEU:HD23	1:C:377:PHE:CZ	2.45	0.51
1:D:116:LYS:HE2	1:D:195:ASP:OD2	2.11	0.51
1:D:362:PHE:CZ	1:D:366:LEU:HD11	2.46	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:B:383:GLY:O	1:B:387:ARG:HG3	2.11	0.50
1:C:628:THR:OG1	1:C:631:THR:HG23	2.10	0.50
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.92	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: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: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
1:D:366:LEU:HB3	1:D:372:LEU:HD13	1.92	0.50
8:B:707:BYC:HDPA	8:B:707:BYC:N8P	2.27	0.50
1:A:489:LYS:O	1:A:493:ILE:HG13	2.11	0.50
1:A:52:GLU:O	1:A:55:SER:HB3	2.11	0.50
2:G:64:TYR:OH	2:G:133:LEU:HD13	2.12	0.50
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
1:C:323:PHE:CD1	8:C:707:BYC:H4B	2.47	0.49
2:E:71:SER:HB2	2:F:146:SER:HB3	1.93	0.49
1:A:622:ASN:N	1:A:626:ILE:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:64:TYR:O	2:G:93:ARG:HD2	2.12	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
1:A:90:MET:HB2	1:A:582:PHE:CD2	2.47	0.49
8:D:707:BYC:HDPA	8:D:707:BYC:N8P	2.28	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
1:D:79:ILE:N	1:D:79:ILE:HD12	2.28	0.48
2:G:76:ARG:O	2:H:13:ILE:N	2.39	0.48
1:A:323:PHE:CG	8:A:707:BYC:H4B	2.48	0.48
1:A:214:PRO:HG3	2:E:40:SER:HA	1.95	0.48
8:A:707:BYC:HDPA	8:A:707:BYC:HN8P	1.78	0.48
1:C:505:MET:O	8:C:707:BYC:N6A	2.47	0.48
2:F:168:VAL:O	2:F:172:VAL:HG23	2.13	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:A:565:THR:CG2	1:A:569:LYS:HE3	2.44	0.47
1:D:445:TYR:OH	1:D:466:GLN:HG2	2.13	0.47
2:E:164:GLY:O	2:E:168:VAL:HG23	2.14	0.47
2:H:32:ALA:HA	2:H:41:SER:O	2.14	0.47
1:C:105:TYR:O	1:C:207:LYS:HB2	2.15	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: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:B:79:ILE:N	1:B:79:ILE:HD12	2.29	0.47
1:C:138:LEU:HD13	1:C:146:THR:HG23	1.97	0.47
1:C:3:TYR:O	1:C:5:GLU:N	2.45	0.47
1:C:508:PHE:CG	1:C:509:PRO:HA	2.50	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:C:486:PRO:HD2	1:C:490:PHE:CE2	2.51	0.46
1:D:44:TRP:O	1:D:585:ARG:NH2	2.34	0.46
1:A:575:TYR:O	1:A:579:VAL:HG23	2.16	0.46
1:B:189:ILE:HD13	1:B:189:ILE:N	2.30	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:D:122:TYR:HD2	1:D:135:ALA:HB2	1.81	0.46
1:D:445:TYR:HA	1:D:448:MET:HE2	1.97	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:189:ILE:HD13	1:D:189:ILE:N	2.29	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
1:D:102:GLU:OE1	1:D:205:GLY:N	2.30	0.46
8:D:707:BYC:HN8P	8:D:707:BYC:HDPA	1.78	0.46
1:A:322:CYS:SG	1:A:323:PHE:N	2.89	0.46
1:C:249:PRO:CG	8:C:707:BYC:H6B	2.46	0.46
1:C:326:LEU:O	1:C:330:MET:HG3	2.15	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:575:TYR:O	1:B:579:VAL:HG23	2.16	0.46
1:B:508:PHE:CG	1:B:509:PRO:HA	2.50	0.46
1:C:478:PHE:CE1	1:C:543:LYS:HE3	2.51	0.46
1:D:212:ALA:O	1:D:214:PRO:HD3	2.15	0.46
1:C:150:ILE:HG21	1:C:202:VAL:HG21	1.97	0.46
1:D:489:LYS:O	1:D:493:ILE:HG13	2.15	0.46
1:D:584:ILE:HD12	1:D:626:ILE:HG12	1.98	0.46
2:G:23:CYS:O	2:G:24:ARG:HB2	2.16	0.46
1:A:32:TYR:O	1:A:34:GLY:N	2.49	0.46
1:A:481:ASP:OD1	1:A:481:ASP:N	2.48	0.46
1:B:214:PRO:HG3	2:F:40:SER:HA	1.98	0.46
1:C:372:LEU:HD23	1:C:377:PHE:HZ	1.81	0.46
1:C:79:ILE:N	1:C:79:ILE:HD12	2.30	0.46
1:D:391:LEU:HD11	1:D:405:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:475:ARG:NH2	1:C:498:GLU:HG2	2.31	0.45
1:D:293:ARG:HD2	1:D:296:LEU:CD2	2.45	0.45
1:C:450:CYS:SG	1:C:595:PRO:HD3	2.57	0.45
1:D:458:THR:HB	7:D:701:UNL:X	2.46	0.45
2:E:13:ILE:N	2:F:76:ARG:O	2.40	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:A:486:PRO:HD3	1:A:520:TRP:CE2	2.52	0.45
1:B:149:ILE:O	1:B:153:GLU:HG3	2.17	0.45
1:A:148:GLU:O	1:A:152:LYS:HG3	2.16	0.45
1:B:32:TYR:O	1:B:34:GLY:N	2.49	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:D:576:ARG:HD3	1:D:576:ARG:O	2.15	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
2:G:93:ARG:NH1	2:H:73:CYS:SG	2.90	0.45
1:A:506:PRO:HG3	1:A:604:PHE:CE1	2.51	0.45
1:A:149:ILE:O	1:A:153:GLU:HG3	2.17	0.45
1:D:237:PRO:O	1:D:239:VAL:HG23	2.17	0.45
1:B:383:GLY:HA3	1:B:386:GLU:OE1	2.17	0.45
1:C:506:PRO:HG3	1:C:604:PHE:CE1	2.51	0.45
1:C:508:PHE:HA	1:C:509:PRO:C	2.37	0.45
2:F:11:LYS:HG2	2:F:137:GLU:HG2	1.99	0.45
2:F:88:GLU:O	2:F:89:CYS:HB2	2.17	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:A:629:LYS:NZ	1:A:642:ASP:OD1	2.50	0.44
1:C:137:HIS:NE2	1:C:153:GLU:OE2	2.48	0.44
1:C:300:TYR:OH	2:G:28:VAL:HG22	2.17	0.44
1:D:125:ILE:HG23	1:D:130:VAL:HG22	1.98	0.44
1:B:481:ASP:N	1:B:481:ASP:OD1	2.48	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:A:383:GLY:HA3	1:A:386:GLU:OE1	2.17	0.44
1:C:538:SER:O	1:C:541:PRO:HD2	2.17	0.44
1:B:629:LYS:NZ	1:B:642:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:ARG:HD3	1:D:576:ARG:C	2.38	0.44
1:A:215:GLU:H	1:A:215:GLU:CD	2.21	0.44
1:A:3:TYR:O	1:A:5:GLU:N	2.49	0.44
1:B:580:ARG:O	1:B:584:ILE:HG12	2.17	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:580:ARG:O	1:A:584:ILE:HG12	2.17	0.44
1:A:69:GLY:HA3	1:A:209:LEU:HD22	2.00	0.44
1:B:69:GLY:HA3	1:B:209:LEU:HD22	2.00	0.44
1:D:475:ARG:NH2	1:D:498:GLU:HG2	2.33	0.44
1:B:215:GLU:CD	1:B:215:GLU:H	2.21	0.44
1:C:486:PRO:HD2	1:C:490:PHE:CD2	2.53	0.44
1:D:238:ASP:HB2	1:D:469:TYR:HE1	1.82	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
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
2:G:63:LEU:HD12	2:G:102:PHE:CE2	2.53	0.43
1:A:448:MET:HE3	1:A:457:ILE:HD11	2.00	0.43
1:D:322:CYS:CB	4:D:703:MTE:S2'	3.03	0.43
2:G:57:ARG:NH1	2:G:85:GLU:O	2.51	0.43
1:A:433:GLN:HE22	1:A:455:ILE:HG22	1.83	0.43
1:A:458:THR:HB	7:A:706:UNL:X	2.48	0.43
1:B:249:PRO:HG2	7:B:705:UNL:X	2.47	0.43
1:D:328:TYR:CE1	1:D:357:PRO:HG3	2.53	0.43
1:B:469:TYR:HB2	1:B:475:ARG:HG2	2.01	0.43
1:D:463:GLN:HB3	1:D:520:TRP:CH2	2.53	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
2:E:12:THR:OG1	2:F:88:GLU:OE2	2.34	0.43
1:A:131:GLU:OE2	1:A:133:ARG:NE	2.39	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
2:H:57:ARG:NH1	2:H:85:GLU:O	2.49	0.43
1:A:253:LYS:HG2	1:A:296:LEU:HD13	2.00	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
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
1:B:294:THR:HB	1:B:309:THR:OG1	2.19	0.42
2:F:109:LEU:HA	2:F:110:PRO:HD3	1.84	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: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:B:505:MET:O	8:B:707:BYC:N6A	2.53	0.42
1:C:48:PRO:HB2	1:C:50:GLU:OE1	2.19	0.42
1:D:105:TYR:O	1:D:207:LYS:HB2	2.18	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
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
2:E:11:LYS:HD3	2:E:115:LEU:CD1	2.50	0.42
1:A:391:LEU:O	1:A:395:ILE:HG13	2.20	0.42
1:C:289:MET:HG3	1:C:293:ARG:NH1	2.35	0.42
1:C:76:ASN:ND2	1:C:300:TYR:O	2.52	0.42
1:B:324:THR:CG2	1:B:353:GLY:HA3	2.49	0.41
1:B:3:TYR:O	1:B:5:GLU:N	2.50	0.41
1:B:42:ILE:O	1:B:46:ARG:HB2	2.20	0.41
2:G:150:THR:O	2:G:154:ILE:HG13	2.20	0.41
1:C:119:GLU:O	1:C:121:VAL:HG13	2.20	0.41
1:C:149:ILE:O	1:C:153:GLU:HG3	2.20	0.41
1:C:73:THR:HG23	1:C:301:ASN:O	2.20	0.41
1:D:215:GLU:CD	1:D:215:GLU:H	2.22	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:A:259:TRP:O	1:A:263:ASN:HB2	2.20	0.41
1:D:328:TYR:CD1	1:D:357:PRO:HG3	2.54	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)
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:E:64:TYR:OH	2:E:133:LEU:HD13	2.19	0.41
1:A:42:ILE:HG23	1:A:46:ARG:HD3	2.03	0.41
2:H:13:ILE:HD11	2:H:115:LEU:HD21	2.03	0.41
2:H:64:TYR:O	2:H:93:ARG:HD2	2.20	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: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:B:513:MET:O	1:B:517:ILE:HG13	2.20	0.41
1:C:349:TYR:CG	1:C:396:VAL:HG11	2.55	0.41
2:F:21:ASN:ND2	2:F:130:VAL:HG11	2.36	0.41
2:G:163:PHE:CD2	2:H:152:MET:HB3	2.56	0.41
1:B:366:LEU:HB3	1:B:372:LEU:HD13	2.03	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:H:152:MET:O	2:H:156:LEU:HG	2.20	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:60:LEU:HD22	1:D:193:MET:HA	2.03	0.40
1:D:322:CYS:SG	1:D:323:PHE:N	2.94	0.40
1:A:576:ARG:O	1:A:576:ARG:HD3	2.22	0.40
1:B:42:ILE:HG23	1:B:46:ARG:HD3	2.03	0.40
1:C:143:ALA:CB	1:C:178:GLU:HB2	2.52	0.40
1:C:225:LEU:O	1:C:229:LYS:HG3	2.21	0.40
1:C:472:LEU:O	1:C:476:GLU: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
2:G:63:LEU:HD12	2:G:102:PHE:CZ	2.56	0.40
2:H:46:ARG:NH1	2:H:104:GLU:OE1	2.53	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:469:TYR:HA	1:D:470:PRO:HD3	1.93	0.40
1:A:135:ALA:HB1	1:A:138:LEU:HD12	2.03	0.40
1:A:366:LEU:HB3	1:A:372:LEU:HD13	2.03	0.40
1:D:239:VAL:CG1	1:D:243:LEU:CB	2.99	0.40
1:A:218:ILE:HD12	1:A:218:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ASP:HA	1:C:26:PRO:HD2	1.92	0.40
1:C:185:SER:O	1:C:352:ASP:HB2	2.21	0.40
1:D:231:ARG:HG2	1:D:246:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	651/653 (100%)	624 (96%)	24 (4%)	3 (0%)	31	34
1	B	651/653 (100%)	624 (96%)	24 (4%)	3 (0%)	31	34
1	C	651/653 (100%)	623 (96%)	24 (4%)	4 (1%)	27	30
1	D	650/653 (100%)	626 (96%)	22 (3%)	2 (0%)	43	50
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%)	36	41

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 ⓘ

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%)	65	77
1	B	548/548 (100%)	539 (98%)	9 (2%)	65	77
1	C	548/548 (100%)	533 (97%)	15 (3%)	48	58
1	D	546/548 (100%)	536 (98%)	10 (2%)	62	73
2	E	133/159 (84%)	132 (99%)	1 (1%)	83	90
2	F	148/159 (93%)	144 (97%)	4 (3%)	48	58
2	G	147/159 (92%)	145 (99%)	2 (1%)	69	80
2	H	132/159 (83%)	132 (100%)	0	100	100
All	All	2749/2828 (97%)	2699 (98%)	50 (2%)	62	73

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	2.98	10 (47%)	19,40,40	2.19	4 (21%)
4	MTE	A	703	5,6	21,26,26	3.02	9 (42%)	19,40,40	2.19	3 (15%)
8	BYC	A	707	-	51,59,59	0.47	0	64,87,87	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	2.97	10 (47%)	19,40,40	2.06	4 (21%)
4	MTE	B	703	5,6	21,26,26	2.89	9 (42%)	19,40,40	2.09	3 (15%)
8	BYC	B	707	-	51,59,59	0.48	0	64,87,87	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	2.93	10 (47%)	19,40,40	2.21	4 (21%)
4	MTE	C	703	5,6	21,26,26	2.95	9 (42%)	19,40,40	2.20	5 (26%)
8	BYC	C	707	-	51,59,59	0.48	0	64,87,87	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	2.96	9 (42%)	19,40,40	2.38	5 (26%)
4	MTE	D	704	5,6	21,26,26	3.01	9 (42%)	19,40,40	2.23	4 (21%)
8	BYC	D	707	-	51,59,59	0.45	0	64,87,87	0.61	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	-	-	1/51/71/71	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	-	-	1/51/71/71	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	-	-	1/51/71/71	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	-	-	1/51/71/71	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 (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	MTE	C9-C10	-6.50	1.29	1.41
4	A	703	MTE	C9-C10	-6.37	1.29	1.41
4	D	704	MTE	C9-C10	-6.36	1.29	1.41
4	D	703	MTE	C9-C10	-6.35	1.29	1.41
4	B	702	MTE	C9-C10	-6.33	1.29	1.41
4	C	702	MTE	C9-C10	-6.32	1.29	1.41
4	C	703	MTE	C9-C10	-6.22	1.29	1.41
4	A	702	MTE	C9-C10	-6.22	1.29	1.41
4	D	704	MTE	C7-C6	-6.14	1.49	1.53
4	A	703	MTE	C7-C6	-5.99	1.49	1.53
4	D	703	MTE	C7-C6	-5.88	1.49	1.53
4	A	702	MTE	C7-C6	-5.59	1.49	1.53
4	C	702	MTE	C7-C6	-5.50	1.49	1.53
4	C	703	MTE	C7-C6	-5.42	1.49	1.53
4	B	702	MTE	C7-C6	-4.88	1.50	1.53
4	B	703	MTE	C7-C6	-4.18	1.50	1.53
4	B	702	MTE	O3'-C7	-3.94	1.38	1.43
4	C	703	MTE	O3'-C7	-3.91	1.38	1.43
4	A	702	MTE	O3'-C7	-3.82	1.38	1.43
4	D	703	MTE	O3'-C7	-3.81	1.38	1.43
4	A	703	MTE	O3'-C7	-3.80	1.38	1.43
4	B	703	MTE	O3'-C7	-3.79	1.38	1.43
4	D	704	MTE	O3'-C7	-3.77	1.38	1.43
4	C	702	MTE	O3'-C7	-3.75	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	MTE	O3'-C3'	-3.33	1.39	1.43
4	C	702	MTE	O3'-C3'	-3.33	1.39	1.43
4	B	702	MTE	O3'-C3'	-3.32	1.39	1.43
4	A	702	MTE	O3'-C3'	-3.27	1.39	1.43
4	C	703	MTE	O3'-C3'	-3.26	1.39	1.43
4	D	703	MTE	O3'-C3'	-3.06	1.39	1.43
4	A	703	MTE	O3'-C3'	-2.88	1.39	1.43
4	D	704	MTE	O3'-C3'	-2.60	1.40	1.43
4	A	702	MTE	C9-N5	2.03	1.42	1.38
4	C	702	MTE	C9-N5	2.04	1.42	1.38
4	B	702	MTE	C9-N5	2.13	1.42	1.38
4	A	702	MTE	C2-N3	2.47	1.39	1.35
4	C	702	MTE	C2-N3	2.47	1.39	1.35
4	D	703	MTE	C2-N3	2.47	1.39	1.35
4	B	702	MTE	C2-N3	2.52	1.39	1.35
4	A	703	MTE	C2-N3	2.54	1.39	1.35
4	B	703	MTE	C2-N3	2.59	1.40	1.35
4	C	703	MTE	C2-N3	2.65	1.40	1.35
4	D	704	MTE	C2-N3	2.70	1.40	1.35
4	B	703	MTE	C4-N3	2.92	1.38	1.33
4	C	702	MTE	C10-N1	2.92	1.39	1.34
4	B	703	MTE	C10-N1	3.02	1.39	1.34
4	A	702	MTE	C10-N1	3.05	1.39	1.34
4	C	703	MTE	C10-N1	3.05	1.39	1.34
4	D	703	MTE	C4-N3	3.05	1.38	1.33
4	A	703	MTE	C4-N3	3.07	1.38	1.33
4	C	703	MTE	C4-N3	3.07	1.38	1.33
4	B	702	MTE	C4-N3	3.11	1.38	1.33
4	C	702	MTE	C4-N3	3.16	1.38	1.33
4	A	703	MTE	C10-N1	3.16	1.39	1.34
4	D	704	MTE	C10-N1	3.16	1.39	1.34
4	B	702	MTE	C10-N1	3.19	1.39	1.34
4	A	702	MTE	C4-N3	3.20	1.38	1.33
4	D	704	MTE	C4-N3	3.22	1.38	1.33
4	D	703	MTE	C10-N1	3.23	1.40	1.34
4	C	702	MTE	C2-N2	4.56	1.43	1.33
4	B	703	MTE	C2-N2	4.65	1.43	1.33
4	D	704	MTE	C2-N2	4.69	1.43	1.33
4	A	703	MTE	C2-N2	4.69	1.43	1.33
4	A	702	MTE	C2-N2	4.69	1.43	1.33
4	B	702	MTE	C2-N2	4.70	1.43	1.33
4	D	703	MTE	C2-N2	4.73	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	MTE	C2-N2	4.74	1.43	1.33
4	D	703	MTE	C4-C9	5.08	1.47	1.41
4	C	702	MTE	C4-C9	5.31	1.47	1.41
4	C	703	MTE	C4-C9	5.39	1.47	1.41
4	B	703	MTE	C4-C9	5.40	1.47	1.41
4	D	704	MTE	C4-C9	5.57	1.48	1.41
4	A	702	MTE	C4-C9	5.65	1.48	1.41
4	B	702	MTE	C4-C9	5.71	1.48	1.41
4	A	703	MTE	C4-C9	5.82	1.48	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	MTE	O3'-C7-C6	-5.34	105.40	108.96
4	C	702	MTE	O3'-C7-C6	-4.45	106.00	108.96
4	A	702	MTE	O3'-C7-C6	-3.97	106.31	108.96
4	C	703	MTE	O3'-C7-C6	-3.75	106.46	108.96
4	D	704	MTE	O3'-C7-C6	-3.66	106.52	108.96
4	B	702	MTE	O3'-C7-C6	-2.78	107.11	108.96
4	A	703	MTE	O3'-C7-C6	-2.69	107.17	108.96
4	C	703	MTE	C10-N8-C7	-2.10	119.56	123.67
4	D	703	MTE	N3-C2-N1	-2.01	122.23	125.43
4	B	702	MTE	C9-C10-N8	2.01	119.97	118.13
4	D	703	MTE	C9-C10-N8	2.01	119.97	118.13
4	D	704	MTE	N8-C10-N1	2.03	120.83	116.90
4	C	702	MTE	C9-C10-N8	2.08	120.04	118.13
8	A	707	BYC	C2P-S1P-C1B	2.09	102.42	99.80
4	C	703	MTE	C9-C10-N8	2.16	120.11	118.13
8	B	707	BYC	C2P-S1P-C1B	2.24	102.61	99.80
8	D	707	BYC	C2P-S1P-C1B	2.32	102.71	99.80
4	A	702	MTE	C9-C10-N8	2.40	120.33	118.13
4	B	703	MTE	C9-C10-N8	2.59	120.50	118.13
4	C	702	MTE	C2-N1-C10	2.71	120.58	114.50
4	C	703	MTE	C2-N1-C10	2.73	120.62	114.50
4	D	704	MTE	C2-N1-C10	2.74	120.65	114.50
4	A	702	MTE	C2-N1-C10	2.75	120.67	114.50
4	B	703	MTE	C2-N1-C10	2.83	120.84	114.50
4	D	703	MTE	C2-N1-C10	2.84	120.87	114.50
4	B	702	MTE	C2-N1-C10	2.84	120.88	114.50
4	A	703	MTE	C2-N1-C10	2.87	120.95	114.50
4	A	702	MTE	C4-C9-C10	6.46	120.41	114.56
4	C	702	MTE	C4-C9-C10	6.53	120.47	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	MTE	C4-C9-C10	6.55	120.49	114.56
4	C	703	MTE	C4-C9-C10	6.78	120.70	114.56
4	D	703	MTE	C4-C9-C10	6.82	120.73	114.56
4	D	704	MTE	C4-C9-C10	7.09	120.98	114.56
4	A	703	MTE	C4-C9-C10	7.11	121.00	114.56
4	B	703	MTE	C4-C9-C10	7.33	121.19	114.56

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	653/653 (100%)	0.90	45 (6%) 17 25	42, 63, 96, 145	0
1	B	653/653 (100%)	2.12	267 (40%) 0 0	46, 116, 167, 195	0
1	C	653/653 (100%)	0.89	60 (9%) 9 14	37, 61, 111, 157	0
1	D	652/653 (99%)	0.82	58 (8%) 9 15	42, 65, 93, 132	0
2	E	162/179 (90%)	0.81	15 (9%) 8 14	38, 59, 95, 127	0
2	F	170/179 (94%)	0.91	18 (10%) 6 10	39, 58, 86, 110	0
2	G	169/179 (94%)	0.76	8 (4%) 31 44	40, 57, 132, 146	0
2	H	161/179 (89%)	0.56	5 (3%) 49 61	44, 63, 125, 149	0
All	All	3273/3328 (98%)	1.10	476 (14%) 2 4	37, 66, 135, 195	0

All (476) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	LEU	13.0
1	B	259	TRP	11.5
1	B	440	MET	11.0
1	C	602	ASN	9.9
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	B	366	LEU	8.8
1	C	259	TRP	8.7
1	A	242	ILE	8.7
1	B	405	LEU	8.6
1	B	434	LEU	8.5
1	B	173	PHE	8.1
1	B	418	ASN	8.0
1	B	641	GLY	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	404	ILE	7.8
1	B	607	LEU	7.7
1	B	369	LYS	7.6
1	B	274	LYS	7.3
1	B	392	LEU	7.3
1	B	323	PHE	7.1
1	B	241	PRO	7.0
1	B	260	HIS	7.0
1	C	243	LEU	6.9
1	B	285	TRP	6.7
1	B	601	LYS	6.7
1	B	439	SER	6.5
1	B	455	ILE	6.5
1	B	625	GLY	6.4
1	B	506	PRO	6.4
1	B	354	PHE	6.3
1	C	274	LYS	6.3
1	B	611	LEU	6.2
1	B	355	SER	6.2
1	B	277	TRP	6.2
1	B	597	ALA	6.2
1	C	241	PRO	6.2
1	C	277	TRP	6.2
1	B	247	GLY	6.1
1	B	258	LYS	6.0
1	B	54	PHE	6.0
1	A	644	PHE	5.9
1	B	600	TRP	5.8
1	B	62	PHE	5.7
1	C	242	ILE	5.7
1	B	577	THR	5.7
1	B	579	VAL	5.7
1	B	377	PHE	5.6
1	B	236	ILE	5.6
1	B	511	VAL	5.5
1	B	240	MET	5.5
1	B	136	SER	5.5
1	B	595	PRO	5.5
1	B	421	GLU	5.5
1	B	120	LEU	5.5
1	B	1	MET	5.4
1	B	239	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	599	HIS	5.4
1	B	446	TYR	5.4
1	B	132	ILE	5.3
1	B	396	VAL	5.3
1	B	509	PRO	5.3
1	B	604	PHE	5.2
1	B	414	GLN	5.2
1	B	618	LEU	5.2
1	C	255	HIS	5.2
1	B	254	VAL	5.2
1	B	379	GLY	5.2
1	B	508	PHE	5.2
1	C	260	HIS	5.1
1	B	438	LEU	5.0
1	B	465	PRO	4.9
2	G	164	GLY	4.9
1	C	280	GLU	4.9
1	C	239	VAL	4.9
1	B	14	LEU	4.9
1	B	174	TYR	4.9
1	B	402	GLY	4.8
1	B	505	MET	4.8
1	B	43	LEU	4.8
1	B	575	TYR	4.8
1	B	498	GLU	4.7
1	B	138	LEU	4.6
1	B	41	LYS	4.6
1	B	61	ILE	4.6
1	B	581	ALA	4.6
1	B	650	LEU	4.6
1	B	167	ALA	4.5
1	B	423	TYR	4.5
2	E	131	GLY	4.5
1	B	388	PHE	4.4
1	B	279	ASP	4.3
2	F	167	VAL	4.3
1	B	255	HIS	4.3
1	C	652	ALA	4.3
1	B	12	VAL	4.3
1	B	359	VAL	4.3
1	B	351	LEU	4.2
2	F	100	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	438	LEU	4.2
1	B	401	ILE	4.2
1	B	428	ILE	4.2
1	B	419	GLY	4.2
1	B	412	ALA	4.1
1	D	323	PHE	4.1
1	B	200	ALA	4.1
1	A	380	LEU	4.1
1	B	362	PHE	4.0
1	B	90	MET	4.0
1	B	490	PHE	4.0
1	B	482	TRP	4.0
1	A	256	ASP	4.0
1	B	276	PHE	4.0
1	B	447	LEU	3.9
1	B	450	CYS	3.9
1	B	602	ASN	3.9
1	B	281	VAL	3.8
1	B	289	MET	3.8
1	A	260	HIS	3.8
1	B	111	ILE	3.8
1	B	37	GLY	3.8
1	C	500	ARG	3.8
1	A	323	PHE	3.7
1	B	269	ALA	3.7
1	B	170	ASN	3.7
1	B	390	TYR	3.7
1	D	33	LEU	3.7
1	B	17	GLY	3.7
1	B	507	ASN	3.7
1	B	122	TYR	3.7
1	B	497	TRP	3.7
1	B	63	ALA	3.7
1	D	283	HIS	3.7
1	B	389	PHE	3.7
1	B	378	PRO	3.6
1	B	464	PHE	3.6
1	B	653	GLY	3.6
1	B	372	LEU	3.6
1	B	441	LEU	3.6
2	G	172	VAL	3.6
1	D	260	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	271	THR	3.6
1	A	27	ARG	3.6
1	B	606	GLU	3.6
1	B	596	PRO	3.6
1	D	281	VAL	3.6
1	B	364	PHE	3.5
2	E	129	LEU	3.5
1	B	520	TRP	3.5
1	B	283	HIS	3.5
1	C	273	ARG	3.5
1	C	285	TRP	3.5
1	B	483	ILE	3.5
1	B	333	TYR	3.5
1	D	634	ASP	3.5
1	B	360	MET	3.4
1	B	242	ILE	3.4
1	C	447	LEU	3.4
1	A	241	PRO	3.4
1	C	31	LEU	3.4
1	B	591	VAL	3.4
1	B	32	TYR	3.4
1	B	572	ALA	3.4
2	E	153	GLU	3.4
1	D	267	GLY	3.3
1	B	615	TYR	3.3
2	F	129	LEU	3.3
1	B	135	ALA	3.3
1	B	496	GLU	3.3
1	D	31	LEU	3.3
1	B	249	PRO	3.3
1	A	240	MET	3.3
2	H	159	LEU	3.3
2	F	168	VAL	3.3
2	F	142	GLU	3.3
1	B	325	LYS	3.2
2	H	8	ARG	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	C	22	VAL	3.2
1	A	279	ASP	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	499	PRO	3.2
1	B	321	LYS	3.2
1	B	278	THR	3.1
1	D	239	VAL	3.1
1	C	275	ASP	3.1
1	B	651	SER	3.1
1	B	371	ILE	3.1
1	B	472	LEU	3.1
1	B	280	GLU	3.1
1	B	548	ILE	3.1
1	D	649	ILE	3.1
1	B	603	ARG	3.1
2	F	115	LEU	3.1
1	B	456	ASN	3.1
1	B	60	LEU	3.1
1	C	440	MET	3.1
1	C	437	LYS	3.1
1	B	616	TYR	3.0
1	B	253	LYS	3.0
1	A	255	HIS	3.0
1	A	1	MET	3.0
1	C	331	ALA	3.0
1	A	653	GLY	3.0
1	B	324	THR	3.0
1	B	444	ILE	3.0
1	A	388	PHE	3.0
1	A	450	CYS	3.0
1	B	160	GLN	3.0
1	B	232	GLU	3.0
1	B	246	LEU	3.0
1	D	635	LEU	3.0
1	D	242	ILE	3.0
1	D	266	TRP	3.0
1	B	503	LYS	3.0
1	B	119	GLU	2.9
1	B	22	VAL	2.9
1	D	240	MET	2.9
2	E	159	LEU	2.9
1	B	473	GLU	2.9
1	D	216	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	254	VAL	2.9
1	B	640	VAL	2.9
2	E	167	VAL	2.9
2	E	172	VAL	2.9
2	F	145	GLU	2.9
1	B	181	ARG	2.9
1	B	308	ALA	2.9
1	A	511	VAL	2.9
1	B	51	VAL	2.9
1	B	67	LEU	2.9
1	B	621	TRP	2.9
1	D	256	ASP	2.9
1	B	244	ALA	2.8
1	B	467	ALA	2.8
1	B	314	GLY	2.8
2	F	156	LEU	2.8
1	B	275	ASP	2.8
1	B	113	PHE	2.8
1	B	363	ALA	2.8
2	F	169	ALA	2.8
1	B	112	ILE	2.8
1	B	318	TYR	2.8
1	A	274	LYS	2.8
1	A	557	ALA	2.8
1	D	27	ARG	2.8
1	B	349	TYR	2.8
1	C	283	HIS	2.8
1	A	597	ALA	2.8
2	F	22	GLY	2.8
1	D	363	ALA	2.7
1	B	95	MET	2.7
1	B	380	LEU	2.7
1	C	445	TYR	2.7
1	B	261	THR	2.7
1	B	270	ARG	2.7
1	B	267	GLY	2.7
1	A	368	GLU	2.7
2	G	169	ALA	2.7
1	B	130	VAL	2.7
1	B	398	ARG	2.7
1	B	263	ASN	2.7
1	D	285	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	379	GLY	2.7
1	C	420	ALA	2.7
1	C	446	TYR	2.7
1	D	287	LYS	2.7
1	B	370	GLY	2.7
1	B	605	PRO	2.7
1	A	615	TYR	2.7
1	C	9	VAL	2.7
2	F	140	VAL	2.7
2	H	171	THR	2.7
1	D	319	MET	2.6
1	A	374	ASP	2.6
1	B	622	ASN	2.6
1	B	331	ALA	2.6
1	B	430	LYS	2.6
1	B	445	TYR	2.6
2	G	115	LEU	2.6
1	A	283	HIS	2.6
1	B	150	ILE	2.6
1	B	327	THR	2.6
1	B	469	TYR	2.6
1	B	494	PHE	2.6
2	E	36	MET	2.6
2	E	112	LYS	2.6
1	A	277	TRP	2.6
1	B	504	SER	2.6
1	B	340	LEU	2.6
1	D	120	LEU	2.6
1	D	218	ILE	2.6
2	F	161	SER	2.6
2	F	147	VAL	2.6
1	B	64	ALA	2.6
1	B	88	LYS	2.6
1	C	472	LEU	2.5
1	D	304	MET	2.5
1	B	373	LYS	2.5
1	B	493	ILE	2.5
1	B	48	PRO	2.5
1	D	172	VAL	2.5
1	C	261	THR	2.5
1	B	570	LYS	2.5
1	D	59	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	255	HIS	2.5
2	F	172	VAL	2.5
1	B	460	ILE	2.5
1	D	395	ILE	2.5
2	F	165	ALA	2.5
1	A	378	PRO	2.5
1	D	3	TYR	2.5
1	D	15	THR	2.4
1	B	168	GLY	2.4
1	D	483	ILE	2.4
1	C	244	ALA	2.4
1	D	232	GLU	2.4
1	B	463	GLN	2.4
1	B	502	GLU	2.4
1	B	332	ALA	2.4
1	B	510	THR	2.4
1	B	400	GLY	2.4
1	B	652	ALA	2.4
1	B	201	VAL	2.4
1	C	323	PHE	2.4
1	C	318	TYR	2.4
1	B	7	GLY	2.4
1	B	175	ALA	2.4
2	G	171	THR	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
2	E	13	ILE	2.3
1	B	237	PRO	2.3
1	C	73	THR	2.3
1	C	651	SER	2.3
1	D	202	VAL	2.3
1	B	620	GLY	2.3
1	B	153	GLU	2.3
1	C	1	MET	2.3
1	A	484	GLN	2.3
1	A	649	ILE	2.3
1	B	322	CYS	2.3
1	B	399	ASP	2.3
2	E	168	VAL	2.3
1	B	381	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	441	LEU	2.3
1	B	449	TYR	2.3
1	C	240	MET	2.3
1	B	121	VAL	2.3
1	B	442	ASN	2.3
1	D	562	GLU	2.3
1	B	129	LYS	2.3
2	G	124	CYS	2.3
1	A	641	GLY	2.3
1	C	307	GLY	2.3
1	A	121	VAL	2.3
1	A	266	TRP	2.3
1	B	645	ILE	2.3
1	B	59	LEU	2.2
1	B	96	GLY	2.2
1	C	449	TYR	2.2
2	F	60	TYR	2.2
1	A	373	LYS	2.2
1	B	13	ASP	2.2
1	B	268	ASN	2.2
1	C	471	LYS	2.2
1	B	479	VAL	2.2
1	B	540	PHE	2.2
1	B	99	TRP	2.2
1	B	125	ILE	2.2
1	A	275	ASP	2.2
2	F	152	MET	2.2
1	B	478	PHE	2.2
1	D	282	SER	2.2
1	D	652	ALA	2.2
1	A	438	LEU	2.2
1	B	134	ASP	2.2
1	B	627	PRO	2.2
1	B	92	PHE	2.2
1	C	388	PHE	2.2
1	D	554	PHE	2.2
1	B	44	TRP	2.2
1	B	309	THR	2.2
1	B	395	ILE	2.2
1	D	82	THR	2.2
1	B	425	HIS	2.2
1	B	367	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	246	LEU	2.2
1	C	558	GLY	2.2
1	D	91	ALA	2.2
1	B	436	LEU	2.2
1	B	495	LEU	2.2
1	C	372	LEU	2.2
1	B	185	SER	2.2
1	B	45	ASP	2.2
1	D	644	PHE	2.2
1	B	146	THR	2.2
2	E	12	THR	2.2
2	E	149	ARG	2.2
1	C	228	ILE	2.2
1	A	497	TRP	2.2
1	B	391	LEU	2.2
1	B	453	GLU	2.2
2	F	90	GLY	2.2
1	A	108	TYR	2.1
1	C	230	HIS	2.1
1	B	336	LEU	2.1
1	C	650	LEU	2.1
1	D	372	LEU	2.1
1	B	452	GLY	2.1
1	C	320	MET	2.1
1	A	281	VAL	2.1
1	B	347	THR	2.1
1	B	571	ALA	2.1
1	D	64	ALA	2.1
1	D	346	ALA	2.1
1	B	481	ASP	2.1
1	C	256	ASP	2.1
1	C	367	LEU	2.1
1	C	258	LYS	2.1
1	C	278	THR	2.1
1	C	332	ALA	2.1
1	D	154	LEU	2.1
2	E	139	GLU	2.1
1	B	319	MET	2.1
1	D	1	MET	2.1
1	A	422	ASP	2.1
1	B	177	ILE	2.1
1	B	342	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	649	ILE	2.1
1	D	195	ASP	2.1
2	G	113	CYS	2.1
1	B	471	LYS	2.1
1	C	357	PRO	2.1
1	D	60	LEU	2.1
1	D	531	LEU	2.1
1	B	516	ASP	2.1
1	D	252	MET	2.1
1	A	285	TRP	2.1
1	C	202	VAL	2.1
2	H	113	CYS	2.1
1	B	480	GLU	2.0
1	C	368	GLU	2.0
1	B	272	ARG	2.0
1	C	493	ILE	2.0
2	E	151	GLU	2.0
2	E	10	VAL	2.0
1	A	210	CYS	2.0
1	B	647	ARG	2.0
1	D	174	TYR	2.0
1	B	209	LEU	2.0
1	B	637	LEU	2.0
1	D	123	LEU	2.0
1	A	625	GLY	2.0
1	A	341	ARG	2.0
1	B	238	ASP	2.0
1	B	487	ASP	2.0
1	D	596	PRO	2.0
2	G	149	ARG	2.0
1	B	411	TRP	2.0
1	A	263	ASN	2.0
1	A	446	TYR	2.0
1	B	210	CYS	2.0
1	B	517	ILE	2.0
1	D	10	LEU	2.0
1	D	138	LEU	2.0
1	B	574	ARG	2.0
1	D	332	ALA	2.0
2	H	165	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	BYC	B	707	56/56	0.59	0.36	39,60,78,94	96
8	BYC	C	707	56/56	0.62	0.38	47,64,86,100	96
5	W	B	704	1/1	0.71	0.41	286,286,286,286	0
8	BYC	A	707	56/56	0.73	0.32	40,56,86,89	96
6	MG	B	706	1/1	0.74	0.12	62,62,62,62	0
6	MG	D	706	1/1	0.77	0.13	44,44,44,44	0
8	BYC	D	707	56/56	0.84	0.24	32,56,98,103	96
4	MTE	C	703	24/24	0.85	0.18	41,50,55,60	0
6	MG	C	704	1/1	0.86	0.22	47,47,47,47	0
4	MTE	B	702	24/24	0.88	0.21	35,82,90,124	0
6	MG	A	705	1/1	0.88	0.23	42,42,42,42	0
7	UNL	C	705	1/-	0.89	0.65	63,63,63,63	0
7	UNL	A	706	1/-	0.89	0.54	55,55,55,55	0
4	MTE	D	704	24/24	0.93	0.20	41,49,58,62	0
4	MTE	B	703	24/24	0.93	0.18	97,106,113,164	0
3	SF4	D	702	8/8	0.93	0.09	53,60,87,104	0
3	SF4	G	1001	8/8	0.93	0.14	36,41,59,60	0
3	SF4	H	1002	8/8	0.94	0.12	50,60,67,69	0
3	SF4	F	1002	8/8	0.94	0.18	36,50,70,91	0
4	MTE	A	703	24/24	0.94	0.19	41,43,56,61	0
3	SF4	A	701	8/8	0.94	0.10	46,56,87,133	0
3	SF4	E	1003	8/8	0.95	0.14	49,52,55,55	0
3	SF4	G	1002	8/8	0.95	0.15	42,46,57,60	0
4	MTE	D	703	24/24	0.95	0.17	26,40,49,68	0
4	MTE	C	702	24/24	0.95	0.18	24,37,48,57	0
3	SF4	F	1001	8/8	0.96	0.12	41,52,54,61	0
3	SF4	C	701	8/8	0.96	0.08	49,52,79,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MTE	A	702	24/24	0.96	0.18	39,46,53,56	0
3	SF4	H	1001	8/8	0.96	0.14	33,46,49,52	0
3	SF4	B	701	8/8	0.96	0.07	79,94,134,153	0
3	SF4	E	1002	8/8	0.97	0.15	52,59,61,66	0
3	SF4	F	1003	8/8	0.97	0.11	52,56,60,66	0
3	SF4	G	1003	8/8	0.97	0.11	45,53,63,68	0
7	UNL	B	705	1/-	0.97	0.43	95,95,95,95	0
3	SF4	H	1003	8/8	0.97	0.13	49,57,70,72	0
3	SF4	E	1001	8/8	0.97	0.15	52,55,56,57	0
7	UNL	D	701	1/-	0.97	0.26	47,47,47,47	0
5	W	D	705	1/1	0.98	0.18	43,43,43,43	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

6.5 Other polymers [i](#)

There are no such residues in this entry.