



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:03 PM GMT

PDB ID : 4Z3Z
Title : Active site complex BamBC of Benzoyl Coenzyme A reductase in complex with Zinc
Authors : Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on : 2015-04-01
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

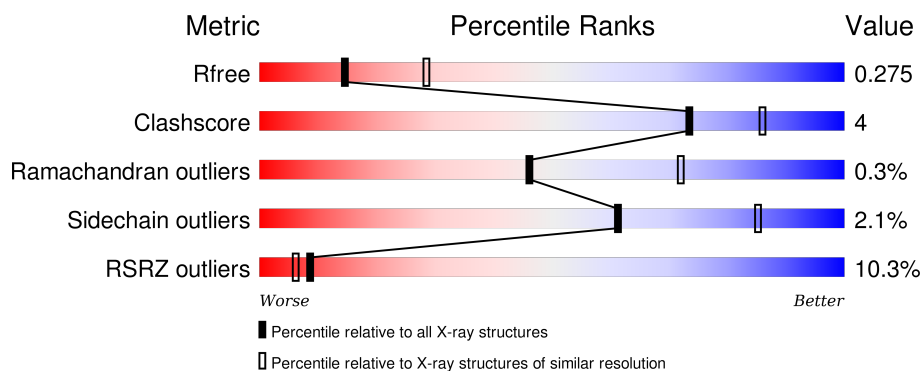
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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>35%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
1	B	653	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
1	C	653	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	D	653	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
2	E	179	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	179	
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
3	UNL	B	701	-	-	-	X
4	SF4	D	702	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26146 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

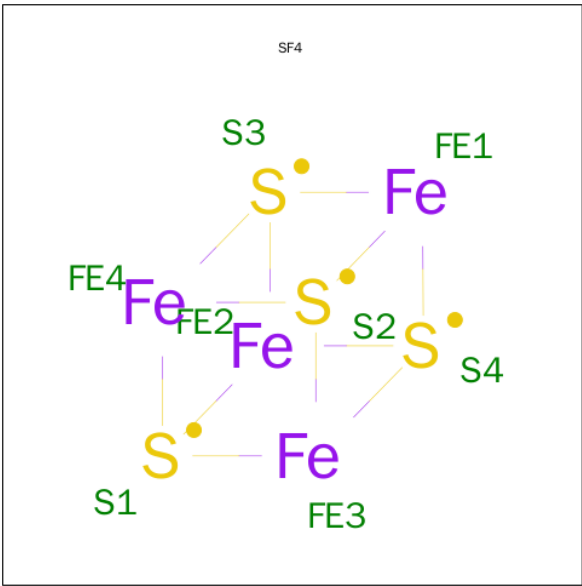
- Molecule 2 is a protein called Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	163	Total	C	N	O	S	0	0	0
			1237	769	218	236	14			
2	F	170	Total	C	N	O	S	0	1	0
			1317	816	226	261	14			
2	G	169	Total	C	N	O	S	0	2	0
			1315	814	228	259	14			
2	H	161	Total	C	N	O	S	0	0	0
			1221	758	213	236	14			

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

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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



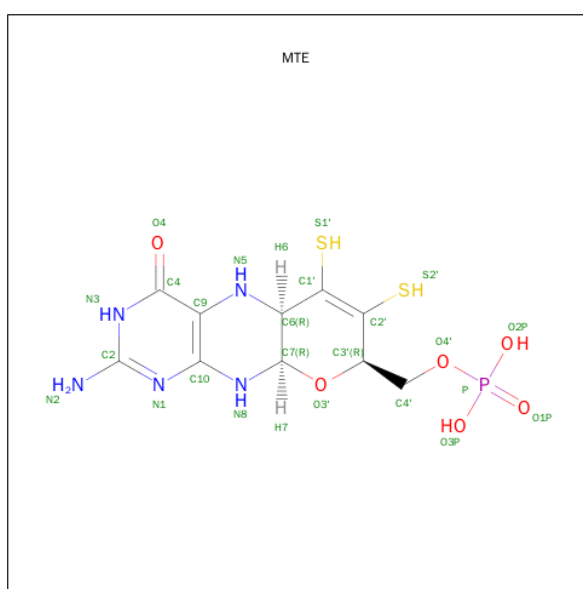
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4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

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

- Molecule 5 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆P₂S₂).



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

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

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

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

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

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

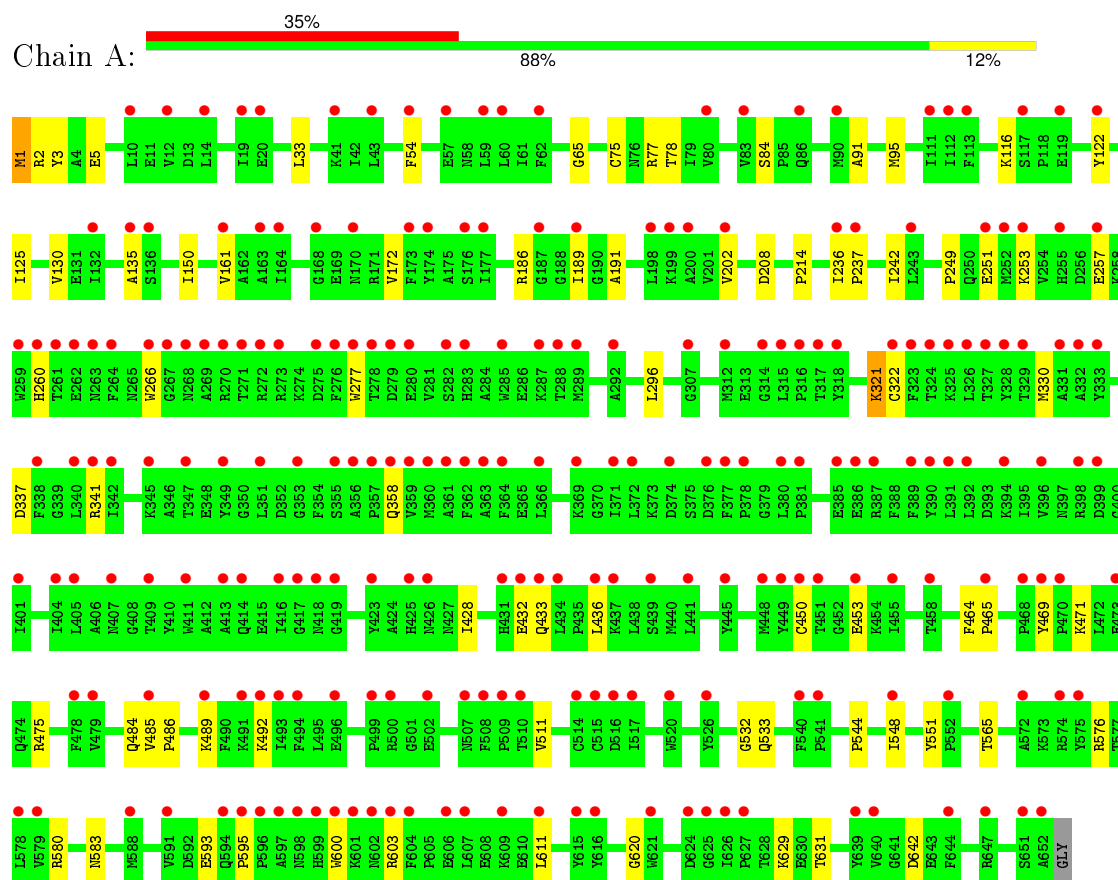
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

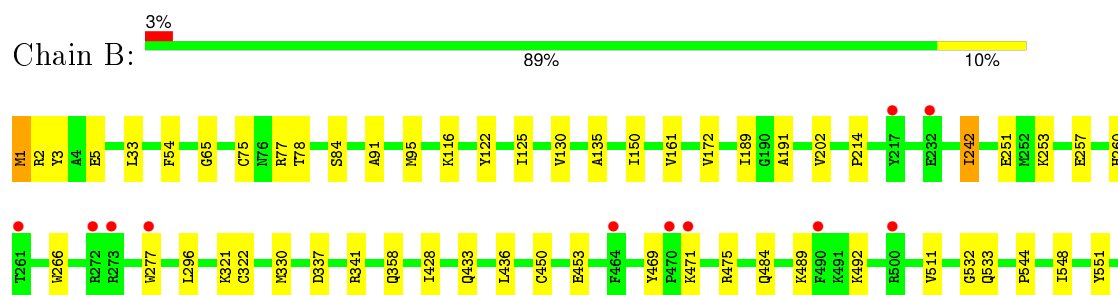
3 Residue-property plots [i](#)

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

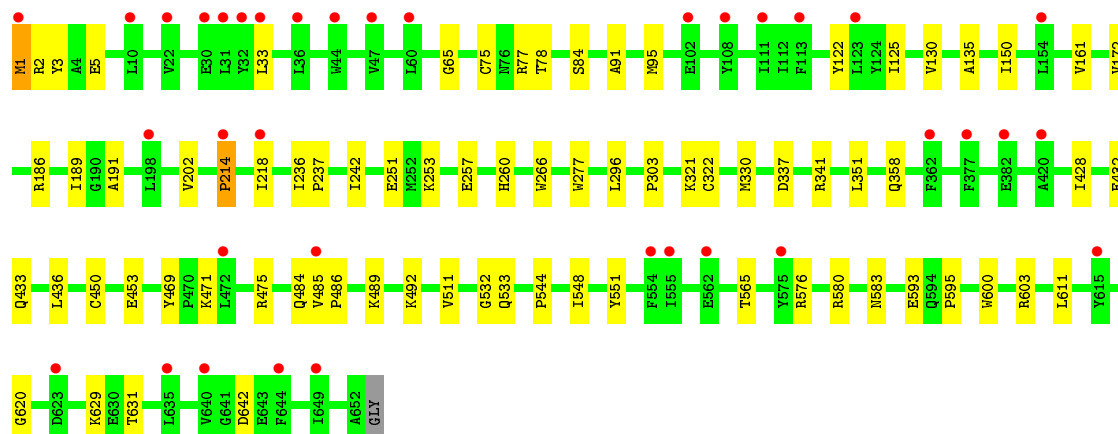
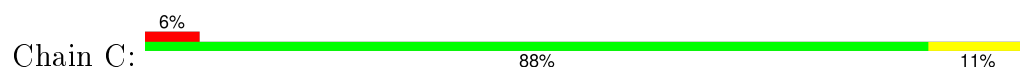


- Molecule 1: Benzoyl-CoA reductase, putative

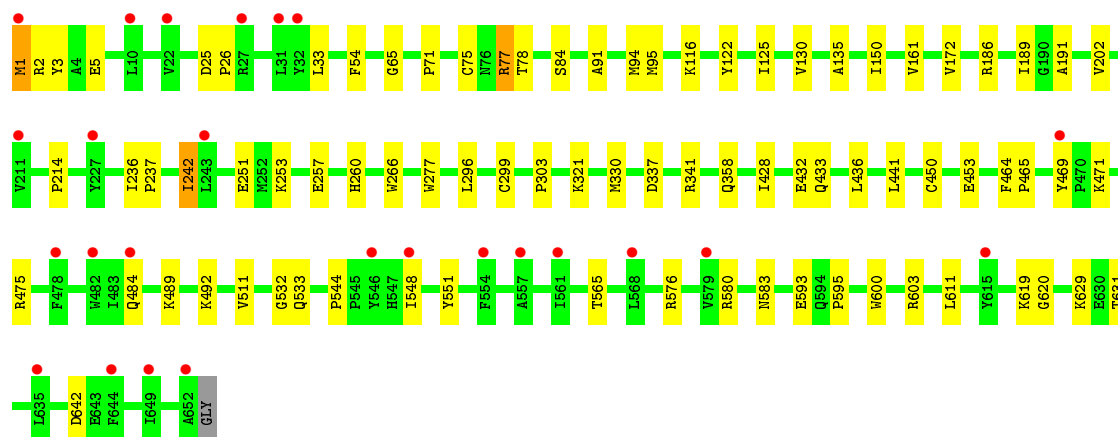
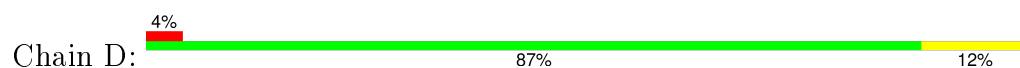




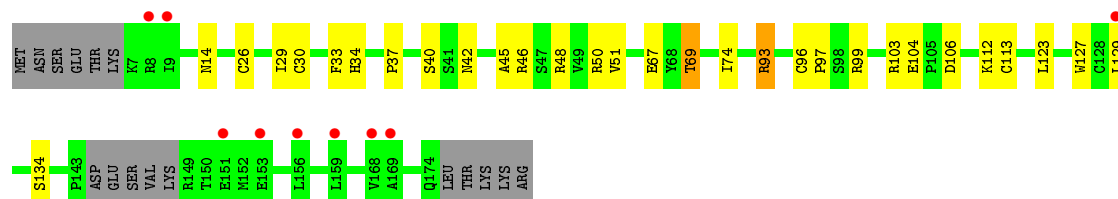
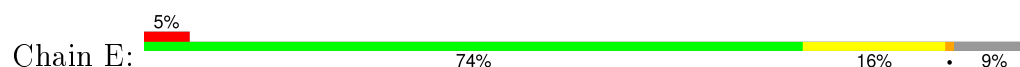
- Molecule 1: Benzoyl-CoA reductase, putative




- Molecule 1: Benzoyl-CoA reductase, putative



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




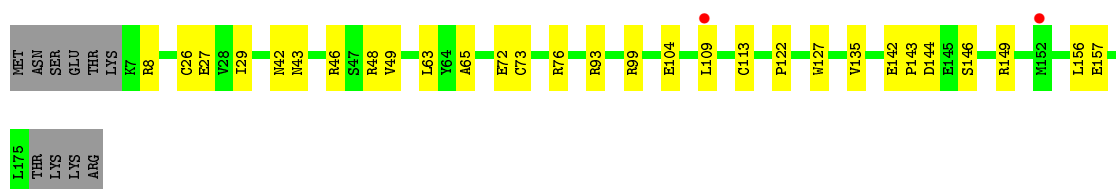
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain F: 




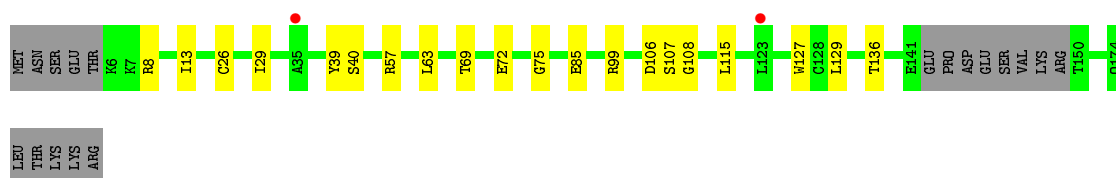
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain G: 



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

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.24Å 117.43Å 143.08Å 90.00° 111.04° 90.00°	Depositor
Resolution (Å)	82.51 – 2.67 82.51 – 2.67	Depositor EDS
% Data completeness (in resolution range)	97.2 (82.51-2.67) 97.4 (82.51-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.232 , 0.274 0.239 , 0.275	Depositor DCC
R_{free} test set	1393 reflections (1.32%)	DCC
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 106724 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26146	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, SF4, MG, W, UNL, MTE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/5306	0.39	0/7172
1	B	0.23	0/5306	0.39	0/7172
1	C	0.23	0/5306	0.39	0/7172
1	D	0.23	0/5306	0.39	0/7172
2	E	0.26	0/1259	0.42	0/1705
2	F	0.27	0/1343	0.44	0/1819
2	G	0.26	0/1344	0.44	0/1819
2	H	0.24	0/1242	0.41	0/1681
All	All	0.24	0/26412	0.40	0/35712

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	5180	0	5110	41	0
1	B	5180	0	5110	33	0
1	C	5180	0	5110	39	0
1	D	5180	0	5110	43	0
2	E	1237	0	1181	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1317	0	1266	16	0
2	G	1315	0	1263	18	0
2	H	1221	0	1158	13	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	2	0
4	E	24	0	0	2	0
4	F	24	0	0	1	0
4	G	24	0	0	2	0
4	H	24	0	0	1	0
5	A	48	0	20	4	0
5	B	48	0	20	1	0
5	C	48	0	20	3	0
5	D	48	0	20	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
All	All	26146	0	25388	210	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 4.

All (210) 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)
2:G:73:CYS:HB2	4:G:1003:SF4:S1	2.03	0.97
3:C:701:UNL:X	5:C:703:MTE:S1'	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:HIS:NE2	4:E:1002:SF4:S1	2.57	0.77
1:D:299:CYS:HB2	4:D:702:SF4:S3	2.29	0.73
1:A:322:CYS:HB3	5:A:704:MTE:S1'	2.30	0.70
2:G:72:GLU:OE1	2:G:76:ARG:NH2	2.21	0.70
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.74	0.69
1:B:84:SER:HB2	1:B:91:ALA:HB2	1.74	0.69
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.74	0.68
1:C:84:SER:HB2	1:C:91:ALA:HB2	1.74	0.68
2:E:93:ARG:NH1	2:F:75:GLY:O	2.31	0.64
2:F:122:PRO:HG2	2:F:135:VAL:HG11	1.79	0.63
1:D:251:GLU:OE1	1:D:260:HIS:HE1	1.80	0.62
2:E:112:LYS:HE2	2:F:74:ILE:HG13	1.81	0.62
1:A:251:GLU:OE1	1:A:260:HIS:HE1	1.80	0.62
1:C:251:GLU:OE1	1:C:260:HIS:HE1	1.80	0.62
1:A:321:LYS:HD3	5:A:703:MTE:H4'2	1.82	0.62
1:A:484:GLN:HG2	1:A:544:PRO:HD2	1.82	0.62
2:G:93:ARG:NH1	2:H:75:GLY:O	2.29	0.62
2:G:72:GLU:OE2	2:H:8:ARG:NH2	2.29	0.62
1:D:484:GLN:HG2	1:D:544:PRO:HD2	1.82	0.61
1:C:484:GLN:HG2	1:C:544:PRO:HD2	1.82	0.61
1:B:251:GLU:OE1	1:B:260:HIS:HE1	1.80	0.61
1:B:484:GLN:HG2	1:B:544:PRO:HD2	1.82	0.61
1:D:629:LYS:NZ	1:D:642:ASP:OD1	2.35	0.60
1:C:629:LYS:NZ	1:C:642:ASP:OD1	2.35	0.60
1:B:629:LYS:NZ	1:B:642:ASP:OD1	2.35	0.60
2:F:11:LYS:HG2	2:F:137:GLU:HG2	1.84	0.60
1:A:629:LYS:NZ	1:A:642:ASP:OD1	2.35	0.59
2:F:99:ARG:HG3	2:F:101:LEU:HB2	1.85	0.59
2:E:106:ASP:N	2:E:106:ASP:OD1	2.35	0.59
1:C:161:VAL:HG22	1:C:202:VAL:HG22	1.85	0.59
1:A:161:VAL:HG22	1:A:202:VAL:HG22	1.85	0.58
1:B:161:VAL:HG22	1:B:202:VAL:HG22	1.85	0.58
1:D:161:VAL:HG22	1:D:202:VAL:HG22	1.85	0.58
2:G:104:GLU:HG3	2:G:109:LEU:HB2	1.86	0.58
1:A:511:VAL:HG13	1:A:611:LEU:HD23	1.85	0.58
1:B:511:VAL:HG13	1:B:611:LEU:HD23	1.85	0.58
1:D:511:VAL:HG13	1:D:611:LEU:HD23	1.85	0.57
1:C:511:VAL:HG13	1:C:611:LEU:HD23	1.85	0.56
1:D:150:ILE:HG21	1:D:202:VAL:HG21	1.88	0.56
1:C:150:ILE:HG21	1:C:202:VAL:HG21	1.88	0.55
1:B:150:ILE:HG21	1:B:202:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:2:ARG:N	2.79	0.55
1:D:620:GLY:HA3	1:D:631:THR:HG21	1.89	0.54
1:A:150:ILE:HG21	1:A:202:VAL:HG21	1.88	0.54
1:B:620:GLY:HA3	1:B:631:THR:HG21	1.89	0.54
1:C:620:GLY:HA3	1:C:631:THR:HG21	1.89	0.54
1:D:358:GLN:NE2	1:D:433:GLN:O	2.40	0.54
1:A:620:GLY:HA3	1:A:631:THR:HG21	1.89	0.54
1:D:303:PRO:HG3	2:E:129:LEU:HD22	1.89	0.54
1:D:75:CYS:HA	1:D:533:GLN:HA	1.90	0.54
1:A:489:LYS:HA	1:A:492:LYS:HD2	1.90	0.53
1:B:489:LYS:HA	1:B:492:LYS:HD2	1.90	0.53
1:C:75:CYS:HA	1:C:533:GLN:HA	1.90	0.53
1:D:489:LYS:HA	1:D:492:LYS:HD2	1.90	0.53
1:C:358:GLN:NE2	1:C:433:GLN:O	2.40	0.53
2:H:57:ARG:NH1	2:H:85:GLU:O	2.41	0.53
1:D:1:MET:SD	1:D:2:ARG:N	2.79	0.53
1:C:1:MET:SD	1:C:2:ARG:N	2.79	0.53
1:C:489:LYS:HA	1:C:492:LYS:HD2	1.90	0.53
1:B:75:CYS:HA	1:B:533:GLN:HA	1.90	0.52
1:A:75:CYS:HA	1:A:533:GLN:HA	1.90	0.52
2:E:30:CYS:SG	2:E:34:HIS:ND1	2.83	0.52
2:G:149:ARG:NH1	2:G:157:GLU:OE1	2.42	0.52
2:H:106:ASP:N	2:H:106:ASP:OD1	2.37	0.51
1:A:469:TYR:HB2	1:A:475:ARG:HG2	1.92	0.51
2:G:65:ALA:HB3	2:G:113:CYS:H	1.75	0.51
1:A:358:GLN:NE2	1:A:433:GLN:O	2.40	0.51
1:C:469:TYR:HB2	1:C:475:ARG:HG2	1.92	0.51
2:E:67:GLU:OE2	2:E:112:LYS:NZ	2.35	0.51
1:B:469:TYR:HB2	1:B:475:ARG:HG2	1.92	0.50
1:D:94:MET:O	5:D:704:MTE:O2P	2.30	0.50
1:A:1:MET:SD	1:A:2:ARG:N	2.79	0.50
2:E:69:THR:HB	2:F:67[B]:GLU:HG3	1.92	0.50
1:D:469:TYR:HB2	1:D:475:ARG:HG2	1.92	0.50
1:B:358:GLN:NE2	1:B:433:GLN:O	2.40	0.49
1:A:322:CYS:CB	5:A:704:MTE:S1'	2.86	0.49
1:C:303:PRO:HG3	2:H:129:LEU:HD22	1.94	0.49
2:E:46:ARG:NH2	2:E:104:GLU:OE1	2.44	0.49
1:D:125:ILE:HG12	1:D:130:VAL:HG13	1.95	0.49
2:G:29:ILE:HD13	2:G:127:TRP:CZ2	2.47	0.49
1:B:600:TRP:HB2	1:B:603:ARG:HD3	1.95	0.49
1:D:600:TRP:HB2	1:D:603:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HG12	1:A:130:VAL:HG13	1.95	0.48
1:C:125:ILE:HG12	1:C:130:VAL:HG13	1.95	0.48
1:C:600:TRP:HB2	1:C:603:ARG:HD3	1.95	0.48
1:C:351:LEU:O	5:C:704:MTE:N2	2.42	0.48
1:A:600:TRP:HB2	1:A:603:ARG:HD3	1.95	0.48
1:B:3:TYR:O	1:B:5:GLU:N	2.47	0.48
1:B:322:CYS:HB3	5:B:704:MTE:S1'	2.54	0.48
2:E:74:ILE:HD12	2:F:114:ASP:HA	1.96	0.48
1:B:125:ILE:HG12	1:B:130:VAL:HG13	1.95	0.48
1:A:548:ILE:HG13	1:A:565:THR:HG23	1.96	0.47
1:A:186:ARG:NH2	1:A:432:GLU:O	2.34	0.47
1:D:186:ARG:NH2	1:D:432:GLU:O	2.34	0.47
2:E:48:ARG:HB3	2:E:113:CYS:HB2	1.97	0.47
1:A:249:PRO:HG2	3:A:701:UNL:X	2.43	0.47
2:G:122:PRO:HB3	4:G:1002:SF4:S2	2.55	0.46
2:G:48:ARG:HB3	2:G:113:CYS:HB2	1.97	0.46
1:C:548:ILE:HG13	1:C:565:THR:HG23	1.97	0.46
1:A:54:PHE:O	1:A:116:LYS:NZ	2.45	0.46
1:B:548:ILE:HG13	1:B:565:THR:HG23	1.96	0.46
1:D:548:ILE:HG13	1:D:565:THR:HG23	1.97	0.46
2:G:8:ARG:NH2	2:H:72:GLU:OE1	2.45	0.46
2:F:122:PRO:HB3	4:F:1002:SF4:S2	2.56	0.46
2:E:29:ILE:HG13	2:E:123:LEU:HB3	1.98	0.46
1:C:322:CYS:HB2	5:C:703:MTE:S2'	2.56	0.46
1:D:453:GLU:OE1	1:D:583:ASN:ND2	2.50	0.45
1:B:337:ASP:O	1:B:341:ARG:HG3	2.16	0.45
2:G:65:ALA:O	2:G:93:ARG:NH2	2.50	0.45
1:C:236:ILE:HA	1:C:237:PRO:HD3	1.82	0.45
1:B:266:TRP:CE3	1:B:330:MET:HA	2.52	0.45
1:D:266:TRP:CE3	1:D:330:MET:HA	2.52	0.45
2:H:115:LEU:HA	4:H:1002:SF4:S1	2.56	0.45
2:F:97:PRO:HA	2:F:103:ARG:NH1	2.32	0.45
1:A:337:ASP:O	1:A:341:ARG:HG3	2.16	0.45
1:D:511:VAL:HG13	1:D:611:LEU:HA	1.99	0.45
1:A:3:TYR:O	1:A:5:GLU:N	2.47	0.45
1:B:453:GLU:OE1	1:B:583:ASN:ND2	2.50	0.45
1:A:453:GLU:OE1	1:A:583:ASN:ND2	2.50	0.45
1:C:218:ILE:HG12	2:H:39:TYR:CE1	2.50	0.45
1:D:54:PHE:O	1:D:116:LYS:NZ	2.46	0.45
1:D:337:ASP:O	1:D:341:ARG:HG3	2.16	0.45
1:D:3:TYR:O	1:D:5:GLU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:VAL:HG13	1:C:611:LEU:HA	1.99	0.45
2:F:64:TYR:OH	2:F:133:LEU:HD13	2.17	0.45
1:C:186:ARG:NH2	1:C:432:GLU:O	2.34	0.45
1:C:266:TRP:CE3	1:C:330:MET:HA	2.52	0.45
1:A:511:VAL:HG13	1:A:611:LEU:HA	1.99	0.44
1:B:511:VAL:HG13	1:B:611:LEU:HA	1.99	0.44
1:D:253:LYS:HE2	1:D:296:LEU:HD13	1.99	0.44
1:A:266:TRP:CE3	1:A:330:MET:HA	2.52	0.44
1:A:253:LYS:HE2	1:A:296:LEU:HD13	1.99	0.44
1:C:337:ASP:O	1:C:341:ARG:HG3	2.17	0.44
1:C:453:GLU:OE1	1:C:583:ASN:ND2	2.50	0.44
1:B:253:LYS:HE2	1:B:296:LEU:HD13	1.99	0.44
1:D:65:GLY:HA3	1:D:532:GLY:HA3	2.00	0.44
1:C:3:TYR:O	1:C:5:GLU:N	2.47	0.44
2:F:104:GLU:HG3	2:F:109:LEU:HB2	2.00	0.44
1:C:253:LYS:HE2	1:C:296:LEU:HD13	1.99	0.44
1:A:65:GLY:HA3	1:A:532:GLY:HA3	2.00	0.44
2:H:29:ILE:HD13	2:H:127:TRP:CZ2	2.53	0.44
1:D:77:ARG:NH1	4:D:702:SF4:S3	2.88	0.43
1:A:580:ARG:NH1	1:A:593:GLU:OE2	2.45	0.43
2:F:14:ASN:HB2	2:F:134:SER:OG	2.18	0.43
2:G:43:ASN:HD22	2:G:46:ARG:NH1	2.16	0.43
2:E:37:PRO:HG2	2:E:40:SER:HB3	2.00	0.43
1:B:54:PHE:O	1:B:116:LYS:NZ	2.45	0.43
1:B:580:ARG:NH1	1:B:593:GLU:OE2	2.45	0.43
1:D:580:ARG:NH1	1:D:593:GLU:OE2	2.45	0.43
1:A:464:PHE:HA	1:A:465:PRO:HD3	1.94	0.43
2:G:156:LEU:HA	2:G:156:LEU:HD23	1.84	0.43
1:C:65:GLY:HA3	1:C:532:GLY:HA3	2.00	0.43
1:B:242:ILE:H	1:B:242:ILE:HG12	1.56	0.43
2:E:34:HIS:CE1	2:E:48:ARG:HD3	2.53	0.42
1:D:78:THR:HB	1:D:95:MET:HG2	2.01	0.42
1:B:257:GLU:HB2	1:B:277:TRP:CH2	2.54	0.42
1:B:65:GLY:HA3	1:B:532:GLY:HA3	2.00	0.42
1:C:214:PRO:HG3	2:H:40:SER:HA	2.00	0.42
1:D:71:PRO:HD3	2:E:42:ASN:ND2	2.33	0.42
2:E:33:PHE:HB2	2:E:123:LEU:HD22	2.01	0.42
1:B:78:THR:HB	1:B:95:MET:HG2	2.01	0.42
1:A:78:THR:HB	1:A:95:MET:HG2	2.01	0.42
1:D:236:ILE:HA	1:D:237:PRO:HD3	1.82	0.42
1:C:257:GLU:HB2	1:C:277:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLU:HB2	1:D:277:TRP:CH2	2.54	0.42
1:C:485:VAL:HA	1:C:486:PRO:HD3	1.91	0.42
1:A:208:ASP:OD1	2:F:46:ARG:NH1	2.52	0.42
1:D:464:PHE:HA	1:D:465:PRO:HD3	1.93	0.42
1:A:257:GLU:HB2	1:A:277:TRP:CH2	2.54	0.42
1:A:428:ILE:HD11	1:A:595:PRO:HA	2.02	0.42
1:C:78:THR:HB	1:C:95:MET:HG2	2.01	0.42
1:B:172:VAL:O	1:B:191:ALA:HB2	2.20	0.41
1:A:172:VAL:O	1:A:191:ALA:HB2	2.20	0.41
1:A:485:VAL:HA	1:A:486:PRO:HD3	1.91	0.41
1:D:172:VAL:O	1:D:191:ALA:HB2	2.20	0.41
1:D:122:TYR:HD2	1:D:135:ALA:HB2	1.85	0.41
1:C:172:VAL:O	1:C:191:ALA:HB2	2.20	0.41
2:E:14:ASN:HB2	2:E:134:SER:O	2.21	0.41
2:F:77:ASP:OD1	2:F:77:ASP:N	2.45	0.41
2:G:142:GLU:HA	2:G:143:PRO:HD3	1.86	0.41
2:E:51:VAL:HG21	4:E:1001:SF4:S2	2.60	0.41
1:D:450:CYS:SG	1:D:595:PRO:HD3	2.61	0.41
1:A:95:MET:HA	5:A:703:MTE:O3P	2.21	0.41
1:B:122:TYR:HD2	1:B:135:ALA:HB2	1.85	0.41
2:F:13:ILE:O	2:F:15:ILE:HG13	2.20	0.41
2:E:29:ILE:HD13	2:E:127:TRP:CZ2	2.56	0.41
1:B:450:CYS:SG	1:B:595:PRO:HD3	2.61	0.41
1:C:450:CYS:SG	1:C:595:PRO:HD3	2.61	0.41
1:A:122:TYR:HD2	1:A:135:ALA:HB2	1.85	0.41
2:H:63:LEU:HA	2:H:63:LEU:HD23	1.89	0.41
1:B:428:ILE:HD11	1:B:595:PRO:HA	2.03	0.41
2:G:144:ASP:OD1	2:G:146:SER:OG	2.25	0.41
1:C:122:TYR:HD2	1:C:135:ALA:HB2	1.85	0.41
2:G:76:ARG:O	2:H:13:ILE:N	2.38	0.41
1:D:428:ILE:HD11	1:D:595:PRO:HA	2.02	0.41
1:D:25:ASP:HA	1:D:26:PRO:HD2	1.92	0.41
1:D:619:LYS:HA	1:D:619:LYS:HD3	1.93	0.40
2:F:160:ILE:HG23	2:F:165:ALA:HA	2.02	0.40
1:C:428:ILE:HD11	1:C:595:PRO:HA	2.02	0.40
1:A:236:ILE:HA	1:A:237:PRO:HD3	1.82	0.40
2:E:45:ALA:HA	2:E:50:ARG:NH1	2.36	0.40
1:A:450:CYS:SG	1:A:595:PRO:HD3	2.61	0.40
1:C:218:ILE:HG12	2:H:39:TYR:CD1	2.57	0.40
1:D:242:ILE:HG12	1:D:242:ILE:H	1.56	0.40
2:G:27:GLU:HG2	2:G:49:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:LEU:HA	1:D:600:TRP:CD1	2.56	0.40
1:C:580:ARG:NH1	1:C:593:GLU:OE2	2.45	0.40
2:E:97:PRO:HA	2:E:103:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	650/653 (100%)	614 (94%)	34 (5%)	2 (0%)	46	72
1	B	650/653 (100%)	613 (94%)	35 (5%)	2 (0%)	46	72
1	C	650/653 (100%)	613 (94%)	35 (5%)	2 (0%)	46	72
1	D	650/653 (100%)	613 (94%)	35 (5%)	2 (0%)	46	72
2	E	159/179 (89%)	151 (95%)	8 (5%)	0	100	100
2	F	169/179 (94%)	157 (93%)	11 (6%)	1 (1%)	30	54
2	G	169/179 (94%)	154 (91%)	15 (9%)	0	100	100
2	H	157/179 (88%)	146 (93%)	9 (6%)	2 (1%)	15	33
All	All	3254/3328 (98%)	3061 (94%)	182 (6%)	11 (0%)	46	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	107	SER
1	A	33	LEU
1	B	33	LEU
1	C	33	LEU
1	D	33	LEU
2	F	42	ASN
1	A	214	PRO

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Mol	Chain	Res	Type
1	B	214	PRO
1	C	214	PRO
1	D	214	PRO
2	H	108	GLY

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	546/548 (100%)	537 (98%)	9 (2%)	70	89
1	B	546/548 (100%)	537 (98%)	9 (2%)	70	89
1	C	546/548 (100%)	537 (98%)	9 (2%)	70	89
1	D	546/548 (100%)	537 (98%)	9 (2%)	70	89
2	E	134/159 (84%)	129 (96%)	5 (4%)	41	69
2	F	148/159 (93%)	141 (95%)	7 (5%)	32	60
2	G	147/159 (92%)	142 (97%)	5 (3%)	44	72
2	H	132/159 (83%)	128 (97%)	4 (3%)	48	77
All	All	2745/2828 (97%)	2688 (98%)	57 (2%)	61	85

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	77	ARG
1	A	189	ILE
1	A	242	ILE
1	A	321	LYS
1	A	436	LEU
1	A	471	LYS
1	A	551	TYR
1	A	576	ARG
1	B	1	MET
1	B	77	ARG

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Mol	Chain	Res	Type
1	B	189	ILE
1	B	242	ILE
1	B	321	LYS
1	B	436	LEU
1	B	471	LYS
1	B	551	TYR
1	B	576	ARG
1	C	1	MET
1	C	77	ARG
1	C	189	ILE
1	C	242	ILE
1	C	321	LYS
1	C	436	LEU
1	C	471	LYS
1	C	551	TYR
1	C	576	ARG
1	D	1	MET
1	D	77	ARG
1	D	189	ILE
1	D	242	ILE
1	D	321	LYS
1	D	436	LEU
1	D	471	LYS
1	D	551	TYR
1	D	576	ARG
2	E	26	CYS
2	E	69	THR
2	E	93	ARG
2	E	96	CYS
2	E	99	ARG
2	F	26	CYS
2	F	41	SER
2	F	46	ARG
2	F	63	LEU
2	F	69	THR
2	F	99	ARG
2	F	156	LEU
2	G	26	CYS
2	G	42	ASN
2	G	63	LEU
2	G	99	ARG
2	G	135	VAL

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Mol	Chain	Res	Type
2	H	26	CYS
2	H	69	THR
2	H	99	ARG
2	H	136	THR

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	463	GLN
1	B	463	GLN
1	C	463	GLN
1	D	463	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are unknown and 12 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	A	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	A	703	5,7,6	21,26,26	3.00	10 (47%)	18,40,40	2.19	6 (33%)
5	MTE	A	704	5,7,6	21,26,26	2.75	11 (52%)	18,40,40	2.47	5 (27%)
4	SF4	B	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	B	703	7,6	21,26,26	2.78	10 (47%)	18,40,40	2.06	3 (16%)
5	MTE	B	704	7,6	21,26,26	2.87	10 (47%)	18,40,40	2.43	4 (22%)
4	SF4	C	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	C	703	7,6	21,26,26	2.78	10 (47%)	18,40,40	2.30	5 (27%)
5	MTE	C	704	7,6	21,26,26	2.83	10 (47%)	18,40,40	2.08	4 (22%)
4	SF4	D	702	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MTE	D	703	7,6	21,26,26	2.69	10 (47%)	18,40,40	2.09	4 (22%)
5	MTE	D	704	7,6	21,26,26	2.75	10 (47%)	18,40,40	2.33	5 (27%)
4	SF4	E	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	G	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	G	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	G	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	1001	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	1002	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	1003	2	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	702	1	-	0/0/48/48	0/6/5/5
5	MTE	A	703	5,7,6	-	0/6/34/34	0/3/3/3
5	MTE	A	704	5,7,6	-	0/6/34/34	0/3/3/3
4	SF4	B	702	1	-	0/0/48/48	0/6/5/5
5	MTE	B	703	7,6	-	0/6/34/34	0/3/3/3
5	MTE	B	704	7,6	-	0/6/34/34	0/3/3/3
4	SF4	C	702	1	-	0/0/48/48	0/6/5/5
5	MTE	C	703	7,6	-	0/6/34/34	0/3/3/3
5	MTE	C	704	7,6	-	0/6/34/34	0/3/3/3
4	SF4	D	702	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MTE	D	703	7,6	-	0/6/34/34	0/3/3/3
5	MTE	D	704	7,6	-	0/6/34/34	0/3/3/3
4	SF4	E	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	E	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	E	1003	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1003	2	-	0/0/48/48	0/6/5/5
4	SF4	G	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	G	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	G	1003	2	-	0/0/48/48	0/6/5/5
4	SF4	H	1001	2	-	0/0/48/48	0/6/5/5
4	SF4	H	1002	2	-	0/0/48/48	0/6/5/5
4	SF4	H	1003	2	-	0/0/48/48	0/6/5/5

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	MTE	C9-C10	-6.89	1.28	1.41
5	A	704	MTE	C9-C10	-6.66	1.28	1.41
5	A	703	MTE	C9-C10	-6.46	1.29	1.41
5	D	704	MTE	C9-C10	-6.35	1.29	1.41
5	B	704	MTE	C7-C6	-6.29	1.48	1.53
5	C	704	MTE	C9-C10	-6.28	1.29	1.41
5	D	703	MTE	C9-C10	-6.26	1.29	1.41
5	B	703	MTE	C9-C10	-6.25	1.29	1.41
5	C	703	MTE	C9-C10	-6.22	1.29	1.41
5	A	703	MTE	C7-C6	-5.50	1.49	1.53
5	C	703	MTE	C7-C6	-5.11	1.49	1.53
5	C	704	MTE	C7-C6	-4.94	1.49	1.53
5	B	703	MTE	C7-C6	-4.91	1.49	1.53
5	D	704	MTE	C7-C6	-4.67	1.50	1.53
5	D	703	MTE	C7-C6	-4.21	1.50	1.53
5	A	703	MTE	O3'-C7	-4.03	1.37	1.43
5	A	704	MTE	C7-C6	-3.92	1.50	1.53
5	B	703	MTE	O3'-C7	-3.66	1.38	1.43
5	C	703	MTE	O3'-C7	-3.40	1.38	1.43
5	D	703	MTE	O3'-C7	-3.35	1.38	1.43
5	C	704	MTE	O3'-C7	-3.30	1.38	1.43
5	A	703	MTE	O3'-C3'	-3.06	1.39	1.43
5	A	704	MTE	O3'-C7	-3.00	1.39	1.43
5	B	704	MTE	O3'-C7	-3.00	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	703	MTE	O3'-C3'	-2.92	1.39	1.43
5	B	704	MTE	O3'-C3'	-2.79	1.39	1.43
5	D	703	MTE	O3'-C3'	-2.77	1.39	1.43
5	C	704	MTE	O3'-C3'	-2.63	1.39	1.43
5	D	704	MTE	O3'-C7	-2.55	1.40	1.43
5	A	704	MTE	O3'-C3'	-2.54	1.40	1.43
5	B	703	MTE	O3'-C3'	-2.25	1.40	1.43
5	D	704	MTE	O3'-C3'	-2.08	1.40	1.43
5	A	704	MTE	C9-N5	2.07	1.42	1.38
5	D	704	MTE	C2-N3	2.09	1.39	1.35
5	B	704	MTE	C2-N3	2.10	1.39	1.35
5	A	704	MTE	C2-N3	2.26	1.39	1.35
5	C	703	MTE	C2-N3	2.29	1.39	1.35
5	C	704	MTE	C2-N3	2.33	1.39	1.35
5	D	703	MTE	C2-N3	2.40	1.39	1.35
5	A	704	MTE	C10-N8	2.46	1.43	1.35
5	B	704	MTE	C10-N1	2.48	1.39	1.34
5	B	703	MTE	C2-N3	2.49	1.40	1.35
5	D	703	MTE	C10-N8	2.53	1.43	1.35
5	A	703	MTE	C2-N3	2.53	1.40	1.35
5	B	704	MTE	C10-N8	2.65	1.43	1.35
5	B	703	MTE	C10-N8	2.67	1.43	1.35
5	B	703	MTE	C10-N1	2.71	1.39	1.34
5	D	703	MTE	C10-N1	2.72	1.39	1.34
5	C	703	MTE	C10-N1	2.73	1.39	1.34
5	A	704	MTE	C10-N1	2.76	1.39	1.34
5	B	703	MTE	C4-N3	2.78	1.38	1.33
5	D	704	MTE	C10-N1	2.80	1.39	1.34
5	A	703	MTE	C10-N8	2.81	1.44	1.35
5	C	703	MTE	C10-N8	2.82	1.44	1.35
5	C	704	MTE	C10-N8	2.82	1.44	1.35
5	A	703	MTE	C10-N1	2.92	1.39	1.34
5	B	704	MTE	C4-N3	2.94	1.38	1.33
5	C	704	MTE	C10-N1	3.00	1.40	1.34
5	A	704	MTE	C4-N3	3.01	1.38	1.33
5	C	703	MTE	C4-N3	3.01	1.38	1.33
5	D	704	MTE	C10-N8	3.02	1.44	1.35
5	D	704	MTE	C4-N3	3.04	1.38	1.33
5	C	704	MTE	C4-N3	3.04	1.38	1.33
5	D	703	MTE	C4-N3	3.11	1.38	1.33
5	A	703	MTE	C4-N3	3.27	1.38	1.33
5	D	703	MTE	C4-C9	3.77	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	MTE	C4-C9	3.91	1.47	1.41
5	D	704	MTE	C2-N2	4.30	1.43	1.34
5	C	703	MTE	C2-N2	4.31	1.43	1.34
5	B	704	MTE	C2-N2	4.34	1.43	1.34
5	C	704	MTE	C2-N2	4.40	1.43	1.34
5	D	703	MTE	C2-N2	4.45	1.43	1.34
5	C	703	MTE	C4-C9	4.49	1.47	1.41
5	A	704	MTE	C2-N2	4.52	1.43	1.34
5	B	703	MTE	C4-C9	4.56	1.47	1.41
5	A	703	MTE	C2-N2	4.56	1.43	1.34
5	B	703	MTE	C2-N2	4.57	1.43	1.34
5	C	704	MTE	C4-C9	5.00	1.48	1.41
5	A	703	MTE	C4-C9	5.03	1.48	1.41
5	A	704	MTE	C4-C9	5.08	1.48	1.41
5	D	704	MTE	C4-C9	5.29	1.49	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	704	MTE	O3'-C7-C6	-4.78	105.69	108.96
5	C	703	MTE	O3'-C7-C6	-3.47	106.59	108.96
5	A	703	MTE	O3'-C7-C6	-2.61	107.18	108.96
5	D	703	MTE	O3'-C7-C6	-2.33	107.37	108.96
5	A	704	MTE	N3-C2-N1	-2.06	122.14	125.51
5	A	703	MTE	N3-C2-N1	-2.01	122.23	125.51
5	B	703	MTE	N8-C10-N1	2.04	119.87	116.62
5	D	703	MTE	C9-C10-N8	2.05	120.14	118.19
5	C	703	MTE	N8-C10-N1	2.12	120.00	116.62
5	A	703	MTE	N8-C10-N1	2.12	120.00	116.62
5	C	704	MTE	O3'-C7-C6	2.13	110.42	108.96
5	D	704	MTE	N8-C10-N1	2.15	120.04	116.62
5	A	703	MTE	C9-C10-N8	2.22	120.30	118.19
5	C	704	MTE	N8-C10-N1	2.29	120.28	116.62
5	A	704	MTE	C9-C10-N8	2.40	120.47	118.19
5	C	703	MTE	C9-C10-N8	2.42	120.49	118.19
5	D	703	MTE	C2-N1-C10	2.49	120.21	114.63
5	D	704	MTE	C9-C10-N8	2.56	120.62	118.19
5	B	704	MTE	N8-C10-N1	2.60	120.77	116.62
5	B	703	MTE	C2-N1-C10	2.65	120.58	114.63
5	C	704	MTE	C2-N1-C10	2.69	120.67	114.63
5	C	703	MTE	C2-N1-C10	2.71	120.71	114.63
5	B	704	MTE	C2-N1-C10	2.75	120.81	114.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	MTE	C2-N1-C10	2.93	121.20	114.63
5	A	704	MTE	C2-N1-C10	2.93	121.22	114.63
5	D	704	MTE	C2-N1-C10	3.01	121.38	114.63
5	D	704	MTE	O3'-C7-C6	4.25	111.87	108.96
5	A	704	MTE	C4-C9-C10	5.83	119.74	114.61
5	A	704	MTE	O3'-C7-C6	6.76	113.59	108.96
5	D	703	MTE	C4-C9-C10	6.88	120.67	114.61
5	B	703	MTE	C4-C9-C10	6.94	120.72	114.61
5	D	704	MTE	C4-C9-C10	6.99	120.76	114.61
5	A	703	MTE	C4-C9-C10	7.02	120.79	114.61
5	C	704	MTE	C4-C9-C10	7.03	120.80	114.61
5	B	704	MTE	C4-C9-C10	7.46	121.18	114.61
5	C	703	MTE	C4-C9-C10	7.48	121.19	114.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	MTE	2	0
5	A	704	MTE	2	0
5	B	704	MTE	1	0
5	C	703	MTE	2	0
5	C	704	MTE	1	0
4	D	702	SF4	2	0
5	D	704	MTE	1	0
4	E	1001	SF4	1	0
4	E	1002	SF4	1	0
4	F	1002	SF4	1	0
4	G	1002	SF4	1	0
4	G	1003	SF4	1	0
4	H	1002	SF4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	652/653 (99%)	1.84	230 (35%) 0 0	60, 173, 256, 390	0
1	B	652/653 (99%)	0.26	19 (2%) 55 53	51, 87, 147, 186	0
1	C	652/653 (99%)	0.34	36 (5%) 29 26	55, 103, 147, 175	0
1	D	652/653 (99%)	0.27	25 (3%) 44 42	45, 93, 145, 185	0
2	E	163/179 (91%)	0.27	9 (5%) 29 26	55, 101, 155, 188	0
2	F	170/179 (94%)	0.39	13 (7%) 17 14	48, 79, 164, 175	0
2	G	169/179 (94%)	0.09	2 (1%) 81 80	56, 92, 167, 178	0
2	H	161/179 (89%)	0.16	2 (1%) 81 80	58, 103, 145, 180	0
All	All	3271/3328 (98%)	0.59	336 (10%) 9 6	45, 103, 209, 390	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	ASP	11.8
1	A	434	LEU	11.1
1	A	357	PRO	10.8
1	A	423	TYR	10.7
1	A	362	PHE	9.7
1	A	611	LEU	9.4
1	A	325	LYS	9.2
1	A	269	ALA	9.1
1	A	625	GLY	9.0
1	A	591	VAL	8.8
1	A	366	LEU	8.4
1	A	272	ARG	8.0
1	A	364	PHE	7.9
1	A	606	GLU	7.9
1	A	331	ALA	7.9
1	A	579	VAL	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	327	THR	7.7
1	A	289	MET	7.6
1	A	261	THR	7.3
1	A	627	PRO	7.2
1	A	377	PHE	7.2
1	A	276	PHE	7.1
1	A	418	ASN	7.1
1	A	361	ALA	7.1
1	A	509	PRO	6.9
1	A	575	TYR	6.8
1	A	405	LEU	6.8
1	A	494	PHE	6.7
1	A	260	HIS	6.7
1	A	599	HIS	6.7
1	A	355	SER	6.7
1	A	264	PHE	6.6
1	A	517	ILE	6.6
1	A	174	TYR	6.5
2	F	152	MET	6.5
1	A	374	ASP	6.5
1	A	595	PRO	6.4
1	A	380	LEU	6.4
1	D	557	ALA	6.4
1	A	359	VAL	6.3
1	A	349	TYR	6.3
1	A	416	ILE	6.3
1	A	329	THR	6.0
1	A	493	ILE	5.9
1	A	315	LEU	5.8
1	A	363	ALA	5.8
1	D	482	TRP	5.8
1	A	526	TYR	5.6
1	A	62	PHE	5.6
1	A	333	TYR	5.6
1	A	439	SER	5.5
1	A	426	ASN	5.5
1	A	479	VAL	5.3
1	A	597	ALA	5.2
1	A	168	GLY	5.2
1	A	262	GLU	5.1
1	A	396	VAL	5.0
1	A	389	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	273	ARG	5.0
1	A	469	TYR	5.0
1	A	243	LEU	4.9
1	A	340	LEU	4.9
1	A	198	LEU	4.8
1	A	135	ALA	4.8
1	A	499	PRO	4.7
1	A	601	LYS	4.7
2	F	168	VAL	4.7
1	A	351	LEU	4.6
1	A	132	ILE	4.6
1	C	1	MET	4.6
1	A	450	CYS	4.5
2	E	151	GLU	4.5
1	B	652	ALA	4.5
1	A	616	TYR	4.4
1	A	381	PRO	4.4
1	A	200	ALA	4.4
1	B	471	LYS	4.3
1	A	414	GLN	4.3
1	A	288	THR	4.3
1	C	640	VAL	4.2
1	A	401	ILE	4.1
2	F	145	GLU	4.1
1	A	111	ILE	4.1
1	A	600	TRP	4.1
1	A	328	TYR	4.1
1	A	353	GLY	4.1
1	A	453	GLU	4.1
1	A	394	LYS	4.1
1	A	271	THR	4.0
1	A	358	GLN	4.0
2	F	156	LEU	4.0
2	F	144	ASP	4.0
1	A	285	TRP	4.0
1	A	392	LEU	4.0
1	A	594	GLN	3.9
1	A	615	TYR	3.9
1	C	562	GLU	3.9
1	A	371	ILE	3.9
1	A	385	GLU	3.8
1	A	390	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	345	LYS	3.8
1	A	324	THR	3.8
1	A	237	PRO	3.8
1	A	491	LYS	3.8
1	A	122	TYR	3.8
1	A	338	PHE	3.8
2	E	169	ALA	3.8
1	A	449	TYR	3.7
1	C	10	LEU	3.7
1	A	508	PHE	3.7
1	A	500	ARG	3.7
1	A	90	MET	3.7
1	A	626	ILE	3.7
1	A	280	GLU	3.7
1	A	314	GLY	3.7
1	D	31	LEU	3.6
1	A	425	HIS	3.6
1	A	455	ILE	3.6
1	A	376	ASP	3.6
1	A	173	PHE	3.6
1	B	490	PHE	3.6
1	A	270	ARG	3.5
1	A	548	ILE	3.5
1	C	108	TYR	3.5
1	A	199	LYS	3.5
1	A	604	PHE	3.5
1	A	432	GLU	3.4
1	A	170	ASN	3.4
1	A	507	ASN	3.4
1	D	568	LEU	3.4
1	A	14	LEU	3.4
1	A	86	GLN	3.3
2	F	176	THR	3.3
1	A	57	GLU	3.3
1	A	164	ILE	3.3
1	A	202	VAL	3.3
1	A	251	GLU	3.3
1	A	515	CYS	3.3
1	C	555	ILE	3.3
2	F	148	LYS	3.3
1	A	263	ASN	3.2
1	A	113	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	ILE	3.2
2	F	154	ILE	3.2
1	A	441	LEU	3.2
1	A	277	TRP	3.2
1	A	640	VAL	3.2
1	A	624	ASP	3.2
1	A	266	TRP	3.1
1	A	448	MET	3.1
1	A	253	LYS	3.1
1	A	268	ASN	3.1
1	A	433	GLN	3.1
1	A	176	SER	3.1
1	A	609	LYS	3.1
1	A	43	LEU	3.1
1	A	20	GLU	3.1
1	A	419	GLY	3.0
1	A	322	CYS	3.0
1	A	117	SER	3.0
1	A	283	HIS	3.0
1	A	387	ARG	3.0
1	A	332	ALA	3.0
1	A	267	GLY	3.0
1	A	470	PRO	3.0
1	C	33	LEU	3.0
1	C	36	LEU	3.0
1	A	411	TRP	3.0
1	A	473	GLU	2.9
1	C	154	LEU	2.9
1	A	259	TRP	2.9
1	A	652	ALA	2.9
1	A	598	ASN	2.9
1	A	502	GLU	2.9
1	D	32	TYR	2.9
1	A	644	PHE	2.9
2	E	156	LEU	2.9
1	A	318	TYR	2.9
1	A	485	VAL	2.9
1	B	470	PRO	2.9
2	F	157	GLU	2.9
1	A	19	ILE	2.9
1	A	588	MET	2.9
1	A	413	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.8
1	A	431	HIS	2.8
1	A	60	LEU	2.8
1	A	489	LYS	2.8
1	D	546	TYR	2.8
1	A	404	ILE	2.8
1	A	651	SER	2.8
1	C	362	PHE	2.8
1	A	278	THR	2.8
1	A	596	PRO	2.8
1	A	341	ARG	2.8
1	A	292	ALA	2.7
1	A	436	LEU	2.7
1	B	572	ALA	2.7
1	A	312	MET	2.7
1	A	369	LYS	2.7
1	A	417	GLY	2.7
1	A	282	SER	2.7
1	D	579	VAL	2.7
2	G	152	MET	2.7
1	A	287	LYS	2.7
1	A	437	LYS	2.7
1	A	399	ASP	2.7
1	A	360	MET	2.7
1	A	307	GLY	2.7
1	A	10	LEU	2.7
1	D	635	LEU	2.7
1	C	615	TYR	2.7
1	D	649	ILE	2.7
1	C	649	ILE	2.7
1	A	458	THR	2.7
1	C	644	PHE	2.6
1	A	621	TRP	2.6
1	C	623	ASP	2.6
1	A	468	PRO	2.6
1	A	326	LEU	2.6
1	C	31	LEU	2.6
1	B	232	GLU	2.6
2	G	109	LEU	2.6
1	A	398	ARG	2.6
1	A	451	THR	2.6
2	E	8	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	514	CYS	2.6
1	D	478	PHE	2.6
1	A	409	THR	2.6
1	C	218	ILE	2.6
1	A	279	ASP	2.6
1	D	10	LEU	2.6
1	C	382	GLU	2.5
1	A	478	PHE	2.5
1	A	119	GLU	2.5
1	A	41	LYS	2.5
1	A	639	TYR	2.5
1	A	540	PHE	2.5
1	A	347	THR	2.5
2	F	163	PHE	2.5
1	A	189	ILE	2.5
1	B	277	TRP	2.5
1	D	469	TYR	2.5
1	A	407	ASN	2.5
2	E	159	LEU	2.5
1	A	236	ILE	2.4
1	A	372	LEU	2.4
1	A	603	ARG	2.4
2	F	161	SER	2.4
1	B	639	TYR	2.4
1	D	211	VAL	2.4
1	C	123	LEU	2.4
1	D	548	ILE	2.4
2	E	9	ILE	2.4
1	C	47	VAL	2.4
1	C	472	LEU	2.4
1	C	102	GLU	2.4
1	A	356	ALA	2.4
2	F	159	LEU	2.4
1	C	22	VAL	2.4
2	E	168	VAL	2.4
1	A	492	LYS	2.4
1	A	445	TYR	2.4
1	C	32	TYR	2.3
1	A	516	ASP	2.3
1	A	80	VAL	2.3
1	D	615	TYR	2.3
1	A	510	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	386	GLU	2.3
1	A	602	ASN	2.3
1	A	161	VAL	2.3
1	A	541	PRO	2.3
1	A	163	ALA	2.3
1	A	136	SER	2.3
2	H	35	ALA	2.3
2	F	60	TYR	2.3
1	A	574	ARG	2.2
1	B	500	ARG	2.2
1	B	615	TYR	2.2
1	C	554	PHE	2.2
1	D	22	VAL	2.2
1	C	30	GLU	2.2
1	A	252	MET	2.2
1	B	644	PHE	2.2
1	C	113	PHE	2.2
1	C	485	VAL	2.2
1	A	378	PRO	2.2
1	C	44	TRP	2.2
1	A	317	THR	2.2
1	A	54	PHE	2.2
1	D	554	PHE	2.2
1	A	112	ILE	2.2
1	B	272	ARG	2.2
1	A	59	LEU	2.2
1	A	391	LEU	2.2
1	A	465	PRO	2.2
1	A	572	ALA	2.2
1	B	261	THR	2.2
1	C	377	PHE	2.2
1	B	217	TYR	2.2
1	A	647	ARG	2.2
1	C	111	ILE	2.1
1	C	198	LEU	2.1
2	E	129	LEU	2.1
1	A	520	TRP	2.1
1	B	464	PHE	2.1
1	D	484	GLN	2.1
1	D	561	ILE	2.1
1	D	27	ARG	2.1
1	B	577	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	552	PRO	2.1
1	C	420	ALA	2.1
1	C	575	TYR	2.1
1	A	83	VAL	2.1
1	A	607	LEU	2.1
1	A	316	PRO	2.1
1	A	187	GLY	2.1
1	A	12	VAL	2.1
1	C	60	LEU	2.1
1	A	177	ILE	2.1
1	B	649	ILE	2.1
1	B	273	ARG	2.1
2	E	153	GLU	2.1
1	D	652	ALA	2.1
1	A	257	GLU	2.1
1	B	640	VAL	2.0
1	C	214	PRO	2.0
1	D	227	TYR	2.0
1	D	644	PHE	2.0
1	A	578	LEU	2.0
2	H	123	LEU	2.0
1	A	496	GLU	2.0
1	A	323	PHE	2.0
1	C	635	LEU	2.0
1	D	243	LEU	2.0
1	A	255	HIS	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	UNL	B	701	1/-	0.98	0.37	4.06	60,60,60,60	0
4	SF4	H	1001	8/8	0.99	0.20	1.25	55,69,76,82	0
4	SF4	F	1002	8/8	0.98	0.20	0.82	41,45,61,70	0
4	SF4	G	1003	8/8	0.99	0.19	0.62	78,80,89,152	0
4	SF4	E	1003	8/8	0.99	0.18	0.35	60,66,75,77	0
5	MTE	D	703	24/24	0.96	0.18	0.30	38,60,70,94	0
5	MTE	B	704	24/24	0.96	0.19	0.29	55,66,73,117	0
4	SF4	E	1001	8/8	0.99	0.19	0.15	56,71,77,117	0
4	SF4	B	702	8/8	0.99	0.16	0.10	44,56,66,73	0
4	SF4	G	1001	8/8	0.99	0.19	0.03	52,55,56,59	0
5	MTE	C	703	24/24	0.96	0.15	-0.08	46,69,86,87	0
5	MTE	B	703	24/24	0.96	0.17	-0.12	31,53,61,142	0
4	SF4	H	1002	8/8	0.99	0.17	-0.16	64,90,98,99	0
5	MTE	C	704	24/24	0.98	0.16	-0.26	39,60,94,112	0
4	SF4	E	1002	8/8	0.99	0.17	-0.30	56,76,99,147	0
5	MTE	D	704	24/24	0.98	0.16	-0.30	38,55,75,82	0
5	MTE	A	703	24/24	0.93	0.19	-0.32	39,93,108,267	0
4	SF4	F	1003	8/8	0.99	0.16	-0.33	54,69,73,85	0
4	SF4	H	1003	8/8	0.98	0.16	-0.35	60,75,90,104	0
4	SF4	D	702	8/8	0.99	0.15	-0.52	59,66,75,83	0
4	SF4	G	1002	8/8	0.99	0.18	-0.56	47,54,65,73	0
4	SF4	F	1001	8/8	0.99	0.15	-0.60	44,49,50,59	0
4	SF4	C	702	8/8	0.99	0.15	-0.73	56,64,74,83	0
8	ZN	A	707	1/1	0.72	0.16	-1.30	67,67,67,67	1
5	MTE	A	704	24/24	0.94	0.15	-1.37	78,82,110,178	0
8	ZN	C	707	1/1	0.96	0.11	-1.50	76,76,76,76	1
7	MG	A	706	1/1	0.75	0.09	-1.52	100,100,100,100	0
4	SF4	A	702	8/8	0.95	0.13	-1.66	65,92,124,143	0
8	ZN	D	707	1/1	0.97	0.07	-2.56	89,89,89,89	1
8	ZN	B	707	1/1	0.99	0.09	-3.01	40,40,40,40	1
6	W	A	705	1/1	0.96	0.14	-	111,111,111,111	0
7	MG	B	706	1/1	0.95	0.22	-	64,64,64,64	0
7	MG	D	706	1/1	0.98	0.13	-	43,43,43,43	0
3	UNL	A	701	1/-	0.91	0.42	-	55,55,55,55	0
6	W	B	705	1/1	1.00	0.26	-	80,80,80,80	0
7	MG	C	706	1/1	0.97	0.18	-	47,47,47,47	0
3	UNL	D	701	1/-	0.99	0.27	-	87,87,87,87	0
6	W	D	705	1/1	0.99	0.21	-	67,67,67,67	0
6	W	C	705	1/1	0.99	0.27	-	78,78,78,78	0
3	UNL	C	701	1/-	0.97	0.39	-	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.