Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 09:08 PM EDT

PDB ID	:	8ECM
Title	:	Crystal Structure Analysis of Acetyl-CoA acetyltransferase from Firmicutes bacterium
Authors	:	Seo, H.S.; Dhe-Paganon, S.
Deposited on	:	2022-09-02
Resolution	:	1.89 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

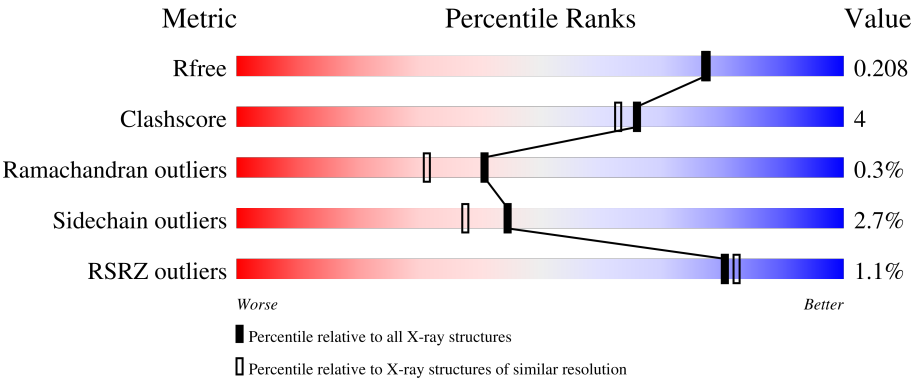
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	86% 12%
1	B	428	88% 10%
1	C	428	87% 11%
1	D	428	90% 8%
1	E	428	88% 9%

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Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25714 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3044	1904	530	584	26			
1	B	420	Total	C	N	O	S	0	0	0
			3056	1911	532	587	26			
1	C	421	Total	C	N	O	S	0	0	0
			3065	1917	534	588	26			
1	D	423	Total	C	N	O	S	0	0	0
			3085	1929	540	590	26			
1	E	421	Total	C	N	O	S	0	0	0
			3077	1925	536	590	26			
1	F	423	Total	C	N	O	S	0	0	0
			3092	1934	540	592	26			
1	G	420	Total	C	N	O	S	0	0	0
			3063	1917	533	587	26			
1	H	417	Total	C	N	O	S	0	0	0
			3039	1902	530	582	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP R6CZ24
A	2	ALA	-	expression tag	UNP R6CZ24
A	421	LEU	-	expression tag	UNP R6CZ24
A	422	GLU	-	expression tag	UNP R6CZ24
A	423	HIS	-	expression tag	UNP R6CZ24
A	424	HIS	-	expression tag	UNP R6CZ24
A	425	HIS	-	expression tag	UNP R6CZ24
A	426	HIS	-	expression tag	UNP R6CZ24
A	427	HIS	-	expression tag	UNP R6CZ24
A	428	HIS	-	expression tag	UNP R6CZ24
B	1	MET	-	initiating methionine	UNP R6CZ24
B	2	ALA	-	expression tag	UNP R6CZ24
B	421	LEU	-	expression tag	UNP R6CZ24

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	GLU	-	expression tag	UNP R6CZ24
B	423	HIS	-	expression tag	UNP R6CZ24
B	424	HIS	-	expression tag	UNP R6CZ24
B	425	HIS	-	expression tag	UNP R6CZ24
B	426	HIS	-	expression tag	UNP R6CZ24
B	427	HIS	-	expression tag	UNP R6CZ24
B	428	HIS	-	expression tag	UNP R6CZ24
C	1	MET	-	initiating methionine	UNP R6CZ24
C	2	ALA	-	expression tag	UNP R6CZ24
C	421	LEU	-	expression tag	UNP R6CZ24
C	422	GLU	-	expression tag	UNP R6CZ24
C	423	HIS	-	expression tag	UNP R6CZ24
C	424	HIS	-	expression tag	UNP R6CZ24
C	425	HIS	-	expression tag	UNP R6CZ24
C	426	HIS	-	expression tag	UNP R6CZ24
C	427	HIS	-	expression tag	UNP R6CZ24
C	428	HIS	-	expression tag	UNP R6CZ24
D	1	MET	-	initiating methionine	UNP R6CZ24
D	2	ALA	-	expression tag	UNP R6CZ24
D	421	LEU	-	expression tag	UNP R6CZ24
D	422	GLU	-	expression tag	UNP R6CZ24
D	423	HIS	-	expression tag	UNP R6CZ24
D	424	HIS	-	expression tag	UNP R6CZ24
D	425	HIS	-	expression tag	UNP R6CZ24
D	426	HIS	-	expression tag	UNP R6CZ24
D	427	HIS	-	expression tag	UNP R6CZ24
D	428	HIS	-	expression tag	UNP R6CZ24
E	1	MET	-	initiating methionine	UNP R6CZ24
E	2	ALA	-	expression tag	UNP R6CZ24
E	421	LEU	-	expression tag	UNP R6CZ24
E	422	GLU	-	expression tag	UNP R6CZ24
E	423	HIS	-	expression tag	UNP R6CZ24
E	424	HIS	-	expression tag	UNP R6CZ24
E	425	HIS	-	expression tag	UNP R6CZ24
E	426	HIS	-	expression tag	UNP R6CZ24
E	427	HIS	-	expression tag	UNP R6CZ24
E	428	HIS	-	expression tag	UNP R6CZ24
F	1	MET	-	initiating methionine	UNP R6CZ24
F	2	ALA	-	expression tag	UNP R6CZ24
F	421	LEU	-	expression tag	UNP R6CZ24
F	422	GLU	-	expression tag	UNP R6CZ24
F	423	HIS	-	expression tag	UNP R6CZ24

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Chain	Residue	Modelled	Actual	Comment	Reference
F	424	HIS	-	expression tag	UNP R6CZ24
F	425	HIS	-	expression tag	UNP R6CZ24
F	426	HIS	-	expression tag	UNP R6CZ24
F	427	HIS	-	expression tag	UNP R6CZ24
F	428	HIS	-	expression tag	UNP R6CZ24
G	1	MET	-	initiating methionine	UNP R6CZ24
G	2	ALA	-	expression tag	UNP R6CZ24
G	421	LEU	-	expression tag	UNP R6CZ24
G	422	GLU	-	expression tag	UNP R6CZ24
G	423	HIS	-	expression tag	UNP R6CZ24
G	424	HIS	-	expression tag	UNP R6CZ24
G	425	HIS	-	expression tag	UNP R6CZ24
G	426	HIS	-	expression tag	UNP R6CZ24
G	427	HIS	-	expression tag	UNP R6CZ24
G	428	HIS	-	expression tag	UNP R6CZ24
H	1	MET	-	initiating methionine	UNP R6CZ24
H	2	ALA	-	expression tag	UNP R6CZ24
H	421	LEU	-	expression tag	UNP R6CZ24
H	422	GLU	-	expression tag	UNP R6CZ24
H	423	HIS	-	expression tag	UNP R6CZ24
H	424	HIS	-	expression tag	UNP R6CZ24
H	425	HIS	-	expression tag	UNP R6CZ24
H	426	HIS	-	expression tag	UNP R6CZ24
H	427	HIS	-	expression tag	UNP R6CZ24
H	428	HIS	-	expression tag	UNP R6CZ24

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	132	Total O 132 132	0	0
2	B	150	Total O 150 150	0	0
2	C	161	Total O 161 161	0	0
2	D	170	Total O 170 170	0	0
2	E	170	Total O 170 170	0	0
2	F	181	Total O 181 181	0	0
2	G	156	Total O 156 156	0	0

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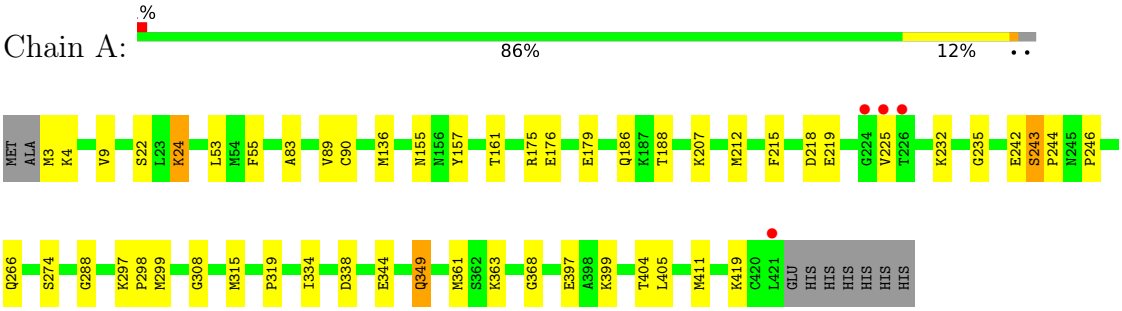
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	73	Total	O	0	0
			73	73		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

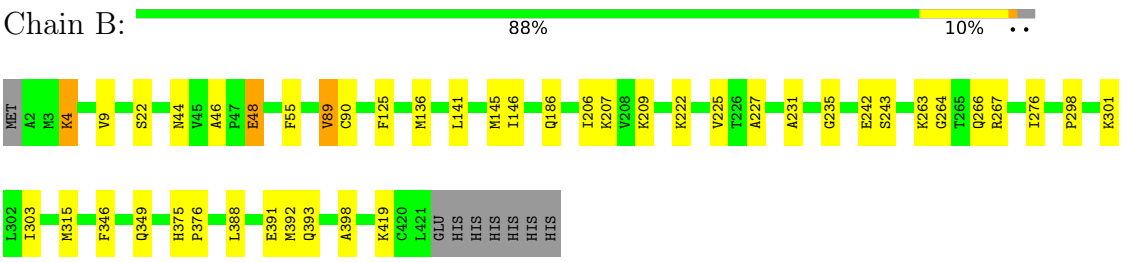
• Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



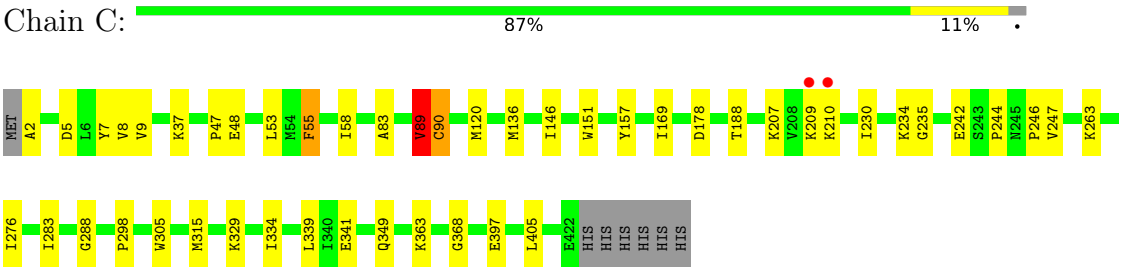
• Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



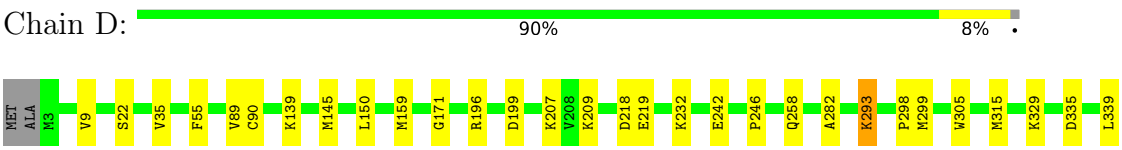
• Molecule 1: Acetyl-CoA acetyltransferase

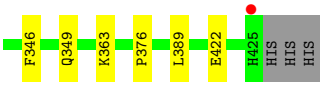
Chain C:



• Molecule 1: Acetyl-CoA acetyltransferase

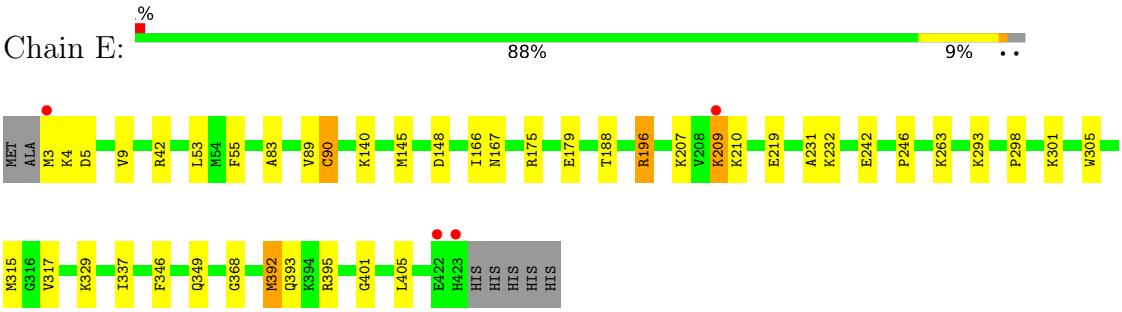
Chain D:





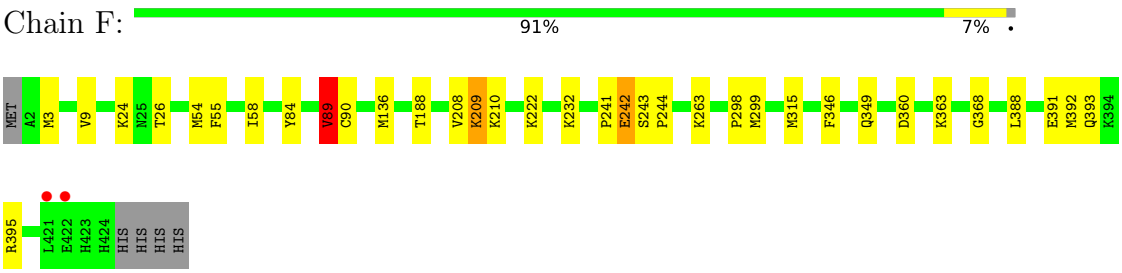
• Molecule 1: Acetyl-CoA acetyltransferase

Chain E:



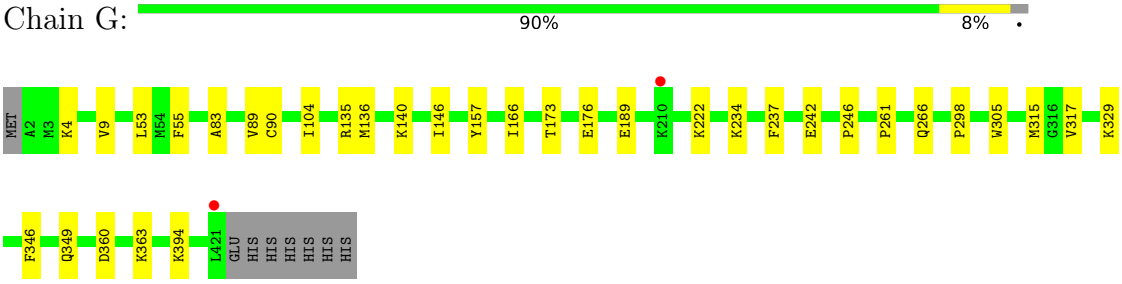
• Molecule 1: Acetyl-CoA acetyltransferase

Chain F:



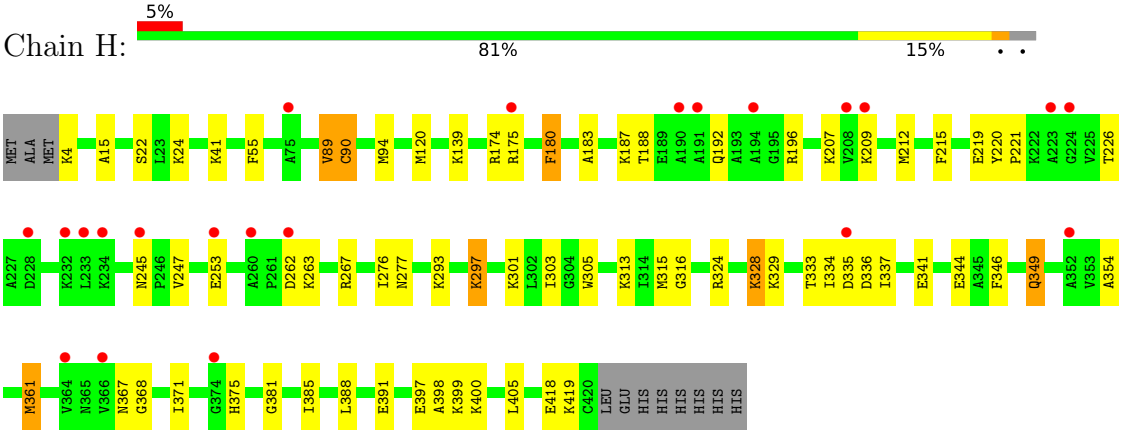
• Molecule 1: Acetyl-CoA acetyltransferase

Chain G:



• Molecule 1: Acetyl-CoA acetyltransferase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.23Å 81.46Å 160.19Å 95.61° 100.45° 108.27°	Depositor
Resolution (Å)	73.46 – 1.89 76.29 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.0 (73.46-1.89) 94.1 (76.29-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.176 , 0.209 0.175 , 0.208	Depositor DCC
R_{free} test set	13245 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25714	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCY

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	0.53	0/3082	0.68	0/4169
1	B	0.61	1/3094 (0.0%)	0.71	0/4184
1	C	0.61	0/3103	0.74	2/4195 (0.0%)
1	D	0.61	0/3126	0.71	2/4229 (0.0%)
1	E	0.67	1/3116 (0.0%)	0.75	2/4212 (0.0%)
1	F	0.66	0/3132	0.72	0/4234
1	G	0.60	0/3101	0.71	0/4192
1	H	0.52	0/3077	0.71	1/4160 (0.0%)
All	All	0.60	2/24831 (0.0%)	0.72	7/33575 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	219	GLU	CB-CG	-5.84	1.41	1.52
1	B	242	GLU	CG-CD	5.32	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	145	MET	CA-CB-CG	6.84	124.93	113.30
1	E	392	MET	CG-SD-CE	-6.41	89.94	100.20
1	C	55	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	C	339	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	H	361	MET	CG-SD-CE	-5.27	91.77	100.20
1	D	339	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	E	145	MET	CG-SD-CE	5.17	108.47	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	376	PRO	Peptide
1	D	376	PRO	Peptide
1	E	196	ARG	Sidechain

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	3044	0	3052	31	0
1	B	3056	0	3070	22	0
1	C	3065	0	3083	30	1
1	D	3085	0	3086	16	0
1	E	3077	0	3098	25	1
1	F	3092	0	3110	18	0
1	G	3063	0	3090	19	0
1	H	3039	0	3063	40	0
2	A	132	0	0	3	0
2	B	150	0	0	5	0
2	C	161	0	0	4	0
2	D	170	0	0	4	0
2	E	170	0	0	5	0
2	F	181	0	0	4	0
2	G	156	0	0	5	0
2	H	73	0	0	2	0
All	All	25714	0	24652	197	1

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 (197) 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:E:392:MET:HE1	1:E:401:GLY:HA3	1.34	1.03
1:E:167:ASN:O	1:E:263:LYS:NZ	1.92	1.02
1:G:242:GLU:HG3	1:G:246:PRO:HA	1.49	0.93
1:D:363:LYS:NZ	2:D:501:HOH:O	2.02	0.91
1:A:176:GLU:OE1	2:A:501:HOH:O	1.90	0.88
1:E:242:GLU:OE2	2:E:501:HOH:O	1.94	0.84
1:E:392:MET:CE	1:E:401:GLY:HA3	2.12	0.79
1:C:207:LYS:HE2	1:C:210:LYS:HD2	1.65	0.79
1:E:4:LYS:N	2:E:502:HOH:O	2.16	0.78
1:H:346:PHE:H	1:H:349:GLN:HE21	1.32	0.77
1:C:334:ILE:HD12	1:C:334:ILE:H	1.49	0.77
1:C:341:GLU:OE1	2:C:501:HOH:O	2.02	0.77
1:G:189:GLU:O	2:G:501:HOH:O	2.03	0.75
1:C:234:LYS:HD2	1:C:235:GLY:N	2.01	0.75
1:A:308:GLY:O	1:A:411:MET:HB3	1.90	0.72
1:C:234:LYS:HD2	1:C:235:GLY:H	1.56	0.71
1:A:22:SER:OG	1:A:219:GLU:OE2	2.09	0.70
1:H:196:ARG:NH2	1:H:391:GLU:OE2	2.23	0.70
1:D:346:PHE:H	1:D:349:GLN:HE21	1.40	0.70
1:F:26:THR:OG1	2:F:501:HOH:O	2.09	0.70
1:B:393:GLN:NE2	2:B:501:HOH:O	2.10	0.70
1:F:244:PRO:HB2	1:F:263:LYS:HG2	1.74	0.70
1:C:363:LYS:NZ	2:C:502:HOH:O	2.26	0.68
1:H:333:THR:HG23	1:H:335:ASP:H	1.59	0.67
1:H:367:ASN:ND2	1:H:391:GLU:OE1	2.21	0.67
1:B:346:PHE:H	1:B:349:GLN:HE21	1.43	0.66
1:D:299:MET:HE2	1:D:389:LEU:HB3	1.78	0.66
1:F:393:GLN:HG2	2:F:541:HOH:O	1.94	0.66
1:H:297:LYS:HD2	1:H:297:LYS:O	1.97	0.65
1:A:242:GLU:HB3	1:A:246:PRO:HA	1.77	0.65
1:A:24:LYS:NZ	2:A:504:HOH:O	2.29	0.64
1:B:46:ALA:HB1	1:B:48:GLU:OE1	1.98	0.64
1:E:346:PHE:H	1:E:349:GLN:HE21	1.46	0.64
1:A:243:SER:HB2	1:A:244:PRO:HD3	1.79	0.64
1:C:37:LYS:NZ	2:C:504:HOH:O	2.30	0.63
1:A:338:ASP:O	1:A:363:LYS:HG2	1.99	0.62
1:H:183:ALA:O	1:H:187:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:GLU:HG3	1:H:371:ILE:HG13	1.83	0.60
1:H:180:PHE:HE1	1:H:344:GLU:OE1	1.84	0.60
1:H:263:LYS:HA	1:H:267:ARG:NH1	2.17	0.59
1:H:305:TRP:O	1:H:329:LYS:HE3	2.02	0.59
1:D:207:LYS:NZ	1:D:209:LYS:O	2.32	0.59
1:A:207:LYS:HG3	1:A:212:MET:HE1	1.85	0.59
1:D:293:LYS:NZ	2:D:503:HOH:O	2.36	0.59
1:C:329:LYS:HG3	2:C:530:HOH:O	2.02	0.58
1:H:22:SER:OG	1:H:219:GLU:OE2	2.15	0.58
1:H:120:MET:HG3	1:H:277:ASN:O	2.03	0.58
1:H:398:ALA:O	1:H:419:LYS:HE2	2.04	0.58
1:G:140:LYS:NZ	2:G:509:HOH:O	2.36	0.58
1:F:388:LEU:O	1:F:392:MET:HG3	2.04	0.58
1:D:22:SER:OG	1:D:219:GLU:OE2	2.11	0.57
1:G:222:LYS:NZ	2:G:505:HOH:O	2.31	0.57
1:F:346:PHE:H	1:F:349:GLN:HE21	1.53	0.56
1:A:175:ARG:O	1:A:179:GLU:HG3	2.05	0.56
1:D:242:GLU:HB2	1:D:246:PRO:HA	1.87	0.56
1:H:400:LYS:NZ	1:H:418:GLU:OE2	2.38	0.55
1:H:301:LYS:HD3	1:H:303:ILE:HG22	1.89	0.55
1:G:135:ARG:HH11	1:G:135:ARG:HG2	1.72	0.55
1:H:94:MET:HG3	1:H:385:ILE:HD11	1.88	0.55
1:C:2:ALA:HA	1:C:5:ASP:OD2	2.08	0.54
1:C:244:PRO:HB2	1:C:263:LYS:HZ3	1.73	0.54
1:G:346:PHE:H	1:G:349:GLN:HE21	1.55	0.54
1:C:120:MET:HE2	1:C:276:ILE:HG23	1.89	0.53
1:F:136:MET:HG2	1:G:146:ILE:HD11	1.90	0.53
1:H:120:MET:HE2	1:H:276:ILE:HG23	1.91	0.53
1:C:334:ILE:H	1:C:334:ILE:CD1	2.19	0.53
1:C:305:TRP:O	1:C:329:LYS:HD3	2.08	0.53
1:E:393:GLN:HG3	2:E:623:HOH:O	2.08	0.53
1:D:299:MET:CE	1:D:389:LEU:HB3	2.39	0.52
1:F:54:MET:HG2	1:F:84:TYR:CE1	2.45	0.52
1:G:394:LYS:NZ	2:G:512:HOH:O	2.42	0.52
1:E:242:GLU:HB2	1:E:246:PRO:HA	1.93	0.51
1:A:9:VAL:HA	1:A:298:PRO:HA	1.91	0.51
1:H:263:LYS:HA	1:H:267:ARG:HH12	1.73	0.51
1:E:140:LYS:HD3	1:H:139:LYS:O	2.10	0.51
1:F:391:GLU:OE2	1:F:395:ARG:NE	2.40	0.50
1:A:207:LYS:HG3	1:A:212:MET:CE	2.40	0.50
1:E:175:ARG:O	1:E:179:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:LYS:NZ	1:G:104:ILE:O	2.36	0.50
1:H:90:SCY:O	2:H:501:HOH:O	2.19	0.50
1:F:9:VAL:O	1:F:299:MET:HG3	2.11	0.50
1:B:146:ILE:HD11	1:C:136:MET:HG2	1.92	0.49
1:E:305:TRP:H	1:E:329:LYS:HD2	1.77	0.49
1:C:188:THR:OG1	1:C:368:GLY:HA3	2.12	0.49
1:E:392:MET:HE1	1:E:401:GLY:CA	2.25	0.49
1:B:231:ALA:HB2	2:B:502:HOH:O	2.13	0.49
1:H:94:MET:HB2	1:H:381:GLY:O	2.12	0.49
1:H:333:THR:N	1:H:336:ASP:OD2	2.41	0.49
1:H:344:GLU:HG3	1:H:371:ILE:H	1.77	0.49
1:B:145:MET:HE1	1:B:276:ILE:HD13	1.95	0.49
1:A:3:MET:HA	1:A:288:GLY:HA3	1.96	0.48
1:A:9:VAL:O	1:A:299:MET:HG3	2.13	0.48
1:F:222:LYS:HE2	2:F:513:HOH:O	2.12	0.48
1:F:9:VAL:HA	1:F:298:PRO:HA	1.96	0.48
1:H:15:ALA:N	2:H:502:HOH:O	2.22	0.48
1:A:90:SCY:O	1:A:405:LEU:HD11	2.14	0.48
1:H:324:ARG:O	1:H:328:LYS:HG3	2.14	0.48
1:B:388:LEU:O	1:B:392:MET:HG3	2.14	0.47
1:C:263:LYS:HZ3	1:C:263:LYS:HB3	1.79	0.47
1:A:235:GLY:HA3	1:A:266:GLN:HB3	1.97	0.47
1:B:227:ALA:O	2:B:502:HOH:O	2.20	0.47
1:D:305:TRP:H	1:D:329:LYS:HD2	1.80	0.47
1:G:237:PHE:O	1:G:266:GLN:HG2	2.14	0.47
1:G:360:ASP:HB3	1:G:363:LYS:HD2	1.95	0.47
1:E:5:ASP:CG	1:E:301:LYS:HE3	2.35	0.47
1:F:360:ASP:HB3	1:F:363:LYS:HD2	1.97	0.47
1:A:188:THR:OG1	1:A:368:GLY:HA3	2.15	0.46
1:B:391:GLU:OE2	2:B:503:HOH:O	2.20	0.46
1:G:9:VAL:HA	1:G:298:PRO:HA	1.97	0.46
1:G:176:GLU:OE1	2:G:502:HOH:O	2.20	0.46
1:F:208:VAL:HG12	1:F:209:LYS:HD2	1.97	0.46
1:H:247:VAL:O	1:H:313:LYS:NZ	2.34	0.46
1:H:354:ALA:HB1	1:H:361:MET:CE	2.46	0.46
1:E:188:THR:OG1	1:E:368:GLY:HA3	2.16	0.45
1:A:186:GLN:NE2	1:A:225:VAL:O	2.48	0.45
1:C:9:VAL:HA	1:C:298:PRO:HA	1.97	0.45
1:B:263:LYS:HA	1:B:267:ARG:NH1	2.31	0.45
1:G:166:ILE:HD13	1:G:317:VAL:HG13	1.99	0.45
1:D:139:LYS:NZ	2:D:502:HOH:O	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:HB3	2:A:583:HOH:O	2.15	0.45
1:C:58:ILE:HD13	1:C:89:VAL:HA	1.98	0.45
1:F:58:ILE:HD13	1:F:89:VAL:HA	1.98	0.45
1:A:243:SER:CB	1:A:244:PRO:HD3	2.46	0.45
1:C:48:GLU:CD	1:C:48:GLU:H	2.21	0.45
1:C:47:PRO:HD2	1:C:48:GLU:OE2	2.17	0.45
1:B:186:GLN:NE2	1:B:225:VAL:O	2.45	0.44
1:E:232:LYS:HD3	1:E:232:LYS:HA	1.58	0.44
1:B:48:GLU:H	1:B:48:GLU:CD	2.20	0.44
1:G:305:TRP:H	1:G:329:LYS:HD2	1.83	0.44
1:B:136:MET:HG3	1:C:146:ILE:HD11	1.99	0.44
1:E:231:ALA:HB3	1:E:232:LYS:HE2	1.99	0.44
1:H:397:GLU:O	1:H:399:LYS:HG2	2.18	0.44
1:H:188:THR:OG1	1:H:368:GLY:HA3	2.19	0.43
1:H:192:GLN:HE22	1:H:221:PRO:HG2	1.83	0.43
1:H:397:GLU:HG2	1:H:398:ALA:N	2.33	0.43
1:A:215:PHE:HE1	1:A:219:GLU:HG3	1.83	0.43
1:B:22:SER:HB3	1:B:206:ILE:HD13	1.99	0.43
1:E:53:LEU:O	1:E:83:ALA:HA	2.18	0.43
1:H:262:ASP:O	1:H:267:ARG:NH1	2.44	0.43
1:A:274:SER:HB3	1:A:344:GLU:O	2.18	0.43
1:B:9:VAL:HA	1:B:298:PRO:HA	1.99	0.43
1:H:41:LYS:HD3	1:H:41:LYS:HA	1.92	0.43
1:D:35:VAL:HG23	1:D:282:ALA:HB2	2.01	0.43
1:C:8:VAL:HG13	1:C:283:ILE:HG23	2.00	0.43
1:G:135:ARG:HG2	1:G:135:ARG:NH1	2.34	0.43
1:H:215:PHE:HE1	1:H:219:GLU:HG3	1.84	0.43
1:H:341:GLU:HG3	1:H:388:LEU:HB2	2.01	0.43
1:C:2:ALA:O	1:C:288:GLY:HA3	2.18	0.43
1:H:220:TYR:N	1:H:221:PRO:HD2	2.34	0.43
1:G:53:LEU:O	1:G:83:ALA:HA	2.19	0.42
1:H:334:ILE:HA	1:H:337:ILE:CD1	2.49	0.42
1:B:398:ALA:O	1:B:419:LYS:HE2	2.19	0.42
1:F:188:THR:OG1	1:F:368:GLY:HA3	2.19	0.42
1:B:207:LYS:HE2	1:B:209:LYS:O	2.20	0.42
1:E:9:VAL:HA	1:E:298:PRO:HA	2.02	0.42
1:E:148:ASP:OD2	2:E:503:HOH:O	2.20	0.42
1:A:155:ASN:HB3	1:A:157:TYR:CE2	2.55	0.42
1:A:349:GLN:HE21	1:A:349:GLN:HB2	1.69	0.42
1:B:125:PHE:HB3	1:B:141:LEU:HD22	2.02	0.42
1:B:301:LYS:HD2	1:B:303:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ALA:HB1	1:C:7:TYR:OH	2.20	0.42
1:C:90:SCY:O	1:C:405:LEU:HD11	2.20	0.42
1:C:151:TRP:CZ2	1:C:157:TYR:HA	2.55	0.42
1:C:169:ILE:HD11	1:C:246:PRO:HB2	2.02	0.42
1:C:242:GLU:OE2	1:C:247:VAL:HG12	2.20	0.41
1:E:90:SCY:O	1:E:405:LEU:HD11	2.19	0.41
1:F:3:MET:HA	2:F:553:HOH:O	2.19	0.41
1:G:242:GLU:H	1:G:242:GLU:HG2	1.65	0.41
1:D:218:ASP:HB3	2:D:543:HOH:O	2.20	0.41
1:D:422:GLU:H	1:D:422:GLU:HG3	1.71	0.41
1:F:241:PRO:O	1:F:242:GLU:HG3	2.20	0.41
1:H:207:LYS:HA	1:H:212:MET:HE3	2.02	0.41
1:A:53:LEU:O	1:A:83:ALA:HA	2.20	0.41
1:B:235:GLY:HA3	1:B:266:GLN:HB3	2.02	0.41
1:C:178:ASP:HB3	1:C:230:ILE:HD11	2.02	0.41
1:E:42:ARG:NH1	2:E:511:HOH:O	2.47	0.41
1:H:207:LYS:HE2	1:H:209:LYS:O	2.21	0.41
1:A:243:SER:CB	1:A:244:PRO:CD	2.99	0.41
1:A:319:PRO:HB3	1:A:404:THR:OG1	2.20	0.41
1:A:243:SER:HB2	1:A:244:PRO:CD	2.48	0.41
1:B:243:SER:OG	1:B:264:GLY:HA2	2.21	0.41
1:A:157:TYR:CD1	1:A:161:THR:HB	2.56	0.41
1:H:316:GLY:HA3	1:H:349:GLN:HB3	2.02	0.41
1:B:4:LYS:NZ	2:B:520:HOH:O	2.50	0.41
1:C:53:LEU:O	1:C:83:ALA:HA	2.20	0.41
1:D:150:LEU:O	1:D:159:MET:HG2	2.21	0.41
1:D:9:VAL:HA	1:D:298:PRO:HA	2.03	0.41
1:E:337:ILE:HG23	1:E:401:GLY:HA2	2.03	0.41
1:A:242:GLU:CB	1:A:246:PRO:HA	2.50	0.40
1:F:241:PRO:O	1:F:243:SER:N	2.54	0.40
1:G:173:THR:HG22	1:G:261:PRO:HD2	2.02	0.40
1:D:171:GLY:HA3	1:D:258:GLN:O	2.22	0.40
1:E:166:ILE:HD13	1:E:317:VAL:HG13	2.03	0.40
1:A:397:GLU:O	1:A:399:LYS:HG2	2.21	0.40
1:E:209:LYS:HB3	1:E:209:LYS:HE2	1.99	0.40
1:E:329:LYS:HB2	1:E:329:LYS:HE3	1.78	0.40
1:A:419:LYS:HB3	1:A:419:LYS:HE2	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLU:OE2	1:E:395:ARG:NH2[1_565]	2.12	0.08

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	416/428 (97%)	403 (97%)	11 (3%)	2 (0%)	29	18
1	B	417/428 (97%)	402 (96%)	14 (3%)	1 (0%)	47	38
1	C	418/428 (98%)	406 (97%)	11 (3%)	1 (0%)	47	38
1	D	420/428 (98%)	409 (97%)	10 (2%)	1 (0%)	47	38
1	E	418/428 (98%)	403 (96%)	14 (3%)	1 (0%)	47	38
1	F	420/428 (98%)	404 (96%)	14 (3%)	2 (0%)	29	18
1	G	417/428 (97%)	400 (96%)	16 (4%)	1 (0%)	47	38
1	H	414/428 (97%)	401 (97%)	12 (3%)	1 (0%)	47	38
All	All	3340/3424 (98%)	3228 (97%)	102 (3%)	10 (0%)	41	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	SER
1	A	89	VAL
1	B	89	VAL
1	C	89	VAL
1	D	89	VAL
1	G	89	VAL
1	H	89	VAL
1	E	89	VAL
1	F	89	VAL
1	F	242	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/321 (96%)	299 (97%)	10 (3%)	39	30
1	B	311/321 (97%)	303 (97%)	8 (3%)	46	39
1	C	312/321 (97%)	307 (98%)	5 (2%)	62	60
1	D	314/321 (98%)	307 (98%)	7 (2%)	52	47
1	E	315/321 (98%)	307 (98%)	8 (2%)	47	41
1	F	316/321 (98%)	309 (98%)	7 (2%)	52	47
1	G	313/321 (98%)	308 (98%)	5 (2%)	62	60
1	H	310/321 (97%)	293 (94%)	17 (6%)	21	12
All	All	2500/2568 (97%)	2433 (97%)	67 (3%)	44	38

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	24	LYS
1	A	55	PHE
1	A	136	MET
1	A	232	LYS
1	A	297	LYS
1	A	315	MET
1	A	334	ILE
1	A	349	GLN
1	A	361	MET
1	B	4	LYS
1	B	44	ASN
1	B	48	GLU
1	B	55	PHE
1	B	89	VAL
1	B	222	LYS
1	B	315	MET
1	B	375	HIS
1	C	55	PHE

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Mol	Chain	Res	Type
1	C	89	VAL
1	C	209	LYS
1	C	315	MET
1	C	349	GLN
1	D	55	PHE
1	D	196	ARG
1	D	199	ASP
1	D	232	LYS
1	D	293	LYS
1	D	315	MET
1	D	335	ASP
1	E	3	MET
1	E	55	PHE
1	E	196	ARG
1	E	207	LYS
1	E	209	LYS
1	E	210	LYS
1	E	293	LYS
1	E	315	MET
1	F	24	LYS
1	F	55	PHE
1	F	89	VAL
1	F	209	LYS
1	F	210	LYS
1	F	232	LYS
1	F	315	MET
1	G	55	PHE
1	G	136	MET
1	G	157	TYR
1	G	234	LYS
1	G	315	MET
1	H	4	LYS
1	H	24	LYS
1	H	55	PHE
1	H	89	VAL
1	H	174	ARG
1	H	175	ARG
1	H	180	PHE
1	H	226	THR
1	H	245	ASN
1	H	253	GLU
1	H	293	LYS

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Mol	Chain	Res	Type
1	H	297	LYS
1	H	315	MET
1	H	328	LYS
1	H	349	GLN
1	H	375	HIS
1	H	405	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	393	GLN
1	B	349	GLN
1	B	367	ASN
1	D	63	GLN
1	D	349	GLN
1	E	349	GLN
1	F	349	GLN
1	G	349	GLN
1	H	192	GLN
1	H	349	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	SCY	F	90	1	7,8,9	1.56	2 (28%)	3,9,11	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SCY	A	90	1	7,8,9	0.95	0	3,9,11	0.47	0
1	SCY	C	90	1	7,8,9	1.64	1 (14%)	3,9,11	0.61	0
1	SCY	E	90	1	7,8,9	2.10	2 (28%)	3,9,11	1.48	0
1	SCY	G	90	1	7,8,9	1.72	2 (28%)	3,9,11	0.28	0
1	SCY	D	90	1	7,8,9	1.48	1 (14%)	3,9,11	0.52	0
1	SCY	H	90	1	7,8,9	1.23	1 (14%)	3,9,11	0.90	0
1	SCY	B	90	1	7,8,9	1.33	2 (28%)	3,9,11	0.60	0

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
1	SCY	F	90	1	-	0/5/7/9	-
1	SCY	A	90	1	-	0/5/7/9	-
1	SCY	C	90	1	-	2/5/7/9	-
1	SCY	E	90	1	-	2/5/7/9	-
1	SCY	G	90	1	-	2/5/7/9	-
1	SCY	D	90	1	-	2/5/7/9	-
1	SCY	H	90	1	-	2/5/7/9	-
1	SCY	B	90	1	-	2/5/7/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	90	SCY	CB-SG	-4.42	1.71	1.81
1	C	90	SCY	CB-SG	-3.67	1.72	1.81
1	F	90	SCY	CB-SG	-3.31	1.73	1.81
1	G	90	SCY	CB-SG	-3.30	1.73	1.81
1	D	90	SCY	CB-SG	-3.06	1.74	1.81
1	B	90	SCY	CB-SG	-2.40	1.75	1.81
1	G	90	SCY	O-C	2.37	1.29	1.19
1	E	90	SCY	CB-CA	2.36	1.59	1.53
1	H	90	SCY	CB-SG	-2.13	1.76	1.81
1	B	90	SCY	O-C	2.05	1.28	1.19
1	F	90	SCY	O-C	2.01	1.27	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	90	SCY	OCD-CD-SG-CB
1	C	90	SCY	CE-CD-SG-CB
1	D	90	SCY	OCD-CD-SG-CB
1	D	90	SCY	CE-CD-SG-CB
1	E	90	SCY	OCD-CD-SG-CB
1	G	90	SCY	OCD-CD-SG-CB
1	G	90	SCY	CE-CD-SG-CB
1	H	90	SCY	OCD-CD-SG-CB
1	H	90	SCY	CE-CD-SG-CB
1	E	90	SCY	CE-CD-SG-CB
1	B	90	SCY	OCD-CD-SG-CB
1	B	90	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	90	SCY	1	0
1	C	90	SCY	1	0
1	E	90	SCY	1	0
1	H	90	SCY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	418/428 (97%)	-0.20	4 (0%) 82 84	35, 51, 80, 98	0
1	B	419/428 (97%)	-0.32	0 100 100	36, 47, 67, 83	0
1	C	420/428 (98%)	-0.32	2 (0%) 91 92	33, 44, 68, 83	0
1	D	422/428 (98%)	-0.36	1 (0%) 95 95	33, 43, 60, 90	0
1	E	420/428 (98%)	-0.25	4 (0%) 82 84	31, 41, 59, 103	0
1	F	422/428 (98%)	-0.24	2 (0%) 91 92	30, 44, 70, 87	0
1	G	419/428 (97%)	-0.36	2 (0%) 91 92	34, 45, 60, 84	0
1	H	416/428 (97%)	0.29	22 (5%) 26 29	36, 68, 98, 113	0
All	All	3356/3424 (98%)	-0.22	37 (1%) 80 82	30, 47, 79, 113	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	228	ASP	4.7
1	E	3	MET	4.2
1	H	232	LYS	3.8
1	E	423	HIS	3.8
1	H	253	GLU	3.4
1	A	225	VAL	3.3
1	H	260	ALA	3.3
1	A	224	GLY	3.2
1	H	175	ARG	3.1
1	G	210	LYS	3.1
1	H	223	ALA	3.1
1	H	208	VAL	3.1
1	A	421	LEU	2.9
1	A	226	THR	2.8
1	D	425	HIS	2.8
1	F	421	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	209	LYS	2.7
1	F	422	GLU	2.7
1	E	422	GLU	2.7
1	H	75	ALA	2.6
1	H	224	GLY	2.4
1	G	421	LEU	2.4
1	H	262	ASP	2.4
1	H	190	ALA	2.4
1	H	366	VAL	2.3
1	H	245	ASN	2.3
1	H	234	LYS	2.3
1	H	191	ALA	2.2
1	H	352	ALA	2.2
1	H	194	ALA	2.2
1	H	374	GLY	2.2
1	E	209	LYS	2.2
1	C	209	LYS	2.1
1	H	335	ASP	2.1
1	H	233	LEU	2.1
1	C	210	LYS	2.1
1	H	364	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SCY	H	90	9/10	0.87	0.14	49,57,65,74	0
1	SCY	G	90	9/10	0.90	0.08	35,41,51,58	0
1	SCY	E	90	9/10	0.90	0.11	33,38,46,71	0
1	SCY	C	90	9/10	0.91	0.10	36,42,48,67	0
1	SCY	B	90	9/10	0.92	0.10	39,42,48,64	0
1	SCY	A	90	9/10	0.92	0.09	41,46,53,69	0
1	SCY	D	90	9/10	0.92	0.11	35,37,47,61	0
1	SCY	F	90	9/10	0.94	0.11	36,41,51,59	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.