Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2019 – 05:04 PM EDT

PDB ID	:	6N3P
Title	:	Crosslinked AcpP=FabZ complex from E. coli Type II FAS
Authors	:	Smith, J.L.; Dodge, G.J.
Deposited on	:	2018-11-15
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

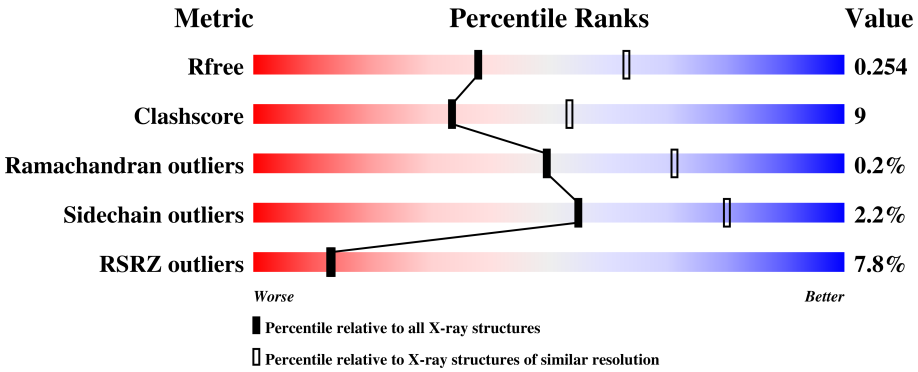
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	154	2% 82% 11% • 6%
1	B	154	77% 17% • 6%
1	C	154	2% 71% 20% • 6%
1	D	154	% 80% 15% 5%
1	E	154	2% 80% 15% 5%

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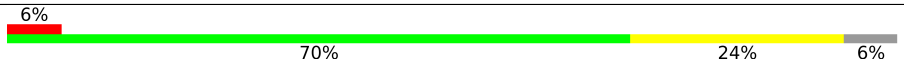
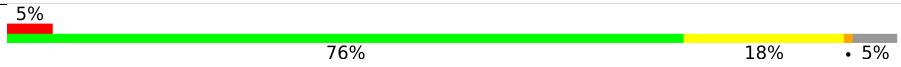
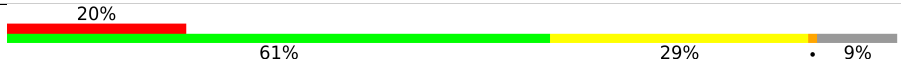
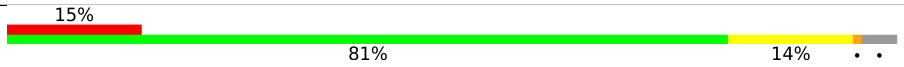
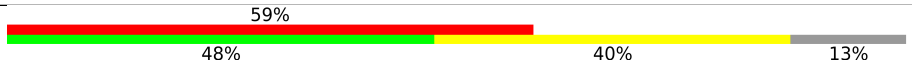
Mol	Chain	Length	Quality of chain
1	F	154	
2	G	80	
2	H	80	
2	I	80	
2	J	80	
2	K	80	
2	L	80	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10775 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 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1146	745	197	197	7			
1	B	145	Total	C	N	O	S	0	0	0
			1153	749	198	199	7			
1	C	144	Total	C	N	O	S	0	0	0
			1142	743	194	198	7			
1	D	146	Total	C	N	O	S	0	0	0
			1161	753	200	201	7			
1	E	146	Total	C	N	O	S	0	0	0
			1162	754	199	202	7			
1	F	146	Total	C	N	O	S	0	0	0
			1162	754	199	202	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B7MBG1
A	-1	ASN	-	expression tag	UNP B7MBG1
A	0	ALA	-	expression tag	UNP B7MBG1
A	151	ALA	-	expression tag	UNP B7MBG1
B	-2	SER	-	expression tag	UNP B7MBG1
B	-1	ASN	-	expression tag	UNP B7MBG1
B	0	ALA	-	expression tag	UNP B7MBG1
B	151	ALA	-	expression tag	UNP B7MBG1
C	-2	SER	-	expression tag	UNP B7MBG1
C	-1	ASN	-	expression tag	UNP B7MBG1
C	0	ALA	-	expression tag	UNP B7MBG1
C	151	ALA	-	expression tag	UNP B7MBG1
D	-2	SER	-	expression tag	UNP B7MBG1
D	-1	ASN	-	expression tag	UNP B7MBG1
D	0	ALA	-	expression tag	UNP B7MBG1
D	151	ALA	-	expression tag	UNP B7MBG1
E	-2	SER	-	expression tag	UNP B7MBG1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP B7MBG1
E	0	ALA	-	expression tag	UNP B7MBG1
E	151	ALA	-	expression tag	UNP B7MBG1
F	-2	SER	-	expression tag	UNP B7MBG1
F	-1	ASN	-	expression tag	UNP B7MBG1
F	0	ALA	-	expression tag	UNP B7MBG1
F	151	ALA	-	expression tag	UNP B7MBG1

- Molecule 2 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	72	Total	C	N	O	S	0	0	0
			562	349	85	127	1			
2	H	75	Total	C	N	O	S	0	0	0
			585	362	91	131	1			
2	I	76	Total	C	N	O	S	0	0	0
			587	363	91	132	1			
2	J	73	Total	C	N	O	S	0	0	0
			566	351	86	128	1			
2	K	77	Total	C	N	O	S	0	0	0
			596	368	93	134	1			
2	L	70	Total	C	N	O	S	0	0	0
			547	341	82	123	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	expression tag	UNP B7MJ81
G	-1	ASN	-	expression tag	UNP B7MJ81
G	0	ALA	-	expression tag	UNP B7MJ81
H	-2	SER	-	expression tag	UNP B7MJ81
H	-1	ASN	-	expression tag	UNP B7MJ81
H	0	ALA	-	expression tag	UNP B7MJ81
I	-2	SER	-	expression tag	UNP B7MJ81
I	-1	ASN	-	expression tag	UNP B7MJ81
I	0	ALA	-	expression tag	UNP B7MJ81
J	-2	SER	-	expression tag	UNP B7MJ81
J	-1	ASN	-	expression tag	UNP B7MJ81
J	0	ALA	-	expression tag	UNP B7MJ81
K	-2	SER	-	expression tag	UNP B7MJ81
K	-1	ASN	-	expression tag	UNP B7MJ81
K	0	ALA	-	expression tag	UNP B7MJ81

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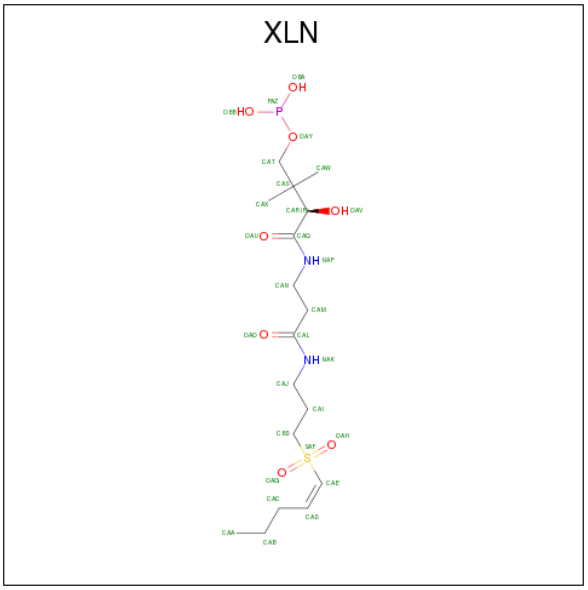
Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP B7MJ81
L	-1	ASN	-	expression tag	UNP B7MJ81
L	0	ALA	-	expression tag	UNP B7MJ81

- Molecule 3 is N 3 -{(2R)-4-[(dihydroxyphosphanyl)oxy]-2-hydroxy-3,3-dimethylbutanoyl}-N-(3-{[(1Z)-pent-1-en-1-yl]sulfonyl}propyl)-beta-alaninamide (three-letter code: XLN) (formula: $C_{17}H_{33}N_2O_8PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	B	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	C	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	D	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	E	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	F	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

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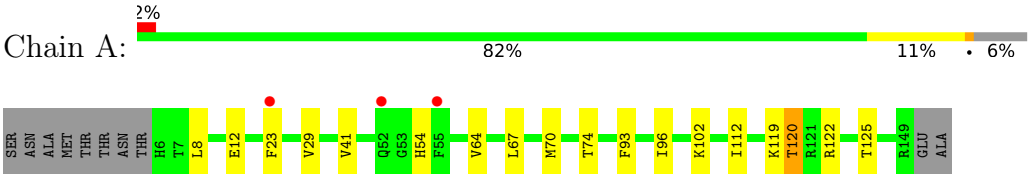
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total O 5 5	0	0
4	C	9	Total O 9 9	0	0
4	D	6	Total O 6 6	0	0
4	E	12	Total O 12 12	0	0
4	F	5	Total O 5 5	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0
4	I	3	Total O 3 3	0	0
4	J	4	Total O 4 4	0	0
4	K	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

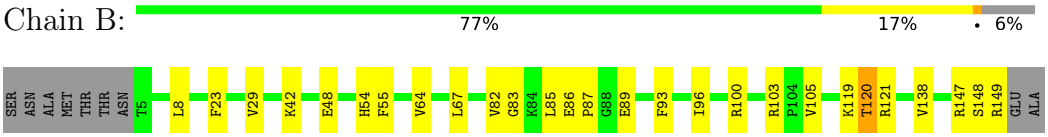
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

Chain A:



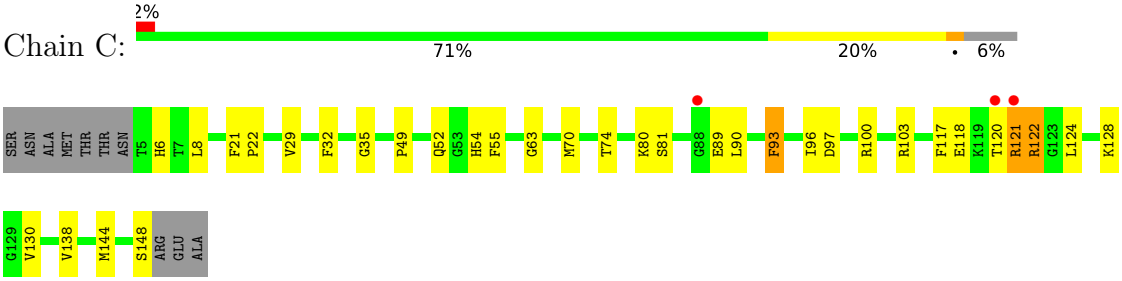
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

Chain B:



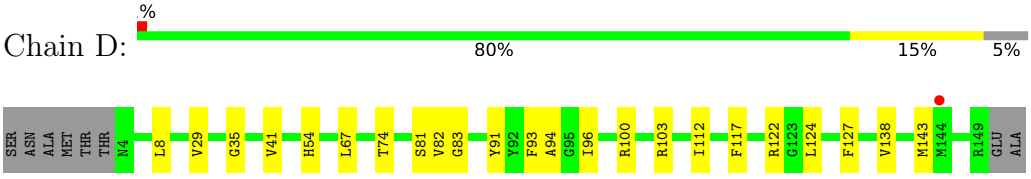
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

Chain C:



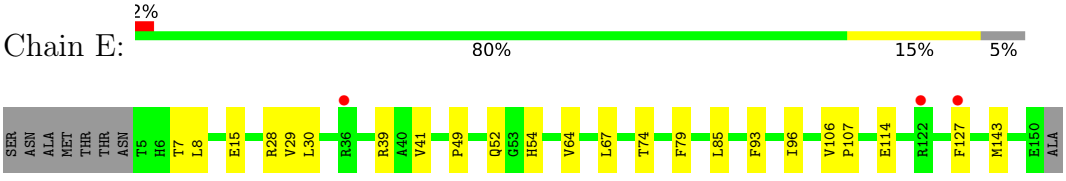
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

Chain D:



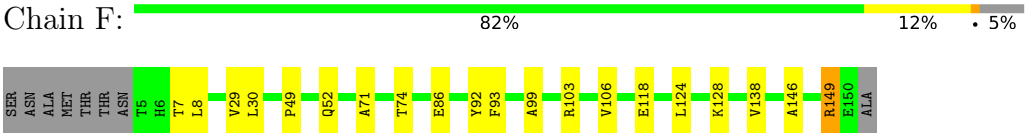
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

Chain E:



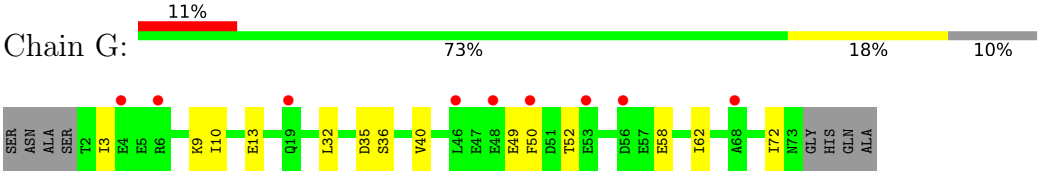
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ

Chain F:



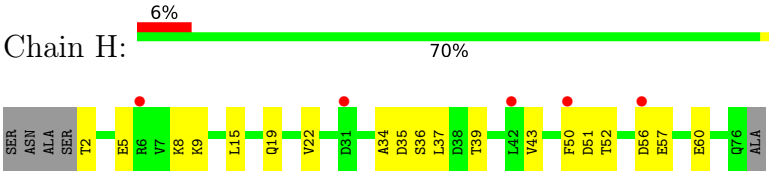
• Molecule 2: Acyl carrier protein

Chain G:



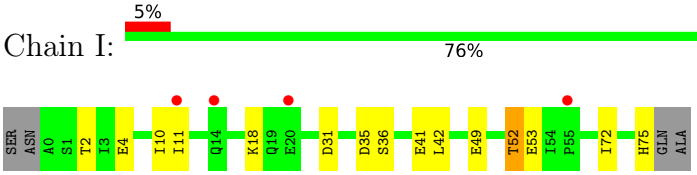
• Molecule 2: Acyl carrier protein

Chain H:



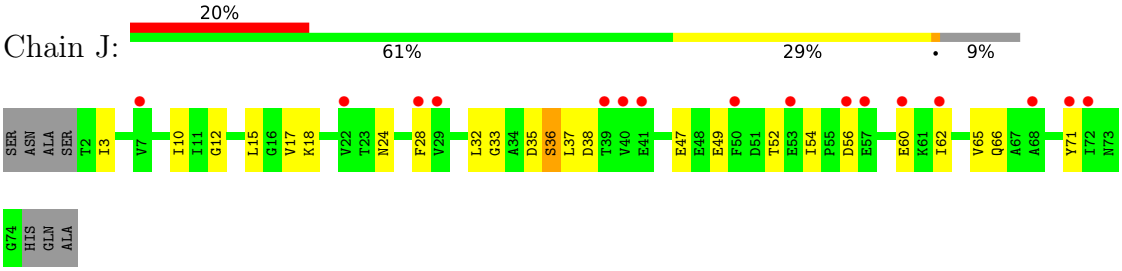
• Molecule 2: Acyl carrier protein

Chain I:



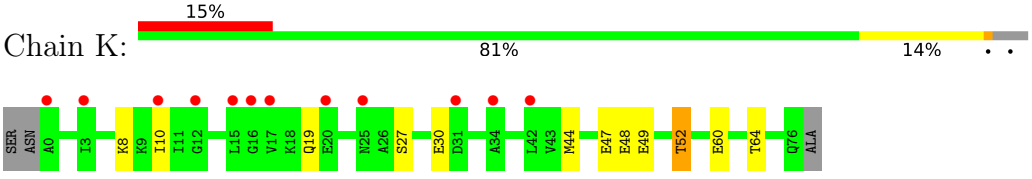
• Molecule 2: Acyl carrier protein

Chain J:



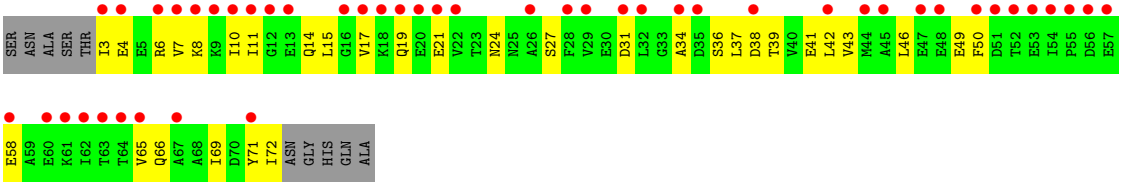
• Molecule 2: Acyl carrier protein

Chain K:



• Molecule 2: Acyl carrier protein

Chain L:


SER
ASN
ALA
SER
THR
I3
E4
E5
R6
V7
K8
K9
I10
I11
G12
E13
Q14
L15
G16
V17
K18
Q19
E20
E21
V22
T23
N24
N25
A26
S27
F28
V29
E30
D31
L32
G33
A34
D35
S36
L37
D38
T39
V40
E41
L42
V43
M44
A45
L46
E47
E48
E49
F50
D51
T52
E53
I54
P55
D56
E57
E58
A59
E60
K61
I62
T63
T64
V65
Q66
A67
A68
I69
D70
Y71
I72
ASN
GLY
HIS
GLN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.14Å 136.19Å 152.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 2.50 49.49 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.49-2.50) 89.3 (49.49-2.41)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.257 0.210 , 0.254	Depositor DCC
R_{free} test set	1997 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10775	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: XLN

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	0.55	0/1172	0.68	0/1579
1	B	0.50	0/1179	0.64	0/1589
1	C	0.47	0/1168	0.62	0/1575
1	D	0.50	0/1187	0.67	0/1600
1	E	0.50	0/1188	0.67	0/1601
1	F	0.43	0/1188	0.62	0/1601
2	G	0.41	0/565	0.53	0/765
2	H	0.46	0/589	0.63	0/797
2	I	0.74	0/591	0.68	0/800
2	J	0.46	0/569	0.64	0/770
2	K	0.43	0/600	0.59	0/812
2	L	0.32	0/550	0.57	0/744
All	All	0.49	0/10546	0.64	0/14233

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1146	0	1173	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1153	0	1180	22	0
1	C	1142	0	1167	26	0
1	D	1161	0	1186	18	0
1	E	1162	0	1186	17	0
1	F	1162	0	1186	18	0
2	G	562	0	542	7	0
2	H	585	0	560	10	0
2	I	587	0	565	10	0
2	J	566	0	545	17	0
2	K	596	0	573	9	0
2	L	547	0	529	36	0
3	A	58	0	0	7	0
3	B	58	0	0	3	0
3	C	58	0	0	12	0
3	D	58	0	0	2	0
3	E	58	0	0	1	0
3	F	58	0	0	0	0
4	A	9	0	0	0	0
4	B	5	0	0	0	0
4	C	9	0	0	0	0
4	D	6	0	0	0	0
4	E	12	0	0	1	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	3	0	0	0	0
4	J	4	0	0	0	0
4	K	3	0	0	0	0
All	All	10775	0	10392	194	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 9.

All (194) 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:F:86:GLU:HG3	1:F:149:ARG:NH2	1.42	1.32
1:F:86:GLU:HG3	1:F:149:ARG:HH22	1.21	1.03
1:F:86:GLU:CG	1:F:149:ARG:NH2	2.22	1.01
1:C:54:HIS:CE1	3:C:400[B]:XLN:CAB	2.44	0.96
2:L:7:VAL:HB	2:L:69:ILE:HD11	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:GLU:HG3	1:F:149:ARG:HH21	1.29	0.91
1:C:54:HIS:HE1	3:C:400[B]:XLN:CAB	1.83	0.91
1:D:54:HIS:CE1	3:D:400[A]:XLN:CAB	2.55	0.90
2:L:7:VAL:HG21	2:L:69:ILE:CD1	2.01	0.88
1:C:63:GLY:H	3:C:400[B]:XLN:CBD	1.90	0.85
2:L:7:VAL:CB	2:L:69:ILE:HD11	2.07	0.84
2:G:35:ASP:OD1	2:G:36:SER:N	2.14	0.81
3:C:400[B]:XLN:CAX	2:L:37:LEU:HD21	2.11	0.79
2:L:7:VAL:HG21	2:L:69:ILE:HD13	1.64	0.78
1:C:89:GLU:HG3	1:C:148:SER:HB2	1.64	0.77
1:B:120:THR:C	1:B:121:ARG:HG2	2.06	0.75
1:B:55:PHE:CD2	3:B:400[B]:XLN:CAB	2.69	0.75
1:F:86:GLU:CG	1:F:149:ARG:HH22	1.93	0.74
1:B:55:PHE:CE2	3:B:400[B]:XLN:CAB	2.71	0.74
2:K:47:GLU:HG3	2:K:52:THR:O	1.87	0.73
1:A:102:LYS:HE2	2:I:41:GLU:OE2	1.89	0.73
3:A:400[B]:XLN:CAX	2:I:35:ASP:OD2	2.36	0.73
2:J:35:ASP:OD1	2:J:38:ASP:N	2.22	0.72
1:D:54:HIS:HE1	3:D:400[A]:XLN:CAB	1.99	0.72
2:L:6:ARG:NH2	2:L:49:GLU:OE2	2.24	0.71
2:I:52:THR:OG1	2:I:53:GLU:N	2.23	0.70
1:F:86:GLU:CB	1:F:149:ARG:NH2	2.55	0.70
2:H:50:PHE:O	2:H:52:THR:N	2.26	0.69
2:L:7:VAL:CG2	2:L:69:ILE:CD1	2.70	0.69
1:A:54:HIS:CD2	3:A:400[A]:XLN:CAD	2.71	0.69
3:A:400[A]:XLN:CAX	2:I:35:ASP:OD2	2.40	0.69
1:C:55:PHE:CD2	3:C:400[B]:XLN:CAA	2.77	0.68
1:C:103:ARG:HB2	1:C:138:VAL:HG12	1.75	0.67
3:C:400[A]:XLN:CAX	2:L:37:LEU:HD21	2.24	0.67
2:H:8:LYS:NZ	2:H:22:VAL:O	2.28	0.67
2:L:11:ILE:HG12	2:L:42:LEU:HD21	1.78	0.66
2:H:15:LEU:HD21	2:H:34:ALA:HB2	1.77	0.66
1:A:54:HIS:CE1	3:A:400[A]:XLN:CAD	2.72	0.66
1:B:54:HIS:CE1	3:B:400[B]:XLN:CAB	2.78	0.66
2:H:9:LYS:HA	2:H:19:GLN:HE22	1.61	0.66
1:E:39:ARG:NH1	1:E:114:GLU:OE2	2.29	0.65
1:C:97:ASP:OD1	1:D:100:ARG:NH2	2.29	0.65
1:C:63:GLY:N	3:C:400[B]:XLN:CBD	2.60	0.65
2:J:15:LEU:HD22	2:J:33:GLY:O	1.96	0.64
1:F:8:LEU:HB2	1:F:29:VAL:HB	1.80	0.64
1:E:74:THR:HG21	1:E:127:PHE:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MET:O	1:C:74:THR:HG23	1.98	0.63
1:C:124:LEU:HD11	1:C:144:MET:HB3	1.81	0.63
1:A:54:HIS:NE2	3:A:400[A]:XLN:CAE	2.29	0.62
2:I:11:ILE:HG12	2:I:42:LEU:HD11	1.81	0.62
1:A:67:LEU:HD13	1:A:96:ILE:HD13	1.81	0.62
2:K:10:ILE:HD11	2:K:49:GLU:HG2	1.81	0.61
1:C:8:LEU:HB2	1:C:29:VAL:HB	1.82	0.60
1:D:8:LEU:HB2	1:D:29:VAL:HB	1.82	0.60
1:B:8:LEU:HB2	1:B:29:VAL:HB	1.83	0.60
2:I:2:THR:HG22	2:I:4:GLU:H	1.66	0.60
2:L:46:LEU:HD13	2:L:72:ILE:HD11	1.83	0.59
2:L:7:VAL:CB	2:L:69:ILE:CD1	2.80	0.59
1:C:121:ARG:NH1	2:H:56:ASP:OD1	2.32	0.59
1:B:67:LEU:HD13	1:B:96:ILE:HD13	1.84	0.59
1:C:55:PHE:CE2	3:C:400[B]:XLN:CAA	2.86	0.59
2:J:24:ASN:O	2:J:66:GLN:N	2.36	0.59
2:H:9:LYS:HA	2:H:19:GLN:NE2	2.17	0.59
1:D:82:VAL:HG12	1:D:83:GLY:H	1.68	0.59
2:K:8:LYS:HB3	2:K:19:GLN:OE1	2.02	0.59
1:C:6:HIS:HB3	1:C:32:PHE:CE1	2.37	0.58
1:A:54:HIS:CE1	3:A:400[B]:XLN:CAB	2.87	0.58
1:B:103:ARG:HB2	1:B:138:VAL:HG22	1.86	0.57
2:J:17:VAL:HG12	2:J:18:LYS:O	2.03	0.57
2:J:10:ILE:HD11	2:J:49:GLU:HG2	1.86	0.57
1:D:67:LEU:HD13	1:D:96:ILE:HD13	1.87	0.57
2:J:24:ASN:HB3	2:J:66:GLN:HG2	1.87	0.56
1:C:118:GLU:OE1	1:C:128:LYS:HB2	2.05	0.56
1:F:118:GLU:OE2	1:F:128:LYS:HB2	2.07	0.55
2:H:35:ASP:O	2:H:37:LEU:N	2.40	0.55
1:A:119:LYS:HZ3	2:K:48:GLU:HG2	1.72	0.54
1:E:74:THR:HG21	1:E:127:PHE:CD1	2.43	0.54
1:E:96:ILE:HB	1:F:99:ALA:HB3	1.89	0.54
1:E:8:LEU:HB2	1:E:29:VAL:HB	1.89	0.54
2:J:47:GLU:HG3	2:J:52:THR:O	2.07	0.54
1:A:41:VAL:HG22	1:A:112:ILE:HD13	1.90	0.53
1:C:100:ARG:NH2	2:L:14:GLN:O	2.42	0.53
2:L:27:SER:O	2:L:31:ASP:HB2	2.09	0.53
1:F:92:TYR:CE2	1:F:146:ALA:HB3	2.44	0.53
1:F:86:GLU:CG	1:F:149:ARG:HH21	2.05	0.53
1:C:90:LEU:H	1:C:148:SER:HA	1.73	0.52
1:A:122:ARG:NH1	2:K:60:GLU:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:ILE:HD11	2:G:49:GLU:HG2	1.91	0.52
1:B:82:VAL:HG12	1:B:83:GLY:H	1.75	0.52
1:A:8:LEU:HB2	1:A:29:VAL:HB	1.92	0.52
1:D:41:VAL:HG22	1:D:112:ILE:HD13	1.90	0.52
2:G:50:PHE:HD2	2:G:72:ILE:HD12	1.74	0.52
1:F:49:PRO:O	1:F:52:GLN:HG2	2.11	0.51
2:L:15:LEU:O	2:L:17:VAL:HG23	2.10	0.51
2:L:10:ILE:HD11	2:L:49:GLU:HG2	1.92	0.51
1:F:103:ARG:HB2	1:F:138:VAL:HG12	1.93	0.51
1:E:106:VAL:HG22	1:E:107:PRO:HD2	1.92	0.51
2:J:17:VAL:CG1	2:J:18:LYS:N	2.74	0.50
1:B:120:THR:O	1:B:121:ARG:HG2	2.12	0.50
3:C:400[B]:XLN:CAX	2:L:37:LEU:CD2	2.85	0.50
2:J:56:ASP:O	2:J:60:GLU:HG2	2.09	0.50
1:C:93:PHE:CZ	1:C:96:ILE:HD11	2.46	0.50
2:L:39:THR:O	2:L:43:VAL:HG23	2.11	0.50
1:D:103:ARG:HB2	1:D:138:VAL:HG12	1.93	0.49
1:B:119:LYS:HD2	1:B:121:ARG:NH2	2.27	0.49
1:C:117:PHE:CE1	1:C:120:THR:OG1	2.64	0.49
2:L:34:ALA:HB1	2:L:38:ASP:HB2	1.94	0.49
2:L:24:ASN:O	2:L:66:GLN:N	2.46	0.49
2:J:12:GLY:O	2:J:15:LEU:O	2.31	0.49
1:D:127:PHE:CZ	1:D:143:MET:HB2	2.48	0.48
1:A:64:VAL:HB	1:B:64:VAL:HB	1.95	0.48
1:D:94:ALA:HB1	2:L:37:LEU:HD13	1.94	0.48
1:E:127:PHE:CZ	1:E:143:MET:HB2	2.49	0.48
2:J:15:LEU:CD2	2:J:33:GLY:O	2.61	0.48
2:I:72:ILE:O	2:I:72:ILE:HG22	2.14	0.48
1:E:7:THR:O	1:E:8:LEU:HD23	2.14	0.48
1:C:49:PRO:O	1:C:52:GLN:HG2	2.13	0.48
1:B:105:VAL:CG2	1:B:138:VAL:HG11	2.43	0.47
1:D:124:LEU:HD12	2:L:37:LEU:HD22	1.96	0.47
1:E:74:THR:HG21	1:E:127:PHE:CD2	2.49	0.47
2:J:28:PHE:HE2	2:J:62:ILE:HG22	1.78	0.47
1:E:28:ARG:HB3	1:E:41:VAL:CG1	2.45	0.47
1:A:8:LEU:HA	1:A:12:GLU:OE2	2.15	0.47
1:F:124:LEU:HD12	2:G:40:VAL:HG21	1.96	0.47
2:G:9:LYS:O	2:G:13:GLU:HG3	2.14	0.47
2:J:54:ILE:HG12	2:J:71:TYR:CE1	2.50	0.47
1:E:49:PRO:O	1:E:52:GLN:HG2	2.15	0.46
2:J:24:ASN:ND2	2:J:66:GLN:OE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:VAL:HG11	2:L:69:ILE:CD1	2.46	0.46
2:G:32:LEU:N	2:G:32:LEU:HD23	2.30	0.46
2:L:11:ILE:HD13	2:L:65:VAL:HG22	1.96	0.46
2:I:18:LYS:HB3	2:I:18:LYS:HE2	1.74	0.46
1:B:119:LYS:CG	1:B:121:ARG:NH2	2.79	0.46
1:D:35:GLY:N	1:D:81:SER:OG	2.45	0.46
1:E:67:LEU:HD13	1:E:96:ILE:HD13	1.97	0.45
1:A:120:THR:HG23	1:A:125:THR:HG23	1.99	0.45
1:A:54:HIS:CE1	3:A:400[A]:XLN:CAE	2.97	0.45
1:F:118:GLU:OE2	1:F:128:LYS:HE3	2.15	0.45
2:J:24:ASN:O	2:J:65:VAL:HB	2.16	0.45
2:I:31:ASP:N	2:I:31:ASP:OD1	2.48	0.45
3:C:400[B]:XLN:CAX	2:L:37:LEU:HD11	2.46	0.45
1:B:89:GLU:OE2	1:B:147:ARG:HD3	2.17	0.45
2:H:57:GLU:O	2:H:60:GLU:HB3	2.17	0.45
2:I:10:ILE:HD11	2:I:49:GLU:HB2	1.98	0.45
1:D:82:VAL:HG12	1:D:83:GLY:N	2.30	0.45
1:B:100:ARG:HD3	1:B:100:ARG:HA	1.78	0.44
2:L:46:LEU:HA	2:L:46:LEU:HD23	1.83	0.44
1:D:124:LEU:CD1	2:L:37:LEU:HD22	2.47	0.44
1:E:28:ARG:HB3	1:E:41:VAL:HG13	2.00	0.44
2:L:7:VAL:CG1	2:L:69:ILE:HD11	2.47	0.44
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.83	0.44
1:E:54:HIS:CE1	3:E:400[B]:XLN:CAB	3.01	0.43
2:H:2:THR:N	2:H:5:GLU:OE1	2.52	0.43
2:L:50:PHE:HE2	2:L:72:ILE:HG21	1.84	0.43
3:C:400[A]:XLN:OAU	2:L:37:LEU:HD11	2.18	0.43
1:A:70:MET:O	1:A:74:THR:HG23	2.19	0.43
1:C:121:ARG:HG3	1:C:122:ARG:HG2	2.01	0.43
1:D:122:ARG:HA	1:D:122:ARG:HD2	1.86	0.43
1:B:148:SER:OG	1:B:149:ARG:N	2.52	0.43
1:F:71:ALA:O	1:F:74:THR:OG1	2.31	0.43
2:H:39:THR:O	2:H:43:VAL:HG23	2.19	0.43
2:K:27:SER:HA	2:K:64:THR:HG22	2.00	0.43
1:E:15:GLU:HG3	4:E:502:HOH:O	2.17	0.43
1:E:7:THR:HG22	1:E:30:LEU:O	2.19	0.43
2:L:37:LEU:O	2:L:41:GLU:HG3	2.20	0.42
1:A:119:LYS:HE2	2:K:44:MET:HG2	2.01	0.42
3:C:400[B]:XLN:CAX	2:L:37:LEU:CG	2.97	0.42
1:B:119:LYS:HD2	1:B:121:ARG:HH21	1.84	0.42
2:L:3:ILE:HG22	2:L:4:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HD11	1:C:80:LYS:HE3	2.02	0.42
1:D:74:THR:HG22	1:D:91:TYR:OH	2.19	0.42
1:B:119:LYS:HG3	1:B:121:ARG:NH2	2.34	0.42
1:B:42:LYS:NZ	1:B:48:GLU:OE1	2.52	0.42
2:L:58:GLU:HB3	2:L:71:TYR:CE2	2.55	0.42
1:B:86:GLU:HB3	1:B:87:PRO:HD2	2.02	0.42
1:C:35:GLY:N	1:C:81:SER:OG	2.50	0.42
2:L:8:LYS:C	2:L:19:GLN:HE22	2.23	0.41
1:A:120:THR:HG22	1:A:125:THR:OG1	2.20	0.41
1:D:74:THR:HG23	1:D:117:PHE:HE1	1.84	0.41
2:G:58:GLU:O	2:G:62:ILE:HD12	2.20	0.41
1:B:85:LEU:HD22	1:B:89:GLU:HB3	2.01	0.41
1:A:119:LYS:HZ1	2:K:47:GLU:HB3	1.85	0.41
1:D:96:ILE:HG12	1:D:143:MET:HG2	2.01	0.41
2:J:17:VAL:HG21	2:J:32:LEU:HD22	2.01	0.41
1:F:128:LYS:HE3	1:F:128:LYS:HB2	1.85	0.41
2:J:36:SER:O	2:J:37:LEU:HD23	2.20	0.41
1:C:90:LEU:O	1:C:148:SER:N	2.37	0.41
1:F:7:THR:HG22	1:F:30:LEU:O	2.21	0.41
1:C:117:PHE:HE1	1:C:120:THR:OG1	2.04	0.41
2:L:6:ARG:O	2:L:10:ILE:HG13	2.21	0.40
2:L:17:VAL:CG1	2:L:21:GLU:HB3	2.52	0.40
1:E:79:PHE:CZ	1:E:85:LEU:HD22	2.56	0.40
2:K:27:SER:OG	2:K:30:GLU:HB2	2.21	0.40
1:C:21:PHE:HA	1:C:22:PRO:HA	1.87	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	142/154 (92%)	137 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	143/154 (93%)	137 (96%)	6 (4%)	0	100 100
1	C	142/154 (92%)	137 (96%)	5 (4%)	0	100 100
1	D	144/154 (94%)	136 (94%)	8 (6%)	0	100 100
1	E	144/154 (94%)	137 (95%)	7 (5%)	0	100 100
1	F	144/154 (94%)	139 (96%)	5 (4%)	0	100 100
2	G	70/80 (88%)	66 (94%)	4 (6%)	0	100 100
2	H	73/80 (91%)	69 (94%)	2 (3%)	2 (3%)	5 8
2	I	74/80 (92%)	71 (96%)	3 (4%)	0	100 100
2	J	71/80 (89%)	67 (94%)	4 (6%)	0	100 100
2	K	75/80 (94%)	70 (93%)	5 (7%)	0	100 100
2	L	68/80 (85%)	62 (91%)	6 (9%)	0	100 100
All	All	1290/1404 (92%)	1228 (95%)	60 (5%)	2 (0%)	49 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	51	ASP
2	H	36	SER

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	122/130 (94%)	119 (98%)	3 (2%)	50 77
1	B	123/130 (95%)	120 (98%)	3 (2%)	52 78
1	C	122/130 (94%)	118 (97%)	4 (3%)	41 68
1	D	124/130 (95%)	123 (99%)	1 (1%)	83 94
1	E	124/130 (95%)	122 (98%)	2 (2%)	65 86
1	F	124/130 (95%)	121 (98%)	3 (2%)	52 78
2	G	63/68 (93%)	61 (97%)	2 (3%)	42 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	65/68 (96%)	65 (100%)	0	100	100
2	I	65/68 (96%)	62 (95%)	3 (5%)	29	53
2	J	63/68 (93%)	61 (97%)	2 (3%)	42	69
2	K	66/68 (97%)	65 (98%)	1 (2%)	67	87
2	L	61/68 (90%)	60 (98%)	1 (2%)	65	86
All	All	1122/1188 (94%)	1097 (98%)	25 (2%)	55	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	93	PHE
1	A	120	THR
1	B	23	PHE
1	B	93	PHE
1	B	120	THR
1	C	93	PHE
1	C	121	ARG
1	C	122	ARG
1	C	130	VAL
1	D	93	PHE
1	E	64	VAL
1	E	93	PHE
1	F	93	PHE
1	F	106	VAL
1	F	149	ARG
2	G	3	ILE
2	G	52	THR
2	I	36	SER
2	I	52	THR
2	I	75	HIS
2	J	3	ILE
2	J	36	SER
2	K	52	THR
2	L	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	6	HIS
2	J	14	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

12 ligands 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	$\#\|Z\| > 2$
3	XLN	A	400[A]	1,2	21,28,28	3.28	7 (33%)	27,37,37	4.13	4 (14%)
3	XLN	A	400[B]	1,2	21,28,28	1.95	3 (14%)	27,37,37	3.35	2 (7%)
3	XLN	B	400[A]	1,2	21,28,28	3.26	4 (19%)	27,37,37	4.27	6 (22%)
3	XLN	B	400[B]	1,2	21,28,28	2.06	3 (14%)	27,37,37	3.61	1 (3%)
3	XLN	C	400[A]	1,2	21,28,28	2.73	3 (14%)	27,37,37	3.85	5 (18%)
3	XLN	C	400[B]	1,2	21,28,28	2.12	3 (14%)	27,37,37	3.20	4 (14%)
3	XLN	D	400[A]	1,2	21,28,28	2.41	3 (14%)	27,37,37	3.67	5 (18%)
3	XLN	D	400[B]	1,2	21,28,28	2.67	3 (14%)	27,37,37	3.78	7 (25%)
3	XLN	E	400[A]	1,2	21,28,28	1.89	2 (9%)	27,37,37	3.86	4 (14%)
3	XLN	E	400[B]	1,2	21,28,28	3.63	7 (33%)	27,37,37	4.54	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	XLN	F	400[A]	1,2	21,28,28	2.45	3 (14%)	27,37,37	3.96	1 (3%)
3	XLN	F	400[B]	1,2	21,28,28	2.55	3 (14%)	27,37,37	3.77	2 (7%)

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	XLN	A	400[A]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	A	400[B]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	B	400[A]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	B	400[B]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	C	400[A]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	C	400[B]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	D	400[A]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	D	400[B]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	E	400[A]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	E	400[B]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	F	400[A]	1,2	-	1/34/36/36	0/0/0/0
3	XLN	F	400[B]	1,2	-	1/34/36/36	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400[A]	XLN	CBD-SAF	-10.06	1.61	1.77
3	E	400[B]	XLN	CBD-SAF	-9.96	1.61	1.77
3	A	400[A]	XLN	CBD-SAF	-9.62	1.62	1.77
3	C	400[A]	XLN	CBD-SAF	-9.27	1.63	1.77
3	D	400[B]	XLN	CBD-SAF	-8.96	1.63	1.77
3	F	400[B]	XLN	CBD-SAF	-8.84	1.63	1.77
3	E	400[B]	XLN	OAH-SAF	-8.69	1.37	1.44
3	D	400[A]	XLN	CBD-SAF	-8.59	1.64	1.77
3	F	400[A]	XLN	CBD-SAF	-8.40	1.64	1.77
3	E	400[B]	XLN	OAG-SAF	-8.09	1.38	1.44
3	B	400[B]	XLN	CBD-SAF	-8.04	1.64	1.77
3	B	400[A]	XLN	OAH-SAF	-8.00	1.38	1.44
3	C	400[B]	XLN	CBD-SAF	-7.98	1.65	1.77
3	E	400[A]	XLN	CBD-SAF	-7.85	1.65	1.77
3	A	400[B]	XLN	CBD-SAF	-7.79	1.65	1.77
3	A	400[A]	XLN	OAH-SAF	-7.12	1.38	1.44
3	A	400[A]	XLN	OAG-SAF	-7.07	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400[A]	XLN	OAG-SAF	-5.97	1.39	1.44
3	D	400[B]	XLN	OAG-SAF	-5.93	1.39	1.44
3	B	400[A]	XLN	OAG-SAF	-5.35	1.40	1.44
3	F	400[B]	XLN	OAH-SAF	-5.12	1.40	1.44
3	F	400[A]	XLN	OAH-SAF	-4.98	1.40	1.44
3	C	400[A]	XLN	OAH-SAF	-4.94	1.40	1.44
3	D	400[A]	XLN	OAG-SAF	-4.88	1.40	1.44
3	F	400[B]	XLN	OAG-SAF	-4.69	1.40	1.44
3	F	400[A]	XLN	OAG-SAF	-4.56	1.40	1.44
3	D	400[B]	XLN	OAH-SAF	-4.41	1.40	1.44
3	D	400[A]	XLN	OAH-SAF	-3.57	1.41	1.44
3	C	400[B]	XLN	OAH-SAF	-3.52	1.41	1.44
3	C	400[B]	XLN	OAG-SAF	-3.51	1.41	1.44
3	B	400[B]	XLN	OAH-SAF	-3.24	1.41	1.44
3	B	400[A]	XLN	OAO-CAL	-2.88	1.17	1.23
3	B	400[B]	XLN	OAG-SAF	-2.61	1.42	1.44
3	E	400[B]	XLN	OAU-CAQ	-2.56	1.18	1.23
3	A	400[B]	XLN	OAG-SAF	-2.50	1.42	1.44
3	A	400[A]	XLN	OAO-CAL	-2.49	1.18	1.23
3	A	400[B]	XLN	OAH-SAF	-2.44	1.42	1.44
3	A	400[A]	XLN	OAU-CAQ	-2.29	1.18	1.23
3	E	400[B]	XLN	OAO-CAL	-2.19	1.18	1.23
3	A	400[A]	XLN	CAW-CAS	-2.14	1.49	1.53
3	E	400[B]	XLN	CAQ-NAP	-2.12	1.29	1.33
3	E	400[A]	XLN	OAH-SAF	-2.07	1.42	1.44
3	E	400[B]	XLN	CAN-NAP	-2.02	1.41	1.46
3	A	400[A]	XLN	CAL-NAK	-2.01	1.28	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	400[B]	XLN	OAH-SAF-OAG	-21.84	106.32	118.22
3	B	400[A]	XLN	OAH-SAF-OAG	-20.73	106.93	118.22
3	A	400[A]	XLN	OAH-SAF-OAG	-20.50	107.05	118.22
3	F	400[A]	XLN	OAH-SAF-OAG	-20.21	107.21	118.22
3	E	400[A]	XLN	OAH-SAF-OAG	-19.01	107.86	118.22
3	F	400[B]	XLN	OAH-SAF-OAG	-18.95	107.89	118.22
3	C	400[A]	XLN	OAH-SAF-OAG	-18.72	108.02	118.22
3	D	400[B]	XLN	OAH-SAF-OAG	-18.15	108.33	118.22
3	B	400[B]	XLN	OAH-SAF-OAG	-18.12	108.35	118.22
3	D	400[A]	XLN	OAH-SAF-OAG	-17.80	108.52	118.22
3	A	400[B]	XLN	OAH-SAF-OAG	-16.84	109.05	118.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	400[B]	XLN	OAH-SAF-OAG	-15.57	109.74	118.22
3	B	400[A]	XLN	CAW-CAS-CAR	-3.18	103.30	108.82
3	E	400[B]	XLN	CAW-CAS-CAR	-3.15	103.36	108.82
3	C	400[A]	XLN	CAN-CAM-CAL	-3.05	107.28	112.36
3	A	400[A]	XLN	CAN-NAP-CAQ	-2.94	117.24	122.59
3	C	400[A]	XLN	CAN-NAP-CAQ	-2.90	117.31	122.59
3	D	400[B]	XLN	CAC-CAD-CAE	-2.88	120.16	125.50
3	B	400[A]	XLN	CAN-NAP-CAQ	-2.73	117.63	122.59
3	C	400[A]	XLN	CAC-CAD-CAE	-2.70	120.48	125.50
3	C	400[B]	XLN	CAN-CAM-CAL	-2.65	107.94	112.36
3	C	400[A]	XLN	CAJ-NAK-CAL	-2.64	117.86	122.84
3	D	400[A]	XLN	CAN-CAM-CAL	-2.63	107.97	112.36
3	D	400[B]	XLN	CAN-NAP-CAQ	-2.51	118.03	122.59
3	E	400[A]	XLN	CAN-CAM-CAL	-2.47	108.24	112.36
3	D	400[A]	XLN	CAN-NAP-CAQ	-2.44	118.15	122.59
3	A	400[A]	XLN	CAW-CAS-CAR	-2.35	104.74	108.82
3	A	400[B]	XLN	CAN-CAM-CAL	-2.27	108.58	112.36
3	C	400[B]	XLN	CAJ-NAK-CAL	-2.25	118.60	122.84
3	D	400[B]	XLN	CAW-CAS-CAR	-2.12	105.14	108.82
3	C	400[B]	XLN	CAN-NAP-CAQ	-2.08	118.81	122.59
3	D	400[B]	XLN	CAN-CAM-CAL	-2.08	108.89	112.36
3	D	400[A]	XLN	CAJ-NAK-CAL	-2.06	118.95	122.84
3	D	400[B]	XLN	CAJ-NAK-CAL	-2.02	119.03	122.84
3	E	400[B]	XLN	CAN-CAM-CAL	-2.02	109.00	112.36
3	B	400[A]	XLN	CAJ-NAK-CAL	-2.01	119.06	122.84
3	A	400[A]	XLN	CAD-CAE-SAF	2.04	127.64	122.33
3	B	400[A]	XLN	CAD-CAE-SAF	2.36	128.46	122.33
3	F	400[B]	XLN	OAH-SAF-CAE	2.72	112.70	108.86
3	E	400[A]	XLN	CAW-CAS-CAT	2.78	112.77	108.23
3	D	400[B]	XLN	OAG-SAF-CAE	2.81	112.82	108.86
3	B	400[A]	XLN	CAX-CAS-CAT	2.89	112.95	108.23
3	E	400[A]	XLN	OAH-SAF-CAE	3.02	113.13	108.86
3	D	400[A]	XLN	OAG-SAF-CAE	3.30	113.51	108.86
3	E	400[B]	XLN	OAH-SAF-CAE	4.30	114.94	108.86
3	E	400[B]	XLN	CAD-CAE-SAF	4.38	133.74	122.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	400[A]	XLN	CAC-CAD-CAE-SAF
3	C	400[A]	XLN	CAC-CAD-CAE-SAF

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Mol	Chain	Res	Type	Atoms
3	B	400[A]	XLN	CAC-CAD-CAE-SAF
3	B	400[B]	XLN	CAC-CAD-CAE-SAF
3	E	400[B]	XLN	CAC-CAD-CAE-SAF
3	F	400[B]	XLN	CAC-CAD-CAE-SAF
3	C	400[B]	XLN	CAC-CAD-CAE-SAF
3	A	400[B]	XLN	CAC-CAD-CAE-SAF
3	D	400[B]	XLN	CAC-CAD-CAE-SAF
3	E	400[A]	XLN	CAC-CAD-CAE-SAF
3	D	400[A]	XLN	CAC-CAD-CAE-SAF
3	A	400[A]	XLN	CAC-CAD-CAE-SAF

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400[A]	XLN	5	0
3	A	400[B]	XLN	2	0
3	B	400[B]	XLN	3	0
3	C	400[A]	XLN	2	0
3	C	400[B]	XLN	10	0
3	D	400[A]	XLN	2	0
3	E	400[B]	XLN	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, 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	144/154 (93%)	0.17	3 (2%) 63 66	39, 62, 90, 130	0
1	B	145/154 (94%)	0.09	0 100 100	41, 59, 92, 112	0
1	C	144/154 (93%)	0.28	3 (2%) 63 66	45, 66, 102, 191	0
1	D	146/154 (94%)	0.15	1 (0%) 87 88	46, 62, 89, 133	0
1	E	146/154 (94%)	0.23	3 (2%) 63 66	43, 62, 95, 120	0
1	F	146/154 (94%)	0.10	0 100 100	40, 61, 96, 129	0
2	G	72/80 (90%)	0.88	9 (12%) 4 3	69, 106, 162, 176	0
2	H	75/80 (93%)	0.39	5 (6%) 18 18	54, 81, 134, 142	0
2	I	76/80 (95%)	0.30	4 (5%) 26 28	55, 76, 121, 126	0
2	J	73/80 (91%)	1.36	16 (21%) 0 0	79, 118, 157, 203	0
2	K	77/80 (96%)	0.90	12 (15%) 2 1	60, 102, 147, 160	0
2	L	70/80 (87%)	3.44	47 (67%) 0 0	115, 159, 205, 224	0
All	All	1314/1404 (93%)	0.51	103 (7%) 13 13	39, 70, 150, 224	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	62	ILE	9.8
2	L	7	VAL	9.4
2	L	17	VAL	8.7
2	L	10	ILE	7.7
2	L	60	GLU	7.3
2	L	44	MET	7.2
2	L	61	LYS	7.0
2	L	55	PRO	7.0
2	J	68	ALA	6.9
2	L	3	ILE	6.5
2	L	56	ASP	6.4

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Mol	Chain	Res	Type	RSRZ
2	L	54	ILE	6.0
2	J	71	TYR	5.8
2	L	42	LEU	5.5
2	L	9	LYS	5.4
2	G	56	ASP	5.3
2	G	48	GLU	5.1
2	L	48	GLU	5.1
2	L	71	TYR	5.1
2	K	0	ALA	5.1
2	L	57	GLU	4.9
2	L	28	PHE	4.8
2	L	19	GLN	4.7
2	L	31	ASP	4.7
2	L	52	THR	4.6
2	K	15	LEU	4.3
2	L	38	ASP	4.2
2	K	17	VAL	4.2
2	L	20	GLU	4.2
2	J	29	VAL	4.2
2	L	45	ALA	4.1
2	K	12	GLY	4.0
2	L	16	GLY	3.9
2	L	8	LYS	3.8
2	L	18	LYS	3.8
2	L	32	LEU	3.7
2	L	22	VAL	3.7
2	J	50	PHE	3.6
2	L	67	ALA	3.6
2	J	62	ILE	3.5
2	L	50	PHE	3.4
2	L	29	VAL	3.3
2	G	50	PHE	3.3
2	J	53	GLU	3.3
2	G	53	GLU	3.2
2	L	35	ASP	3.2
2	L	53	GLU	3.2
2	L	47	GLU	3.2
2	J	40	VAL	3.1
2	L	6	ARG	3.1
2	K	16	GLY	3.0
2	K	20	GLU	3.0
2	J	57	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	G	46	LEU	2.9
2	L	21	GLU	2.8
2	I	11	ILE	2.7
2	G	68	ALA	2.7
2	H	56	ASP	2.7
2	L	58	GLU	2.7
1	C	120	THR	2.7
1	E	127	PHE	2.7
2	J	22	VAL	2.6
1	E	122	ARG	2.6
2	L	64	THR	2.6
1	A	23	PHE	2.6
2	J	72	ILE	2.6
2	J	56	ASP	2.6
2	L	65	VAL	2.5
2	J	7	VAL	2.5
2	L	13	GLU	2.5
2	L	26	ALA	2.5
1	A	55	PHE	2.4
2	G	19	GLN	2.4
2	H	50	PHE	2.4
2	J	28	PHE	2.4
2	H	31	ASP	2.4
2	J	60	GLU	2.3
2	H	42	LEU	2.3
2	I	14	GLN	2.3
2	K	10	ILE	2.3
2	I	20	GLU	2.3
2	K	31	ASP	2.3
2	L	63	THR	2.3
1	E	36	ARG	2.2
2	K	3	ILE	2.2
2	G	4	GLU	2.2
2	L	11	ILE	2.2
1	A	52	GLN	2.2
2	L	4	GLU	2.2
2	L	34	ALA	2.1
2	H	6	ARG	2.1
2	J	41	GLU	2.1
2	G	6	ARG	2.1
2	K	25	ASN	2.1
1	C	88	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	42	LEU	2.1
2	K	34	ALA	2.1
2	J	39	THR	2.1
2	L	51	ASP	2.1
2	L	12	GLY	2.1
2	I	55	PRO	2.0
1	C	121	ARG	2.0
1	D	144	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	XLN	C	400[A]	29/29	0.80	0.29	65,93,118,121	29
3	XLN	C	400[B]	29/29	0.80	0.29	77,93,118,120	29
3	XLN	F	400[A]	29/29	0.86	0.19	59,71,100,103	29
3	XLN	F	400[B]	29/29	0.86	0.19	49,71,99,104	29
3	XLN	E	400[B]	29/29	0.88	0.17	46,69,84,92	29
3	XLN	B	400[A]	29/29	0.88	0.20	62,78,83,90	29
3	XLN	E	400[A]	29/29	0.88	0.17	53,69,83,90	29
3	XLN	B	400[B]	29/29	0.88	0.20	63,77,83,88	29
3	XLN	A	400[B]	29/29	0.89	0.19	57,71,85,86	29
3	XLN	A	400[A]	29/29	0.89	0.19	54,72,87,88	29
3	XLN	D	400[A]	29/29	0.91	0.17	67,78,86,96	29
3	XLN	D	400[B]	29/29	0.91	0.17	62,76,87,96	29

6.5 Other polymers (i)

There are no such residues in this entry.