Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 06:36 AM EST

PDB ID	:	6BZF
Title	:	Structure of S. cerevisiae Zip2:Spo16 complex, C2 form
Authors	:	Arora, K.; Corbett, K.D.
Deposited on	:	2017-12-23
Resolution	:	2.29 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

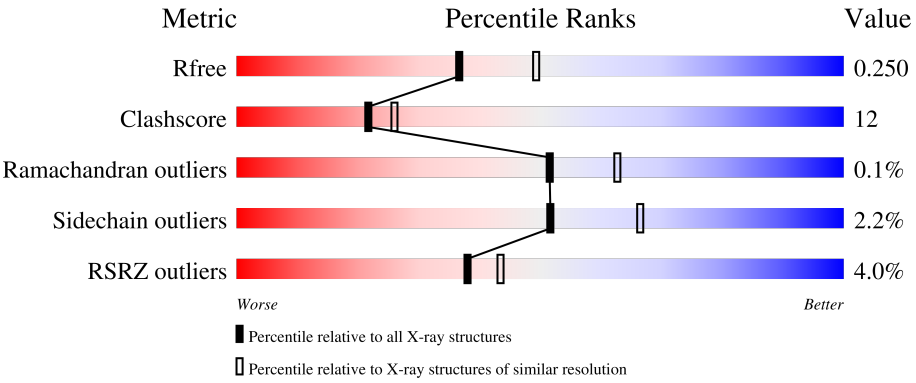
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.29 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	216	4% 62% 29% 9%
1	E	216	6% 57% 23% · 19%
2	B	206	2% 78% 21% ·
3	C	216	3% 72% 19% 9%
3	G	216	7% 59% 20% · 19%

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Mol	Chain	Length	Quality of chain
4	D	206	
5	F	206	
5	H	206	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13182 atoms, of which 1 is hydrogen 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 Sporulation-specific protein 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1627	1044	272	308	3			
1	E	175	Total	C	N	O	S	0	0	0
			1440	936	235	267	2			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP P17122
A	-16	LYS	-	expression tag	UNP P17122
A	-15	SER	-	expression tag	UNP P17122
A	-14	SER	-	expression tag	UNP P17122
A	-13	HIS	-	expression tag	UNP P17122
A	-12	HIS	-	expression tag	UNP P17122
A	-11	HIS	-	expression tag	UNP P17122
A	-10	HIS	-	expression tag	UNP P17122
A	-9	HIS	-	expression tag	UNP P17122
A	-8	HIS	-	expression tag	UNP P17122
A	-7	GLU	-	expression tag	UNP P17122
A	-6	ASN	-	expression tag	UNP P17122
A	-5	LEU	-	expression tag	UNP P17122
A	-4	TYR	-	expression tag	UNP P17122
A	-3	PHE	-	expression tag	UNP P17122
A	-2	GLN	-	expression tag	UNP P17122
A	-1	SER	-	expression tag	UNP P17122
A	0	ASN	-	expression tag	UNP P17122
A	1	ALA	-	expression tag	UNP P17122
E	-17	MET	-	expression tag	UNP P17122
E	-16	LYS	-	expression tag	UNP P17122
E	-15	SER	-	expression tag	UNP P17122
E	-14	SER	-	expression tag	UNP P17122
E	-13	HIS	-	expression tag	UNP P17122
E	-12	HIS	-	expression tag	UNP P17122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP P17122
E	-10	HIS	-	expression tag	UNP P17122
E	-9	HIS	-	expression tag	UNP P17122
E	-8	HIS	-	expression tag	UNP P17122
E	-7	GLU	-	expression tag	UNP P17122
E	-6	ASN	-	expression tag	UNP P17122
E	-5	LEU	-	expression tag	UNP P17122
E	-4	TYR	-	expression tag	UNP P17122
E	-3	PHE	-	expression tag	UNP P17122
E	-2	GLN	-	expression tag	UNP P17122
E	-1	SER	-	expression tag	UNP P17122
E	0	ASN	-	expression tag	UNP P17122
E	1	ALA	-	expression tag	UNP P17122

- Molecule 2 is a protein called Protein ZIP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1735	1131	279	316	9			

- Molecule 3 is a protein called Sporulation-specific protein 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	197	Total	C	N	O	S	0	0	0
			1625	1046	267	309	3			
3	G	174	Total	C	N	O	S	0	0	0
			1411	910	236	262	3			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	expression tag	UNP P17122
C	-16	LYS	-	expression tag	UNP P17122
C	-15	SER	-	expression tag	UNP P17122
C	-14	SER	-	expression tag	UNP P17122
C	-13	HIS	-	expression tag	UNP P17122
C	-12	HIS	-	expression tag	UNP P17122
C	-11	HIS	-	expression tag	UNP P17122
C	-10	HIS	-	expression tag	UNP P17122
C	-9	HIS	-	expression tag	UNP P17122
C	-8	HIS	-	expression tag	UNP P17122
C	-7	GLU	-	expression tag	UNP P17122

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	expression tag	UNP P17122
C	-5	LEU	-	expression tag	UNP P17122
C	-4	TYR	-	expression tag	UNP P17122
C	-3	PHE	-	expression tag	UNP P17122
C	-2	GLN	-	expression tag	UNP P17122
C	-1	SER	-	expression tag	UNP P17122
C	0	ASN	-	expression tag	UNP P17122
C	1	ALA	-	expression tag	UNP P17122
G	-17	MET	-	expression tag	UNP P17122
G	-16	LYS	-	expression tag	UNP P17122
G	-15	SER	-	expression tag	UNP P17122
G	-14	SER	-	expression tag	UNP P17122
G	-13	HIS	-	expression tag	UNP P17122
G	-12	HIS	-	expression tag	UNP P17122
G	-11	HIS	-	expression tag	UNP P17122
G	-10	HIS	-	expression tag	UNP P17122
G	-9	HIS	-	expression tag	UNP P17122
G	-8	HIS	-	expression tag	UNP P17122
G	-7	GLU	-	expression tag	UNP P17122
G	-6	ASN	-	expression tag	UNP P17122
G	-5	LEU	-	expression tag	UNP P17122
G	-4	TYR	-	expression tag	UNP P17122
G	-3	PHE	-	expression tag	UNP P17122
G	-2	GLN	-	expression tag	UNP P17122
G	-1	SER	-	expression tag	UNP P17122
G	0	ASN	-	expression tag	UNP P17122
G	1	ALA	-	expression tag	UNP P17122

- Molecule 4 is a protein called Protein ZIP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	206	Total	C	N	O	S	0	0	0
			1737	1133	279	316	9			

- Molecule 5 is a protein called Protein ZIP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	F	204	Total	C	H	N	O	S	0	0	0
			1705	1112	1	274	309	9			
5	H	200	Total	C		N	O	S	0	0	0
			1678	1096		270	303	9			

- Molecule 6 is water.

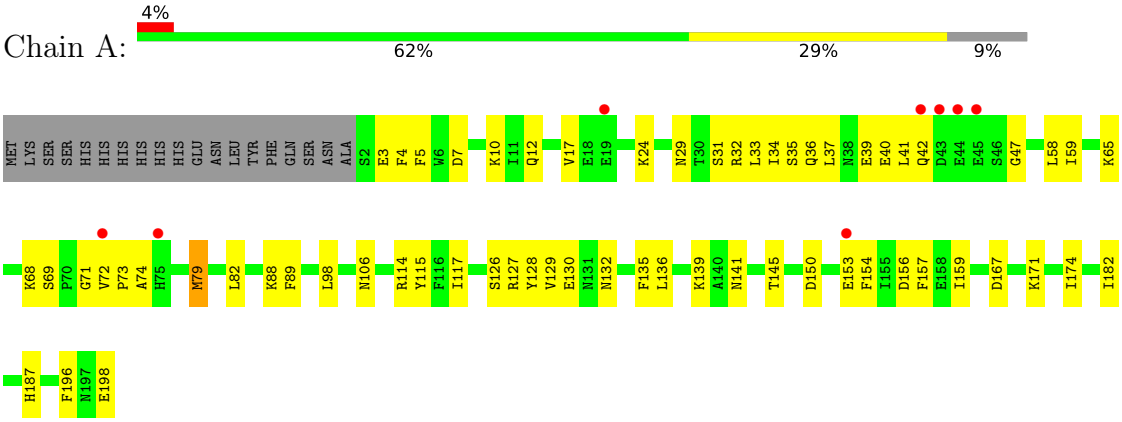
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total O 26 26	0	0
6	B	50	Total O 50 50	0	0
6	C	25	Total O 25 25	0	0
6	D	57	Total O 57 57	0	0
6	E	9	Total O 9 9	0	0
6	F	22	Total O 22 22	0	0
6	G	9	Total O 9 9	0	0
6	H	26	Total O 26 26	0	0

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.

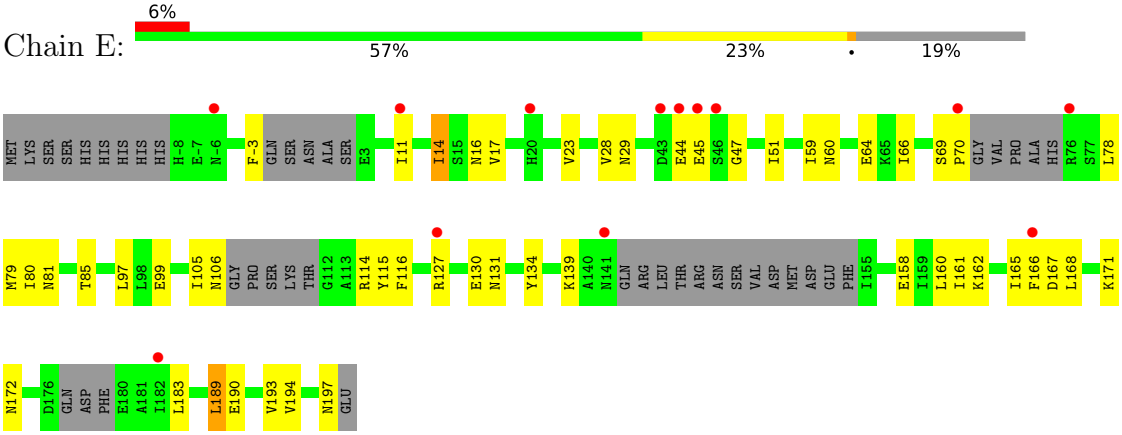
• Molecule 1: Sporulation-specific protein 16

Chain A:



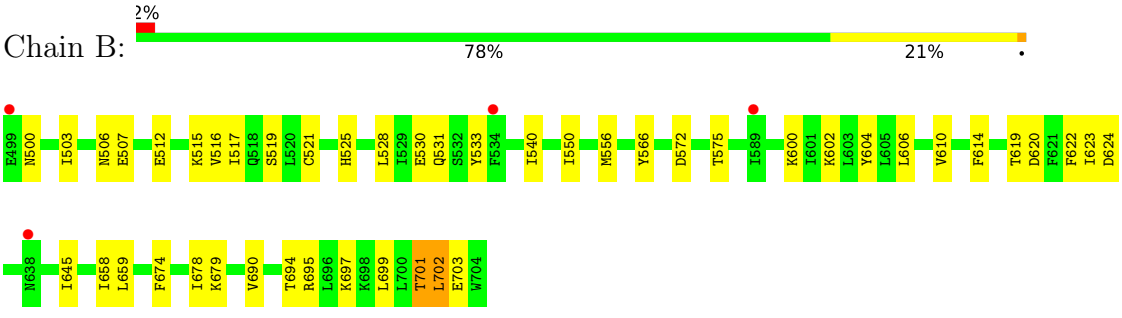
• Molecule 1: Sporulation-specific protein 16

Chain E:



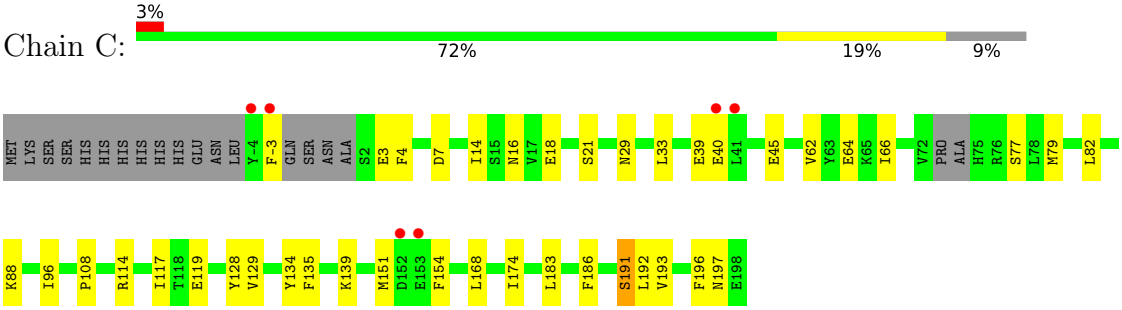
• Molecule 2: Protein ZIP2

Chain B:



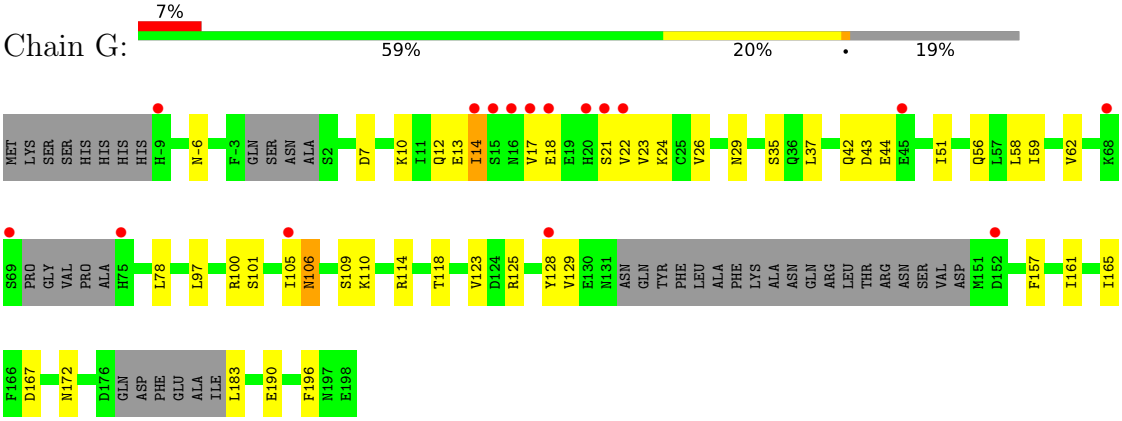
• Molecule 3: Sporulation-specific protein 16

Chain C:



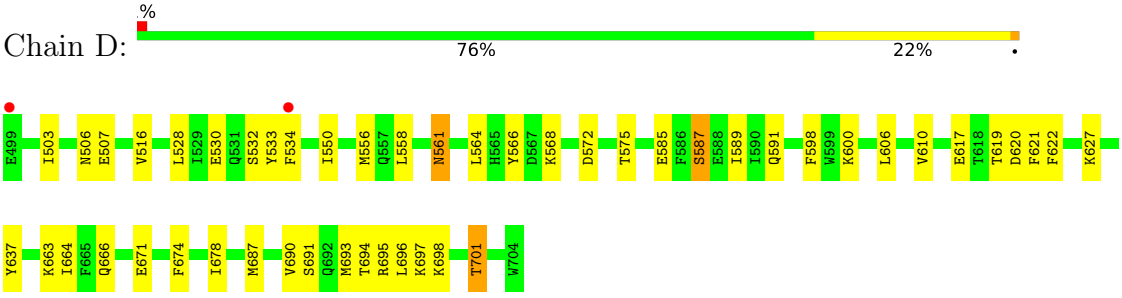
• Molecule 3: Sporulation-specific protein 16

Chain G:



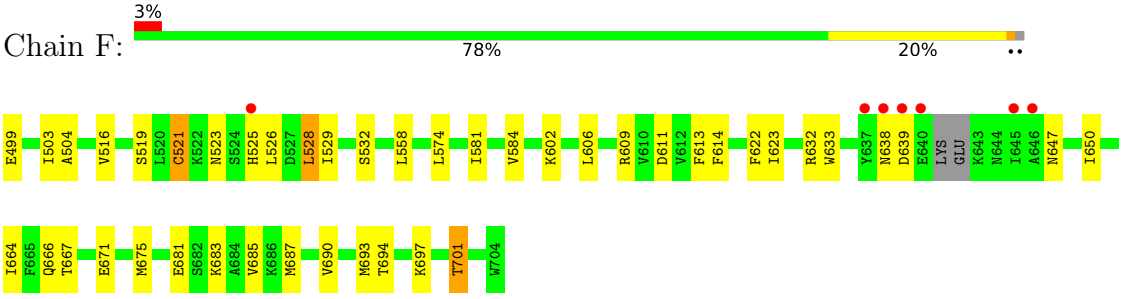
• Molecule 4: Protein ZIP2

Chain D:



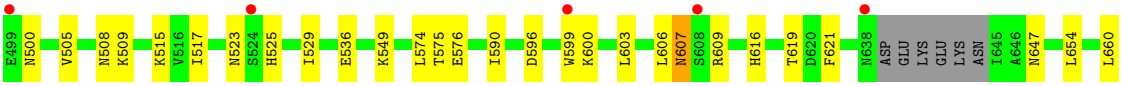
• Molecule 5: Protein ZIP2

Chain F:



• Molecule 5: Protein ZIP2

Chain H:


E499
N500
V505
N508
K509
K515
V516
I517
N523
S524
H525
I529
E536
K549
L574
T575
E576
I590
D596
W599
K600
L603
L606
N607
S608
R609
H616
T619
D620
F621
N638
ASP
GLU
LYS
GLU
LYS
ASN
I645
A646
N647
L654
L660


V661
R662
Q666
F674
I678
E681
V685
S691
K697
K698
L699
L700
T701
W704

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.40Å 63.59Å 199.04Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	57.09 – 2.29 99.52 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.3 (57.09-2.29) 98.4 (99.52-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.196 , 0.250 0.196 , 0.250	Depositor DCC
R_{free} test set	4807 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13182	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1553e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: M0H, MLY

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	0.38	0/1647	0.53	0/2230
1	E	0.36	0/1452	0.50	0/1961
2	B	0.45	0/1728	0.57	0/2331
3	C	0.39	0/1654	0.51	0/2235
3	G	0.36	0/1434	0.51	0/1937
4	D	0.45	0/1719	0.56	0/2320
5	F	0.42	0/1707	0.55	0/2303
5	H	0.42	0/1681	0.56	0/2267
All	All	0.41	0/13022	0.54	0/17584

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
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	14	ILE	Peptide

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	1627	0	1613	55	0
1	E	1440	0	1420	52	0
2	B	1735	0	1743	46	0
3	C	1625	0	1602	36	0
3	G	1411	0	1387	44	0
4	D	1737	0	1746	52	0
5	F	1704	1	1700	47	0
5	H	1678	0	1681	32	0
6	A	26	0	0	1	0
6	B	50	0	0	3	0
6	C	25	0	0	6	0
6	D	57	0	0	6	0
6	E	9	0	0	2	0
6	F	22	0	0	0	0
6	G	9	0	0	0	0
6	H	26	0	0	0	0
All	All	13181	1	12892	307	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 12.

All (307) 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:193:VAL:HG12	5:F:675:MET:HE1	1.06	1.03
3:C:79:MET:HE2	4:D:606:LEU:HD11	1.52	0.92
1:E:193:VAL:CG1	5:F:675:MET:HE1	1.98	0.89
3:G:56:GLN:HG2	3:G:105:ILE:HD11	1.57	0.86
1:A:37:LEU:HD23	1:A:41:LEU:HD12	1.58	0.86
1:E:193:VAL:HG12	5:F:675:MET:CE	2.01	0.86
2:B:645:ILE:HD12	4:D:619:THR:HB	1.60	0.82
3:C:119:GLU:OE1	6:C:201:HOH:O	1.97	0.81
2:B:531:GLN:HE21	2:B:658:ILE:HG21	1.45	0.81
4:D:637:TYR:HA	4:D:666:GLN:NE2	1.96	0.80
1:E:44:GLU:HG3	1:E:47:GLY:HA3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ILE:HD11	1:E:66:ILE:CG1	2.13	0.79
4:D:534:PHE:O	6:D:801:HOH:O	2.00	0.79
2:B:690:VAL:O	2:B:694:THR:HG23	1.84	0.78
5:F:690:VAL:O	5:F:694:THR:HG23	1.84	0.77
1:A:72:VAL:HG12	1:A:74:ALA:HB2	1.68	0.76
5:F:526:LEU:HD21	5:F:528:LEU:HD21	1.69	0.75
4:D:690:VAL:O	4:D:694:THR:HG23	1.87	0.74
5:H:515:LYS:HD2	5:H:619:THR:HG21	1.67	0.74
1:E:14:ILE:HD12	1:E:23:VAL:CG1	2.17	0.74
5:F:499:GLU:HG2	5:F:638:ASN:HD21	1.52	0.74
2:B:697:LYS:O	2:B:701:THR:HB	1.88	0.74
6:C:207:HOH:O	4:D:556:MET:HE1	1.86	0.74
1:E:172:ASN:OD1	6:E:201:HOH:O	2.06	0.73
3:G:114:ARG:HG2	3:G:114:ARG:HH11	1.53	0.73
1:E:11:ILE:HD11	1:E:66:ILE:HG13	1.71	0.73
5:H:697:LYS:O	5:H:701:THR:HB	1.87	0.73
2:B:620:ASP:OD2	6:B:801:HOH:O	2.06	0.72
5:H:500:ASN:OD1	5:H:525:HIS:HA	1.90	0.72
3:G:128:TYR:CZ	5:H:600:MLY:HH23	2.25	0.72
3:C:135:PHE:CE1	3:C:139:LYS:HD2	2.26	0.71
1:A:132:ASN:O	1:A:136:LEU:HD13	1.91	0.71
5:F:574:LEU:O	5:F:609:ARG:NH2	2.24	0.71
4:D:663:MLY:HH12	6:D:802:HOH:O	1.91	0.69
5:H:574:LEU:O	5:H:609:ARG:NH2	2.22	0.69
3:C:197:ASN:ND2	4:D:671:GLU:OE1	2.25	0.69
3:C:174:ILE:HD11	3:C:196:PHE:HE2	1.58	0.69
5:F:521:M0H:HD1	5:F:528:LEU:HG	1.74	0.69
3:C:64:GLU:OE1	6:C:202:HOH:O	2.11	0.69
5:F:581:ILE:HD11	5:F:633:TRP:HZ3	1.59	0.68
1:E:167:ASP:O	1:E:171:LYS:HG2	1.93	0.68
4:D:558:LEU:HD23	4:D:564:LEU:HD23	1.75	0.68
3:C:174:ILE:HD11	3:C:196:PHE:CE2	2.28	0.68
4:D:506:ASN:HB2	4:D:533:TYR:OH	1.93	0.68
2:B:645:ILE:HD11	6:D:832:HOH:O	1.95	0.66
4:D:663:MLY:HG2	4:D:687:MET:CE	2.25	0.66
5:F:499:GLU:HG2	5:F:638:ASN:ND2	2.10	0.66
1:E:168:LEU:CD2	5:F:671:GLU:HG3	2.26	0.66
2:B:506:ASN:HB2	2:B:533:TYR:OH	1.96	0.66
4:D:587:SER:OG	4:D:589:ILE:HG13	1.95	0.66
5:F:581:ILE:HD11	5:F:633:TRP:CZ3	2.31	0.66
1:E:14:ILE:HD12	1:E:23:VAL:HG12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:123:VAL:HG21	5:H:596:ASP:OD2	1.97	0.65
1:E:114:ARG:NH2	5:F:611:ASP:OD1	2.22	0.65
4:D:637:TYR:HA	4:D:666:GLN:HE21	1.61	0.65
2:B:702:LEU:HD12	2:B:703:GLU:N	2.11	0.65
1:E:51:ILE:HG21	1:E:97:LEU:HD13	1.79	0.65
5:F:693:MET:CE	5:F:697:LYS:HE3	2.26	0.65
1:A:174:ILE:HD13	1:A:182:ILE:CD1	2.26	0.65
1:A:72:VAL:CG1	1:A:74:ALA:HB2	2.27	0.64
1:A:128:TYR:CZ	2:B:600:MLY:HD2	2.32	0.64
4:D:664:ILE:HG13	4:D:687:MET:HE2	1.80	0.64
1:E:134:TYR:CZ	5:F:558:LEU:HD11	2.33	0.64
4:D:697:LYS:O	4:D:701:THR:HB	1.97	0.63
3:G:128:TYR:HD2	5:H:599:TRP:CZ2	2.16	0.63
3:C:135:PHE:CZ	3:C:139:LYS:HD2	2.33	0.63
1:A:10:LYS:HD2	1:A:12:GLN:HE21	1.63	0.62
3:G:128:TYR:CE1	5:H:600:MLY:HH12	2.33	0.62
3:G:118:THR:HG21	5:H:599:TRP:HB3	1.81	0.62
1:A:29:ASN:ND2	1:A:31:SER:OG	2.33	0.62
3:G:13:GLU:OE1	3:G:24:LYS:NZ	2.26	0.62
6:C:220:HOH:O	4:D:556:MET:HE1	2.00	0.61
1:A:65:LYS:HA	1:A:68:LYS:HE2	1.81	0.61
1:E:14:ILE:HD12	1:E:23:VAL:HG11	1.83	0.61
1:A:40:GLU:O	1:A:41:LEU:HD23	2.01	0.61
1:E:44:GLU:HG2	1:E:44:GLU:O	2.01	0.60
5:F:602:LYS:HE3	5:F:614:PHE:CE2	2.36	0.60
5:F:664:ILE:HG12	5:F:687:MET:CE	2.32	0.60
4:D:550:ILE:HB	4:D:566:TYR:CZ	2.36	0.60
2:B:515:LYS:NZ	6:B:807:HOH:O	2.34	0.60
3:G:7:ASP:HB2	3:G:29:ASN:HB3	1.82	0.60
5:H:515:LYS:CD	5:H:619:THR:HG21	2.32	0.60
1:E:79:MET:HE2	5:F:606:LEU:HD11	1.83	0.59
3:G:157:PHE:O	3:G:161:ILE:HG13	2.02	0.59
1:E:11:ILE:HD11	1:E:66:ILE:HG12	1.84	0.59
1:E:69:SER:HB3	1:E:70:PRO:HD2	1.83	0.59
4:D:568:MLY:HH12	4:D:572:ASP:OD2	2.01	0.59
3:G:51:ILE:HG21	3:G:97:LEU:HD13	1.85	0.59
5:F:693:MET:HE1	5:F:697:LYS:HE3	1.85	0.58
5:H:509:LYS:HE3	5:H:536:GLU:O	2.03	0.58
1:A:34:ILE:HG23	1:A:88:LYS:HD2	1.85	0.58
3:G:37:LEU:HD11	3:G:51:ILE:HD11	1.84	0.58
3:G:17:VAL:HG22	3:G:129:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:663:MLY:HG2	4:D:687:MET:HE3	1.85	0.58
4:D:561:ASN:OD1	4:D:561:ASN:N	2.37	0.57
4:D:693:MET:HG3	4:D:697:LYS:HE2	1.87	0.57
5:F:667:THR:HG21	5:F:683:LYS:HE2	1.86	0.57
4:D:568:MLY:HH23	4:D:572:ASP:OD1	2.04	0.57
1:A:24:MLY:HH21	1:A:71:GLY:HA3	1.87	0.56
2:B:550:ILE:HB	2:B:566:TYR:CZ	2.40	0.56
4:D:568:MLY:HE2	4:D:572:ASP:OD2	2.05	0.56
5:F:681:GLU:O	5:F:685:VAL:HG23	2.04	0.56
2:B:531:GLN:HA	2:B:531:GLN:OE1	2.06	0.56
5:F:519:SER:CB	5:F:623:ILE:HD13	2.36	0.56
3:C:7:ASP:HB2	3:C:29:ASN:HB3	1.88	0.56
1:A:154:PHE:CZ	2:B:695:ARG:HD3	2.40	0.56
4:D:503:ILE:CG1	4:D:528:LEU:HD13	2.36	0.56
3:C:134:TYR:CZ	4:D:558:LEU:HD21	2.41	0.56
3:G:101:SER:O	3:G:105:ILE:HG13	2.05	0.56
1:A:98:LEU:HD22	1:A:117:ILE:HG13	1.87	0.56
5:F:504:ALA:HA	5:F:529:ILE:O	2.06	0.56
3:G:114:ARG:HG2	3:G:114:ARG:NH1	2.21	0.56
3:C:128:TYR:CE1	4:D:600:MLY:HE3	2.41	0.55
3:G:26:VAL:HG21	3:G:62:VAL:CG1	2.35	0.55
3:G:58:LEU:O	3:G:62:VAL:HG23	2.07	0.55
3:G:26:VAL:HG21	3:G:62:VAL:HG11	1.88	0.55
1:A:157:PHE:CE1	2:B:699:LEU:HB2	2.41	0.55
2:B:624:ASP:HB3	1:E:-3:PHE:CE2	2.42	0.55
2:B:624:ASP:HB3	1:E:-3:PHE:CD2	2.42	0.55
1:E:127:ARG:NH1	1:E:131:ASN:HB2	2.21	0.55
5:F:519:SER:HB2	5:F:623:ILE:HD13	1.88	0.55
3:C:154:PHE:CE2	4:D:695:ARG:HD3	2.42	0.55
1:E:29:ASN:HA	1:E:85:THR:CG2	2.38	0.55
1:A:129:VAL:HG13	1:A:135:PHE:HE2	1.72	0.54
3:G:56:GLN:HG2	3:G:105:ILE:CD1	2.34	0.54
1:A:35:SER:O	1:A:39:GLU:HB2	2.08	0.54
2:B:645:ILE:CD1	4:D:619:THR:HB	2.34	0.54
5:F:639:ASP:HB2	5:F:666:GLN:HG2	1.90	0.54
6:C:220:HOH:O	4:D:556:MET:CE	2.56	0.54
1:A:65:LYS:O	1:A:68:LYS:HG2	2.08	0.53
3:C:96:ILE:HD11	4:D:621:PHE:CE1	2.43	0.53
3:G:14:ILE:HB	3:G:23:VAL:HB	1.90	0.53
5:F:697:LYS:O	5:F:701:THR:HB	2.09	0.53
1:A:127:ARG:NH1	1:A:130:GLU:OE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:503:ILE:HG13	5:F:528:LEU:HD22	1.91	0.53
1:A:106:ASN:HD22	1:E:105:ILE:CG2	2.22	0.52
2:B:619:THR:HG22	2:B:623:ILE:CD1	2.39	0.52
4:D:506:ASN:HB2	4:D:533:TYR:HH	1.74	0.52
1:E:29:ASN:HA	1:E:85:THR:HG23	1.91	0.52
5:H:654:LEU:HD11	5:H:699:LEU:HD22	1.91	0.52
5:F:516:VAL:HG21	5:F:622:PHE:HD2	1.74	0.52
1:E:190:GLU:O	1:E:194:VAL:HG13	2.10	0.52
1:A:7:ASP:OD2	1:A:32:ARG:HD3	2.10	0.52
4:D:572:ASP:O	4:D:575:THR:HB	2.10	0.52
1:E:11:ILE:HG23	1:E:11:ILE:O	2.09	0.52
5:H:523:ASN:OD1	5:H:525:HIS:N	2.32	0.52
1:A:69:SER:O	1:A:71:GLY:N	2.39	0.52
4:D:507:GLU:HG3	4:D:530:GLU:OE2	2.11	0.51
5:F:632:ARG:HG2	5:F:633:TRP:CD1	2.46	0.51
5:F:664:ILE:HG12	5:F:687:MET:HE3	1.92	0.51
3:G:18:GLU:N	3:G:21:SER:OG	2.43	0.51
4:D:507:GLU:OE1	4:D:532:SER:HB2	2.10	0.51
1:E:16:ASN:HD22	1:E:130:GLU:HG2	1.75	0.51
3:G:128:TYR:CD1	5:H:600:MLY:HH12	2.45	0.51
3:G:165:ILE:HD13	3:G:183:LEU:HD21	1.92	0.51
1:A:157:PHE:HE1	2:B:699:LEU:HB2	1.74	0.51
1:A:42:GLN:HA	1:A:42:GLN:OE1	2.10	0.51
1:E:81:ASN:HB2	1:E:116:PHE:CZ	2.45	0.51
5:F:584:VAL:HG11	5:F:614:PHE:CE1	2.46	0.51
3:G:59:ILE:HG22	3:G:109:SER:HB3	1.92	0.51
2:B:602:LYS:HE3	2:B:614:PHE:CE2	2.46	0.51
1:E:11:ILE:CD1	1:E:66:ILE:HG13	2.40	0.51
1:E:17:VAL:O	1:E:139:LYS:HE3	2.11	0.50
3:C:96:ILE:HD11	4:D:621:PHE:HE1	1.76	0.50
1:A:141:ASN:O	1:A:145:THR:HG23	2.10	0.50
3:C:114:ARG:NH2	4:D:610:VAL:O	2.45	0.50
4:D:664:ILE:CG1	4:D:687:MET:HE2	2.42	0.50
5:F:503:ILE:CG1	5:F:528:LEU:HD22	2.42	0.50
3:C:108:PRO:HD2	6:C:217:HOH:O	2.11	0.50
1:A:41:LEU:HD13	1:A:47:GLY:HA2	1.94	0.50
1:E:45:GLU:HA	1:E:45:GLU:OE1	2.11	0.50
3:G:167:ASP:OD2	5:H:647:ASN:OD1	2.30	0.50
4:D:620:ASP:HB2	6:D:817:HOH:O	2.11	0.49
2:B:517:ILE:HG23	2:B:528:LEU:HD12	1.93	0.49
2:B:531:GLN:NE2	2:B:658:ILE:HG21	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:MET:HE1	4:D:698:LYS:HE2	1.94	0.49
1:A:174:ILE:HD12	1:A:196:PHE:HZ	1.77	0.49
1:A:150:ASP:HB3	1:A:153:GLU:OE2	2.13	0.49
4:D:606:LEU:HA	6:D:827:HOH:O	2.12	0.49
1:A:135:PHE:CE1	2:B:604:TYR:HA	2.48	0.48
1:A:40:GLU:O	1:E:45:GLU:HG2	2.13	0.48
4:D:663:MLY:HG2	4:D:687:MET:HE1	1.93	0.48
5:F:664:ILE:HG12	5:F:687:MET:HE1	1.95	0.48
5:F:602:LYS:HE3	5:F:614:PHE:HE2	1.78	0.48
3:C:39:GLU:HG3	3:C:40:GLU:N	2.28	0.48
2:B:503:ILE:HD11	2:B:528:LEU:HD21	1.95	0.48
1:E:105:ILE:HG22	1:E:106:ASN:OD1	2.14	0.47
1:E:161:ILE:O	1:E:165:ILE:HG13	2.15	0.47
3:G:13:GLU:C	3:G:14:ILE:HG13	2.34	0.47
2:B:500:ASN:OD1	2:B:525:HIS:C	2.53	0.47
1:A:174:ILE:HD12	1:A:196:PHE:CZ	2.49	0.47
5:H:575:THR:HG22	5:H:576:GLU:HG2	1.97	0.47
4:D:516:VAL:HG21	4:D:622:PHE:HD2	1.78	0.47
1:E:79:MET:HE1	6:E:203:HOH:O	2.15	0.47
5:H:616:HIS:HD2	5:H:621:PHE:CE2	2.33	0.47
3:C:79:MET:HE3	3:C:114:ARG:HB2	1.97	0.46
4:D:558:LEU:HD23	4:D:564:LEU:CD2	2.45	0.46
5:H:603:LEU:HD23	5:H:603:LEU:HA	1.71	0.46
1:A:154:PHE:CE2	2:B:695:ARG:HD3	2.50	0.46
3:C:39:GLU:OE2	3:C:40:GLU:HG3	2.15	0.46
3:C:174:ILE:CD1	3:C:196:PHE:CE2	2.97	0.46
1:E:60:ASN:O	1:E:64:GLU:HG3	2.14	0.46
3:G:-6:ASN:OD1	3:G:-6:ASN:N	2.48	0.46
3:G:14:ILE:HG22	3:G:129:VAL:HG11	1.97	0.46
5:F:693:MET:HE3	5:F:697:LYS:HE3	1.94	0.46
1:A:187:HIS:O	2:B:703:GLU:HA	2.15	0.46
5:H:606:LEU:HD23	5:H:606:LEU:HA	1.71	0.46
3:G:56:GLN:HA	3:G:105:ILE:HD11	1.97	0.46
5:H:529:ILE:HD11	5:H:662:ARG:NH2	2.31	0.46
3:G:42:GLN:H	3:G:42:GLN:HG2	1.54	0.46
3:G:128:TYR:CD2	5:H:599:TRP:CZ2	3.03	0.46
5:H:607:ASN:OD1	5:H:607:ASN:C	2.53	0.46
5:F:523:ASN:OD1	5:F:525:HIS:HB2	2.16	0.46
3:G:128:TYR:HD2	5:H:599:TRP:CH2	2.33	0.45
1:E:197:ASN:HB2	5:F:675:MET:HE3	1.96	0.45
1:A:79:MET:CE	2:B:606:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:GLU:HG3	6:B:829:HOH:O	2.16	0.45
4:D:674:PHE:O	4:D:678:ILE:HG13	2.16	0.45
2:B:507:GLU:HG3	2:B:530:GLU:OE2	2.17	0.45
3:C:186:PHE:HB3	3:C:191:SER:HB2	1.99	0.45
3:G:17:VAL:HG22	3:G:129:VAL:CG2	2.46	0.44
1:A:79:MET:HG3	2:B:606:LEU:HD21	1.99	0.44
3:C:79:MET:CE	3:C:114:ARG:HB2	2.47	0.44
1:E:79:MET:CE	5:F:606:LEU:HD11	2.46	0.44
3:G:44:GLU:H	3:G:44:GLU:HG3	1.63	0.44
1:A:7:ASP:HB2	1:A:29:ASN:HB3	1.99	0.44
1:A:65:LYS:HG3	1:A:68:LYS:HE2	1.99	0.44
2:B:516:VAL:HG21	2:B:622:PHE:HD2	1.82	0.44
1:E:79:MET:HE2	1:E:79:MET:HB3	1.86	0.44
4:D:627:MLY:HD3	4:D:627:MLY:HH22	1.72	0.44
5:H:660:LEU:HD12	5:H:660:LEU:O	2.17	0.44
1:A:128:TYR:CE1	2:B:600:MLY:HD2	2.52	0.44
1:A:174:ILE:HD13	1:A:182:ILE:HD12	1.98	0.44
5:F:521:M0H:HD2	5:F:521:M0H:HA	1.89	0.44
3:G:172:ASN:ND2	3:G:196:PHE:CD1	2.86	0.44
1:E:134:TYR:OH	5:F:558:LEU:HD11	2.17	0.44
1:E:162:LYS:O	1:E:166:PHE:HD2	1.98	0.44
1:A:3:GLU:HG2	1:A:4:PHE:N	2.33	0.44
4:D:585:GLU:HB3	4:D:617:GLU:HG3	2.00	0.43
5:H:549:MLY:HD3	5:H:549:MLY:HH22	1.83	0.43
1:E:99:GLU:HG2	5:F:613:PHE:CE1	2.52	0.43
5:F:639:ASP:HB2	5:F:666:GLN:HA	1.99	0.43
1:A:37:LEU:O	1:A:41:LEU:HB2	2.18	0.43
5:F:584:VAL:HG11	5:F:614:PHE:HE1	1.81	0.43
1:E:193:VAL:O	5:F:675:MET:HE3	2.18	0.43
1:A:129:VAL:HG13	1:A:135:PHE:CE2	2.53	0.43
2:B:503:ILE:CG1	2:B:528:LEU:HD22	2.49	0.43
1:A:58:LEU:HD23	1:A:82:LEU:HD13	2.01	0.43
2:B:702:LEU:HD12	2:B:702:LEU:C	2.36	0.43
3:G:106:ASN:HD22	3:G:106:ASN:HA	1.63	0.43
1:E:80:ILE:HD12	1:E:115:TYR:CE2	2.54	0.43
5:F:584:VAL:HB	5:F:614:PHE:CD1	2.54	0.43
5:H:674:PHE:O	5:H:678:ILE:HD12	2.19	0.42
1:A:167:ASP:O	1:A:171:LYS:HB2	2.19	0.42
2:B:503:ILE:HD11	2:B:528:LEU:CD2	2.48	0.42
2:B:503:ILE:CG1	2:B:528:LEU:CD2	2.98	0.42
2:B:674:PHE:O	2:B:678:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:GLU:HG3	3:C:40:GLU:CG	2.49	0.42
4:D:696:LEU:HA	4:D:696:LEU:HD12	1.73	0.42
2:B:624:ASP:CB	1:E:-3:PHE:CE2	3.02	0.42
3:G:17:VAL:CG2	3:G:129:VAL:HG11	2.49	0.42
1:A:5:PHE:CE1	1:A:36:GLN:HG3	2.54	0.42
3:C:3:GLU:HG2	3:C:4:PHE:H	1.85	0.42
3:G:190:GLU:HG3	5:H:678:ILE:HG12	2.01	0.42
3:G:17:VAL:HG22	3:G:129:VAL:HG11	2.01	0.42
3:C:79:MET:HE2	4:D:606:LEU:CD1	2.35	0.42
5:F:667:THR:CG2	5:F:683:LYS:HE2	2.48	0.42
4:D:663:MLY:HH23	6:D:802:HOH:O	2.20	0.42
3:G:22:VAL:O	3:G:78:LEU:HD12	2.20	0.42
1:E:28:VAL:O	1:E:85:THR:HG23	2.20	0.42
1:E:59:ILE:HG23	1:E:115:TYR:CZ	2.55	0.42
1:E:189:LEU:HA	1:E:189:LEU:HD23	1.76	0.42
3:G:10:LYS:HE3	3:G:12:GLN:HE21	1.85	0.42
1:A:59:ILE:HG23	1:A:115:TYR:CZ	2.55	0.41
1:A:79:MET:HE2	2:B:606:LEU:CD1	2.50	0.41
1:A:198:GLU:OE2	2:B:679:LYS:HE3	2.21	0.41
3:G:128:TYR:OH	5:H:600:MLY:HH23	2.20	0.41
5:H:681:GLU:O	5:H:685:VAL:HG23	2.20	0.41
3:C:3:GLU:HG2	3:C:4:PHE:N	2.35	0.41
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.67	0.41
1:A:29:ASN:ND2	1:A:31:SER:H	2.18	0.41
2:B:572:ASP:O	2:B:575:THR:HB	2.20	0.41
3:C:16:ASN:O	3:C:129:VAL:CG1	2.68	0.41
5:F:647:ASN:HA	5:F:650:ILE:HD12	2.01	0.41
1:A:5:PHE:CZ	1:A:36:GLN:HG3	2.56	0.41
1:A:79:MET:HE2	2:B:606:LEU:HD11	2.01	0.41
1:E:158:GLU:H	1:E:158:GLU:HG2	1.73	0.41
3:G:105:ILE:O	3:G:110:LYS:HB2	2.20	0.41
3:C:62:VAL:O	3:C:66:ILE:HG13	2.20	0.41
3:C:151:MET:CE	4:D:698:LYS:HE2	2.50	0.41
1:A:114:ARG:NH2	2:B:610:VAL:O	2.54	0.41
3:C:18:GLU:HB3	3:C:21:SER:OG	2.20	0.41
3:C:82:LEU:O	3:C:117:ILE:HA	2.20	0.41
3:C:154:PHE:CZ	4:D:695:ARG:HD3	2.56	0.41
1:E:78:LEU:HD12	1:E:79:MET:H	1.84	0.41
3:C:168:LEU:HD11	3:C:193:VAL:HG22	2.03	0.41
5:H:590:ILE:HD12	5:H:590:ILE:HA	1.82	0.40
1:A:156:ASP:HB2	1:A:159:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:LEU:O	3:C:196:PHE:HD1	2.04	0.40
4:D:591:GLN:HA	4:D:598:PHE:HE2	1.86	0.40
1:A:71:GLY:O	1:A:73:PRO:HD3	2.22	0.40
3:C:183:LEU:HD23	3:C:183:LEU:HA	1.85	0.40
6:A:216:HOH:O	2:B:556:MET:HE2	2.20	0.40
3:G:125:ARG:HB3	5:H:599:TRP:CH2	2.56	0.40
5:H:505:VAL:HG21	5:H:517:ILE:HD11	2.02	0.40
1:A:17:VAL:O	1:A:139:LYS:NZ	2.49	0.40
2:B:540:ILE:HG22	2:B:659:LEU:HD12	2.04	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	194/216 (90%)	188 (97%)	6 (3%)	0	100	100
1	E	162/216 (75%)	158 (98%)	4 (2%)	0	100	100
2	B	200/206 (97%)	191 (96%)	9 (4%)	0	100	100
3	C	191/216 (88%)	185 (97%)	5 (3%)	1 (0%)	29	34
3	G	164/216 (76%)	158 (96%)	5 (3%)	1 (1%)	25	29
4	D	199/206 (97%)	193 (97%)	6 (3%)	0	100	100
5	F	197/206 (96%)	194 (98%)	3 (2%)	0	100	100
5	H	193/206 (94%)	189 (98%)	4 (2%)	0	100	100
All	All	1500/1688 (89%)	1456 (97%)	42 (3%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	88	LYS

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Mol	Chain	Res	Type
3	G	14	ILE

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	184/202 (91%)	180 (98%)	4 (2%)	52	66
1	E	159/202 (79%)	156 (98%)	3 (2%)	57	71
2	B	190/190 (100%)	187 (98%)	3 (2%)	62	76
3	C	184/203 (91%)	179 (97%)	5 (3%)	44	59
3	G	158/203 (78%)	154 (98%)	4 (2%)	47	62
4	D	189/189 (100%)	185 (98%)	4 (2%)	53	68
5	F	186/191 (97%)	183 (98%)	3 (2%)	62	76
5	H	184/191 (96%)	179 (97%)	5 (3%)	44	59
All	All	1434/1571 (91%)	1403 (98%)	31 (2%)	52	66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	79	MET
1	A	89	PHE
1	A	126	SER
2	B	519	SER
2	B	701	THR
2	B	702	LEU
3	C	-3	PHE
3	C	33	LEU
3	C	45	GLU
3	C	77	SER
3	C	191	SER
4	D	561	ASN
4	D	587	SER

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Mol	Chain	Res	Type
4	D	691	SER
4	D	701	THR
1	E	14	ILE
1	E	160	LEU
1	E	189	LEU
5	F	528	LEU
5	F	532	SER
5	F	701	THR
3	G	35	SER
3	G	43	ASP
3	G	100	ARG
3	G	106	ASN
5	H	508	ASN
5	H	607	ASN
5	H	666	GLN
5	H	691	SER
5	H	701	THR

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	12	GLN
1	A	29	ASN
1	A	49	ASN
2	B	531	GLN
4	D	666	GLN
1	E	16	ASN
5	F	638	ASN
3	G	12	GLN
3	G	67	GLN
3	G	106	ASN
5	H	647	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

17 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	$\#\|Z\| > 2$
2	MLY	B	627	2	9,10,11	0.54	0	6,11,13	0.97	0
5	MLY	F	600	5	9,10,11	0.72	0	6,11,13	0.76	0
1	MLY	E	24	1	9,10,11	0.58	0	6,11,13	0.85	0
5	M0H	H	521	5	5,7,8	0.87	0	2,7,9	0.78	0
2	MLY	B	600	2	9,10,11	0.46	0	6,11,13	0.66	0
5	MLY	H	600	5	9,10,11	0.73	0	6,11,13	0.84	0
4	MLY	D	568	4	9,10,11	0.63	0	6,11,13	0.64	0
4	MLY	D	600	4	9,10,11	0.48	0	6,11,13	0.73	0
1	MLY	A	24	1	9,10,11	0.58	0	6,11,13	1.12	0
4	MLY	D	663	4	9,10,11	0.68	0	6,11,13	0.76	0
2	MLY	B	663	2	9,10,11	0.76	0	6,11,13	0.72	0
5	M0H	F	521	5	5,7,8	0.72	0	2,7,9	2.37	1 (50%)
5	MLY	F	549	5	9,10,11	0.57	0	6,11,13	0.92	0
4	M0H	D	521	4	5,7,8	0.78	0	2,7,9	0.93	0
4	MLY	D	627	4	9,10,11	0.48	0	6,11,13	0.96	0
5	MLY	H	549	5	9,10,11	0.48	0	6,11,13	1.19	0
2	M0H	B	521	2	5,7,8	1.04	0	2,7,9	1.75	1 (50%)

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
2	MLY	B	627	2	-	1/8/9/11	-
5	MLY	F	600	5	-	7/8/9/11	-
1	MLY	E	24	1	-	1/8/9/11	-
5	M0H	H	521	5	-	1/5/6/8	-
2	MLY	B	600	2	-	1/8/9/11	-
5	MLY	H	600	5	-	2/8/9/11	-
4	MLY	D	568	4	-	5/8/9/11	-
4	MLY	D	600	4	-	2/8/9/11	-
1	MLY	A	24	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLY	D	663	4	-	2/8/9/11	-
2	MLY	B	663	2	-	2/8/9/11	-
5	M0H	F	521	5	-	1/5/6/8	-
5	MLY	F	549	5	-	1/8/9/11	-
4	M0H	D	521	4	-	2/5/6/8	-
4	MLY	D	627	4	-	2/8/9/11	-
5	MLY	H	549	5	-	0/8/9/11	-
2	M0H	B	521	2	-	3/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	521	M0H	CB-SG-CD	3.25	107.47	102.06
2	B	521	M0H	CB-SG-CD	2.24	105.79	102.06

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	568	MLY	C-CA-CB-CG
4	D	627	MLY	C-CA-CB-CG
5	F	600	MLY	N-CA-CB-CG
5	F	600	MLY	C-CA-CB-CG
1	A	24	MLY	CD-CE-NZ-CH2
5	F	600	MLY	CD-CE-NZ-CH1
5	H	600	MLY	CD-CE-NZ-CH1
5	H	600	MLY	CD-CE-NZ-CH2
5	F	600	MLY	CG-CD-CE-NZ
5	F	549	MLY	CG-CD-CE-NZ
1	A	24	MLY	CD-CE-NZ-CH1
2	B	663	MLY	CD-CE-NZ-CH1
2	B	663	MLY	CD-CE-NZ-CH2
4	D	663	MLY	CD-CE-NZ-CH2
5	F	600	MLY	CD-CE-NZ-CH2
1	A	24	MLY	CA-CB-CG-CD
5	F	600	MLY	CA-CB-CG-CD
4	D	568	MLY	CD-CE-NZ-CH1
4	D	568	MLY	CD-CE-NZ-CH2
4	D	600	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
4	D	600	MLY	CD-CE-NZ-CH1
1	E	24	MLY	CD-CE-NZ-CH2
1	A	24	MLY	CE-CD-CG-CB
4	D	568	MLY	CA-CB-CG-CD
4	D	627	MLY	CA-CB-CG-CD
5	F	600	MLY	CE-CD-CG-CB
2	B	600	MLY	CE-CD-CG-CB
2	B	521	M0H	C-CA-CB-SG
4	D	521	M0H	C-CA-CB-SG
2	B	627	MLY	CG-CD-CE-NZ
4	D	663	MLY	CD-CE-NZ-CH1
4	D	568	MLY	N-CA-CB-CG
2	B	521	M0H	N-CA-CB-SG
2	B	521	M0H	OXT-C-CA-N
4	D	521	M0H	OXT-C-CA-N
5	F	521	M0H	OXT-C-CA-N
5	H	521	M0H	OXT-C-CA-N

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	MLY	2	0
5	H	600	MLY	4	0
4	D	568	MLY	3	0
4	D	600	MLY	1	0
1	A	24	MLY	1	0
4	D	663	MLY	5	0
5	F	521	M0H	2	0
4	D	627	MLY	1	0
5	H	549	MLY	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	196/216 (90%)	0.21	8 (4%)	37	42	31, 53, 112, 155	0
1	E	174/216 (80%)	0.44	13 (7%)	14	18	35, 60, 116, 150	0
2	B	202/206 (98%)	0.03	4 (1%)	65	70	27, 41, 64, 134	0
3	C	197/216 (91%)	0.14	6 (3%)	50	56	30, 52, 97, 117	0
3	G	174/216 (80%)	0.50	16 (9%)	9	11	35, 61, 129, 164	0
4	D	201/206 (97%)	0.02	2 (0%)	82	86	28, 41, 68, 117	0
5	F	201/206 (97%)	0.19	7 (3%)	44	49	29, 47, 94, 211	0
5	H	197/206 (95%)	0.07	5 (2%)	57	63	28, 44, 75, 111	0
All	All	1542/1688 (91%)	0.19	61 (3%)	38	43	27, 50, 100, 211	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	17	VAL	14.6
5	F	638	ASN	7.5
1	A	45	GLU	7.1
5	F	639	ASP	6.6
1	E	44	GLU	5.7
1	E	182	ILE	5.5
5	F	646	ALA	5.4
5	F	645	ILE	5.3
5	H	524	SER	5.1
3	G	20	HIS	4.9
1	A	75	HIS	4.5
1	A	72	VAL	4.4
5	F	640	GLU	3.9
3	G	45	GLU	3.9
1	A	153	GLU	3.8
3	G	68	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	499	GLU	3.6
3	G	21	SER	3.6
1	E	46	SER	3.5
3	G	105	ILE	3.5
1	E	45	GLU	3.5
1	E	70	PRO	3.4
1	E	11	ILE	3.4
3	G	15	SER	3.3
1	E	-6	ASN	3.2
1	A	42	GLN	3.2
3	G	18	GLU	3.1
1	E	43	ASP	3.1
3	C	-4	TYR	3.1
3	G	22	VAL	3.1
1	E	166	PHE	3.0
3	G	-9	HIS	3.0
4	D	534	PHE	2.9
5	F	637	TYR	2.9
3	G	69	SER	2.8
3	C	-3	PHE	2.8
1	E	76	ARG	2.8
3	C	41	LEU	2.8
1	A	43	ASP	2.7
5	H	499	GLU	2.7
3	G	16	ASN	2.6
2	B	589	ILE	2.6
5	H	608	SER	2.5
3	C	153	GLU	2.5
5	H	599	TRP	2.5
3	G	75	HIS	2.5
2	B	499	GLU	2.4
1	A	19	GLU	2.4
3	G	128	TYR	2.4
3	C	152	ASP	2.4
3	G	14	ILE	2.3
1	E	141	ASN	2.3
1	E	20	HIS	2.2
3	C	40	GLU	2.2
2	B	534	PHE	2.2
3	G	152	ASP	2.1
5	F	525	HIS	2.0
1	E	127	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
5	H	638	ASN	2.0
2	B	638	ASN	2.0
1	A	44	GLU	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
5	M0H	H	521	8/9	0.92	0.12	46,57,64,69	0
5	M0H	F	521	8/9	0.94	0.12	42,47,55,63	0
4	M0H	D	521	8/9	0.95	0.12	40,45,65,67	0
4	MLY	D	627	11/12	0.95	0.15	34,37,63,65	0
1	MLY	E	24	11/12	0.95	0.21	58,65,69,76	0
1	MLY	A	24	11/12	0.95	0.14	36,51,65,69	0
2	M0H	B	521	8/9	0.95	0.10	39,47,53,56	0
5	MLY	H	600	11/12	0.95	0.16	30,48,56,59	0
2	MLY	B	663	11/12	0.96	0.15	33,36,68,68	0
5	MLY	F	600	11/12	0.96	0.15	37,46,53,54	0
4	MLY	D	663	11/12	0.96	0.17	32,41,71,75	0
4	MLY	D	568	11/12	0.96	0.24	31,37,80,81	0
2	MLY	B	627	11/12	0.97	0.17	28,31,50,50	0
2	MLY	B	600	11/12	0.97	0.13	34,42,47,50	0
5	MLY	F	549	11/12	0.97	0.12	32,36,66,69	0
5	MLY	H	549	11/12	0.98	0.16	30,37,67,71	0
4	MLY	D	600	11/12	0.98	0.13	29,33,42,46	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.