



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2022 – 04:11 pm BST

PDB ID : 7Q5N  
Title : Crystal structure of Chaetomium thermophilum Ahp1-Urm1 complex  
Authors : Ravichandran, K.E.; Wilk, P.; Grudnik, P.; Glatt, S.  
Deposited on : 2021-11-04  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

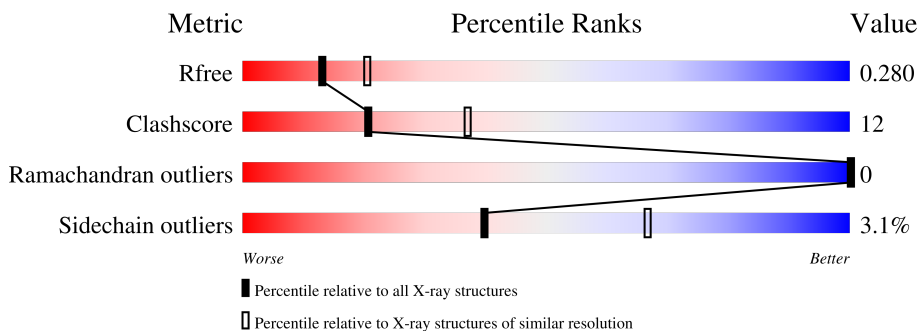
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	174	90% 8% ..
1	B	174	86% 11% ..
1	C	174	71% 26% .
1	D	174	75% 23% .
1	E	174	82% 14% ..
1	F	174	69% 27% ..
2	G	111	80% 12% . 7%

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Mol	Chain	Length	Quality of chain
2	H	111	 76% 17% • 6%
2	I	111	 69% 24% 6%
2	J	111	 55% 36% • 7%
2	K	111	 81% 13% 6%
2	L	111	 62% 30% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSS	A	60	-	-	X	-
1	CSS	B	60	-	-	X	-
1	CSS	D	60	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12664 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 Thioredoxin domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1256	795	212	245	4	0	0	0
1	B	172	1268	804	214	246	4	0	0	0
1	C	169	1247	790	210	243	4	0	0	0
1	D	170	1251	792	211	244	4	0	0	0
1	E	169	1247	790	210	243	4	0	0	0
1	F	168	1239	785	209	242	3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0S1P8
A	0	ALA	-	expression tag	UNP G0S1P8
A	30	SER	CYS	engineered mutation	UNP G0S1P8
B	-1	GLY	-	expression tag	UNP G0S1P8
B	0	ALA	-	expression tag	UNP G0S1P8
B	30	SER	CYS	engineered mutation	UNP G0S1P8
C	-1	GLY	-	expression tag	UNP G0S1P8
C	0	ALA	-	expression tag	UNP G0S1P8
C	30	SER	CYS	engineered mutation	UNP G0S1P8
D	-1	GLY	-	expression tag	UNP G0S1P8
D	0	ALA	-	expression tag	UNP G0S1P8
D	30	SER	CYS	engineered mutation	UNP G0S1P8
E	-1	GLY	-	expression tag	UNP G0S1P8
E	0	ALA	-	expression tag	UNP G0S1P8
E	30	SER	CYS	engineered mutation	UNP G0S1P8
F	-1	GLY	-	expression tag	UNP G0S1P8
F	0	ALA	-	expression tag	UNP G0S1P8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	SER	CYS	engineered mutation	UNP G0S1P8

- Molecule 2 is a protein called Ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	103	821	525	134	160	2	0	0	0
2	H	104	829	531	135	161	2	1	0	0
2	I	104	829	531	135	161	2	0	0	0
2	J	103	821	525	134	160	2	0	0	0
2	K	104	829	531	135	161	2	0	0	0
2	L	104	829	531	135	161	2	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP G0SE11
G	2	ALA	-	expression tag	UNP G0SE11
G	55	SER	CYS	engineered mutation	UNP G0SE11
H	1	MET	-	initiating methionine	UNP G0SE11
H	2	ALA	-	expression tag	UNP G0SE11
H	55	SER	CYS	engineered mutation	UNP G0SE11
I	1	MET	-	initiating methionine	UNP G0SE11
I	2	ALA	-	expression tag	UNP G0SE11
I	55	SER	CYS	engineered mutation	UNP G0SE11
J	1	MET	-	initiating methionine	UNP G0SE11
J	2	ALA	-	expression tag	UNP G0SE11
J	55	SER	CYS	engineered mutation	UNP G0SE11
K	1	MET	-	initiating methionine	UNP G0SE11
K	2	ALA	-	expression tag	UNP G0SE11
K	55	SER	CYS	engineered mutation	UNP G0SE11
L	1	MET	-	initiating methionine	UNP G0SE11
L	2	ALA	-	expression tag	UNP G0SE11
L	55	SER	CYS	engineered mutation	UNP G0SE11

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	3	Total Zn 3 3	0	0
3	C	3	Total Zn 3 3	0	0
3	D	2	Total Zn 2 2	0	0
3	E	3	Total Zn 3 3	0	0
3	F	2	Total Zn 2 2	0	0
3	G	1	Total Zn 1 1	0	0
3	H	8	Total Zn 8 8	0	0
3	I	5	Total Zn 5 5	0	0
3	J	4	Total Zn 4 4	0	0
3	K	6	Total Zn 6 6	0	0
3	L	3	Total Zn 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	22	Total O 22 22	0	0
4	C	9	Total O 9 9	0	0
4	D	11	Total O 11 11	0	0
4	E	15	Total O 15 15	0	0
4	F	4	Total O 4 4	0	0
4	G	6	Total O 6 6	0	0
4	H	12	Total O 12 12	0	0

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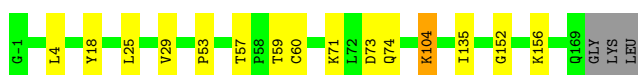
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	I	9	Total O 9 9	0	0
4	J	6	Total O 6 6	0	0
4	K	21	Total O 21 21	0	0
4	L	9	Total O 9 9	0	0

### 3 Residue-property plots


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. 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. 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.

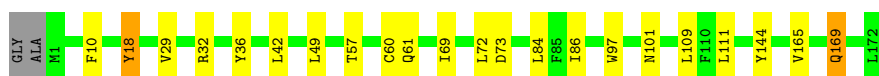
- Molecule 1: Thioredoxin domain-containing protein

Chain A:  90% 8% ..



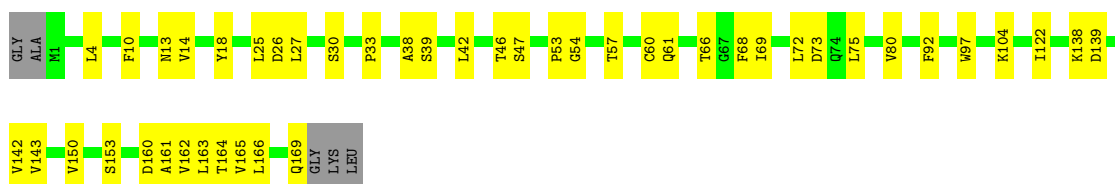
- Molecule 1: Thioredoxin domain-containing protein

Chain B:  86% 11% ..




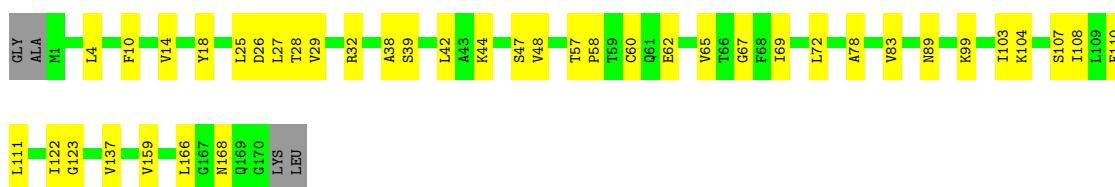
- Molecule 1: Thioredoxin domain-containing protein

Chain C:  71% 26% .




- Molecule 1: Thioredoxin domain-containing protein

Chain D:  75% 23% .



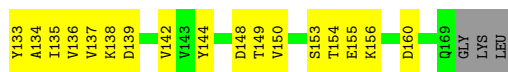
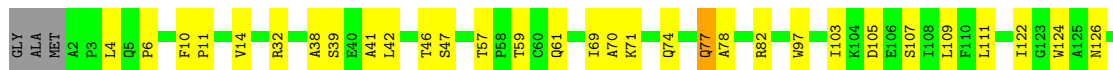
- Molecule 1: Thioredoxin domain-containing protein

Chain E:  82% 14% ..

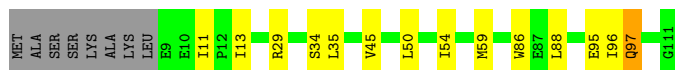
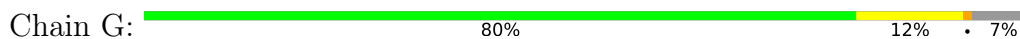




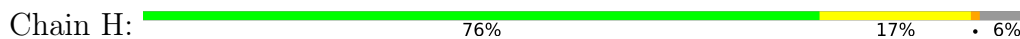
- Molecule 1: Thioredoxin domain-containing protein



- Molecule 2: Ubiquitin-related modifier 1



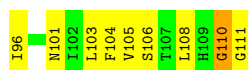
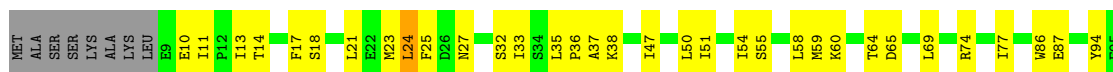
- Molecule 2: Ubiquitin-related modifier 1



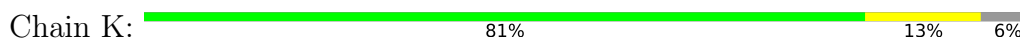
- Molecule 2: Ubiquitin-related modifier 1



- Molecule 2: Ubiquitin-related modifier 1



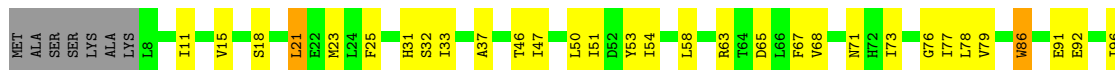
- Molecule 2: Ubiquitin-related modifier 1





- Molecule 2: Ubiquitin-related modifier 1

Chain L: 62% 30% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.43Å 197.22Å 139.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.50 48.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.47-2.50) 99.3 (48.47-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.5, PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.234 , 0.272 0.244 , 0.280	Depositor DCC
$R_{free}$ test set	4366 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.1	Xtrriage
Anisotropy	0.449	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/1272	0.56	0/1730
1	B	0.30	0/1284	0.52	0/1745
1	C	0.32	0/1263	0.52	0/1718
1	D	0.35	0/1267	0.59	0/1723
1	E	0.43	0/1263	0.63	0/1718
1	F	0.39	0/1255	0.63	1/1708 (0.1%)
2	G	0.31	0/838	0.54	0/1137
2	H	0.30	0/846	0.53	0/1148
2	I	0.45	0/846	0.72	0/1148
2	J	0.56	3/838 (0.4%)	0.74	3/1137 (0.3%)
2	K	0.27	0/846	0.52	0/1148
2	L	0.29	0/846	0.56	0/1148
All	All	0.37	3/12664 (0.0%)	0.59	4/17208 (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
2	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	111	GLY	C-O	8.45	1.37	1.23
2	J	111	GLY	CA-C	-6.08	1.42	1.51
2	J	110	GLY	C-N	-5.17	1.23	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	110	GLY	CA-C-N	-6.71	102.79	116.20
2	J	110	GLY	O-C-N	6.54	134.31	123.20
1	F	57	THR	CA-CB-OG1	-5.52	97.40	109.00
2	J	24	LEU	CB-CG-CD1	-5.02	102.47	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	110	GLY	Mainchain

## 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	1256	0	1250	14	0
1	B	1268	0	1269	22	0
1	C	1247	0	1242	38	0
1	D	1251	0	1245	40	0
1	E	1247	0	1242	18	0
1	F	1239	0	1230	42	0
2	G	821	0	809	12	0
2	H	829	0	820	15	0
2	I	829	0	820	29	0
2	J	821	0	809	41	0
2	K	829	0	820	8	0
2	L	829	0	820	42	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	8	0	0	0	0
3	I	5	0	0	0	0
3	J	4	0	0	1	0
3	K	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	3	0	0	0	0
4	A	33	0	0	1	0
4	B	22	0	0	5	0
4	C	9	0	0	3	0
4	D	11	0	0	3	0
4	E	15	0	0	4	0
4	F	4	0	0	0	0
4	G	6	0	0	0	0
4	H	12	0	0	2	0
4	I	9	0	0	5	0
4	J	6	0	0	0	0
4	K	21	0	0	2	0
4	L	9	0	0	6	0
All	All	12664	0	12376	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.

The worst 5 of 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:53:PRO:HB2	4:E:302:HOH:O	1.33	1.21
2:L:54:ILE:HA	2:L:58:LEU:HD23	1.32	1.11
2:L:25:PHE:HB3	4:L:302:HOH:O	1.55	1.06
2:I:9:GLU:HB2	4:I:402:HOH:O	1.55	1.04
2:L:25:PHE:CB	4:L:302:HOH:O	2.03	1.03

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	168/174 (97%)	160 (95%)	8 (5%)	0	100	100
1	B	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
1	C	166/174 (95%)	160 (96%)	6 (4%)	0	100	100
1	D	167/174 (96%)	158 (95%)	9 (5%)	0	100	100
1	E	166/174 (95%)	160 (96%)	6 (4%)	0	100	100
1	F	165/174 (95%)	155 (94%)	10 (6%)	0	100	100
2	G	101/111 (91%)	96 (95%)	5 (5%)	0	100	100
2	H	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
2	I	102/111 (92%)	96 (94%)	6 (6%)	0	100	100
2	J	101/111 (91%)	92 (91%)	9 (9%)	0	100	100
2	K	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
2	L	102/111 (92%)	95 (93%)	7 (7%)	0	100	100
All	All	1611/1710 (94%)	1529 (95%)	82 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	132/134 (98%)	130 (98%)	2 (2%)	65	85
1	B	134/134 (100%)	132 (98%)	2 (2%)	65	85
1	C	132/134 (98%)	127 (96%)	5 (4%)	33	58
1	D	132/134 (98%)	129 (98%)	3 (2%)	50	76
1	E	132/134 (98%)	126 (96%)	6 (4%)	27	51
1	F	131/134 (98%)	127 (97%)	4 (3%)	40	67
2	G	92/98 (94%)	89 (97%)	3 (3%)	38	64
2	H	93/98 (95%)	90 (97%)	3 (3%)	39	65
2	I	93/98 (95%)	90 (97%)	3 (3%)	39	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	92/98 (94%)	89 (97%)	3 (3%)	38 64
2	K	93/98 (95%)	88 (95%)	5 (5%)	22 42
2	L	93/98 (95%)	90 (97%)	3 (3%)	39 65
All	All	1349/1392 (97%)	1307 (97%)	42 (3%)	40 67

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	18	SER
2	K	18	SER
2	I	61	ASP
2	J	58	LEU
2	K	65	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	168	ASN
1	F	77	GLN
2	L	71	ASN
2	G	82	ASN
2	I	31	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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	CSS	D	60	1	4,6,7	0.94	0	1,6,8	0.49	0
1	CSS	E	60	1	4,6,7	0.75	0	1,6,8	0.09	0
1	CSS	A	60	1	4,6,7	1.20	0	1,6,8	0.21	0
1	CSS	F	60	1	4,6,7	1.05	0	1,6,8	0.03	0
1	CSS	B	60	1	4,6,7	1.03	0	1,6,8	0.06	0
1	CSS	C	60	1	4,6,7	0.97	0	1,6,8	0.33	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	D	60	1	-	0/1/5/7	-
1	CSS	E	60	1	-	0/1/5/7	-
1	CSS	A	60	1	-	0/1/5/7	-
1	CSS	F	60	1	-	0/1/5/7	-
1	CSS	B	60	1	-	0/1/5/7	-
1	CSS	C	60	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	60	CSS	5	0
1	E	60	CSS	3	0
1	A	60	CSS	5	0
1	B	60	CSS	4	0
1	C	60	CSS	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 41 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.