WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:09 AM GMT

PDB ID	:	3DHW
Title	:	Crystal structure of methionine importer MetNI
Authors	:	Rees, D.C.; Kaiser, J.T.; Kadaba, N.S.; Johnson, E.; Lee, A.T.
Deposited on	:	2008-06-18
Resolution	:	3.70 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

A user guide is available at

http://wwpdb.org/validation/2016/XrayValidationReportHelp

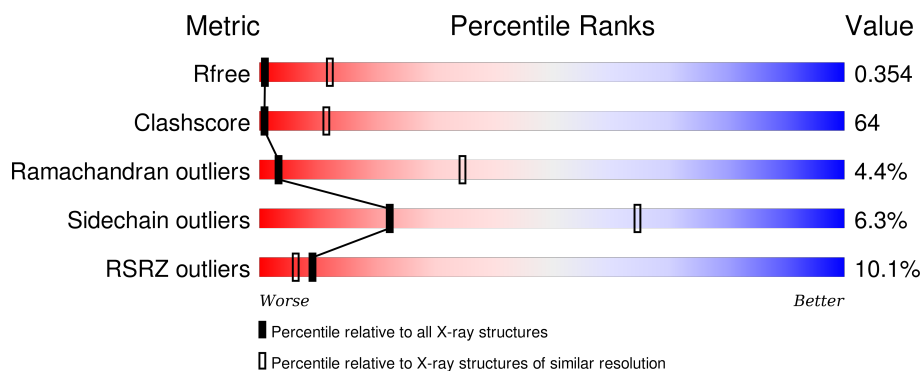with specific help available everywhere you see the ⓘ symbol.

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 3.70 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	Percentile Ranks	Value
Rfree		0.354
Clashscore		64
Ramachandran outliers		4.4%
Sidechain outliers		6.3%
RSRZ outliers		10.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	217	3% · 18% 60% 12% · 6%
1	B	217	7% · 25% 57% 10% · 6%
1	E	217	7% · 24% 59% 10% 6%
1	F	217	2% · 21% 59% 12% · 6%
2	C	343	3% · 28% 56% 15% ·

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Mol	Chain	Length	Quality of chain
2	D	343	7% · · · 38% · · · 54% · · · 7% ·
2	G	343	27% · · · 37% · · · 59% · · ·
2	H	343	14% · · · 38% · · · 55% · · · 6% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16688 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 D-methionine transport system permease protein metI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1520	1014	244	254	8			
1	B	203	Total	C	N	O	S	0	0	0
			1520	1014	244	254	8			
1	E	203	Total	C	N	O	S	0	0	0
			1520	1014	244	254	8			
1	F	203	Total	C	N	O	S	0	0	0
			1520	1014	244	254	8			

- Molecule 2 is a protein called Methionine import ATP-binding protein metN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	343	Total	C	N	O	S	0	0	0
			2652	1664	467	509	12			
2	D	343	Total	C	N	O	S	0	0	0
			2652	1664	467	509	12			
2	G	343	Total	C	N	O	S	0	0	0
			2652	1664	467	509	12			
2	H	343	Total	C	N	O	S	0	0	0
			2652	1664	467	509	12			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by iss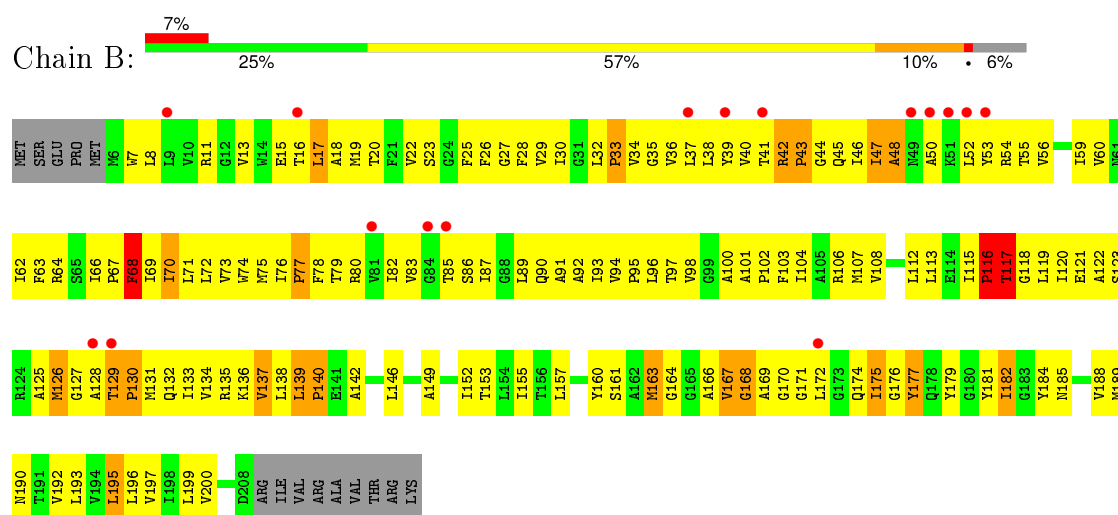ues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches 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.

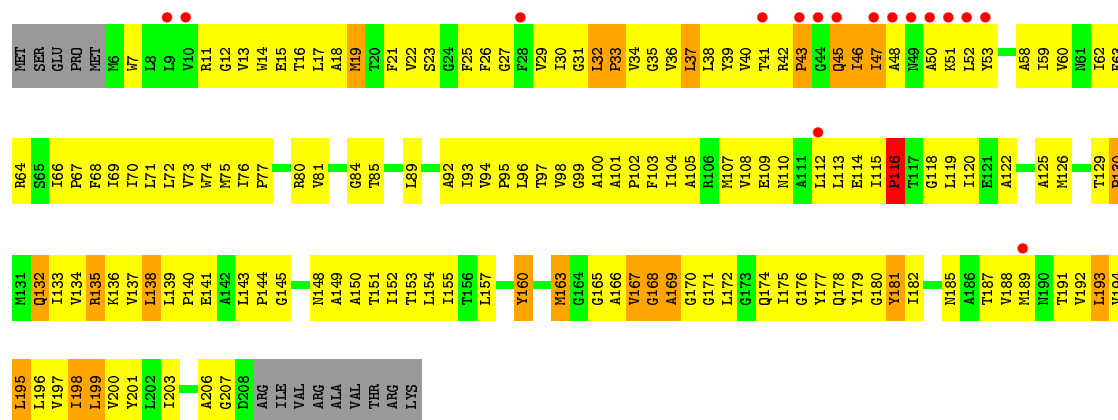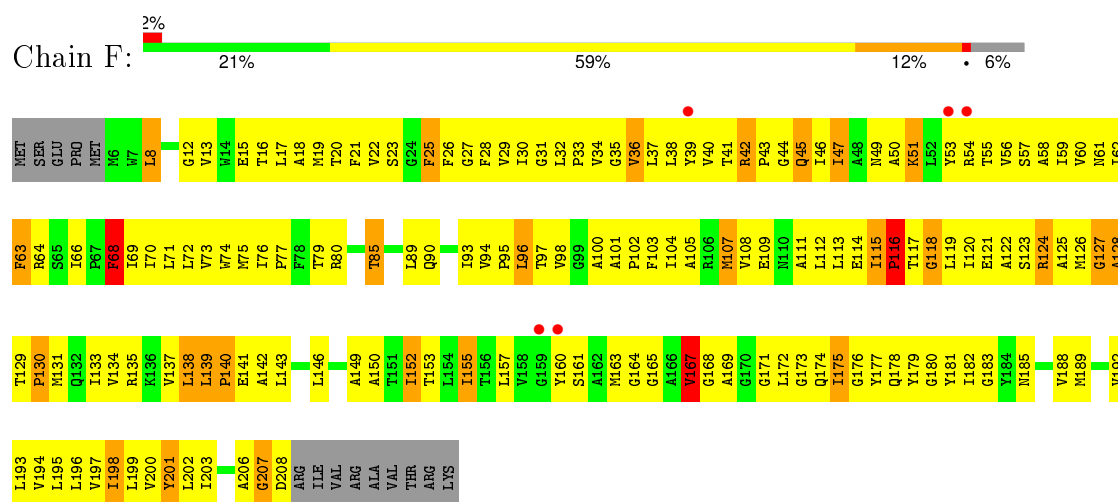• Molecule 1: D-methionine transport system permease protein metI

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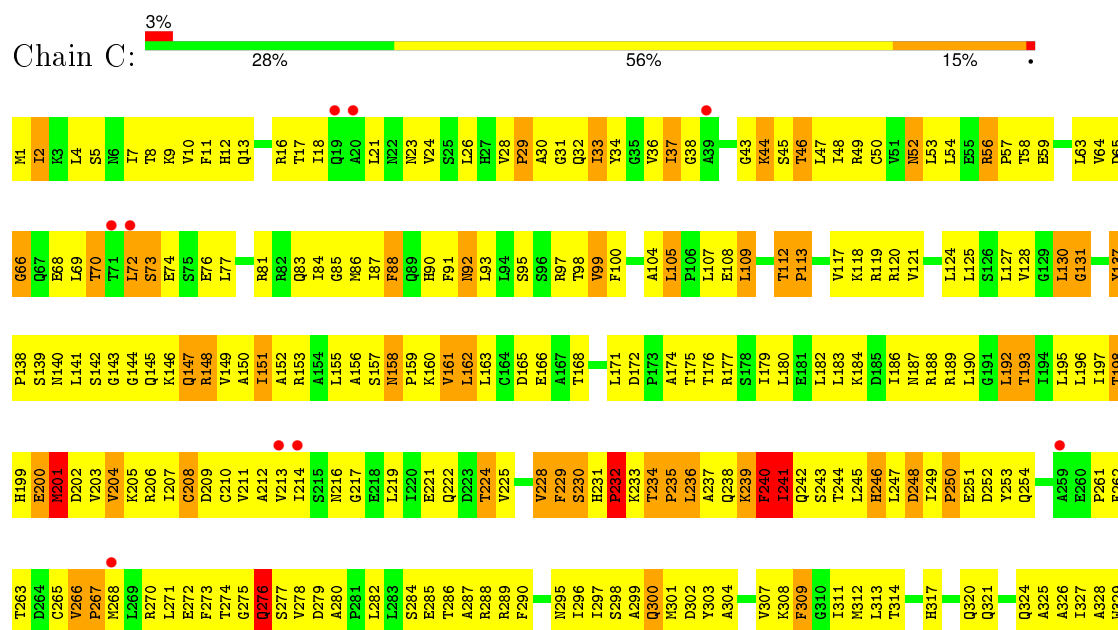• Molecule 1: D-methionine transport system permease protein metI

• Molecule 1: D-methionine transport system permease protein metI

Chain F:

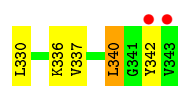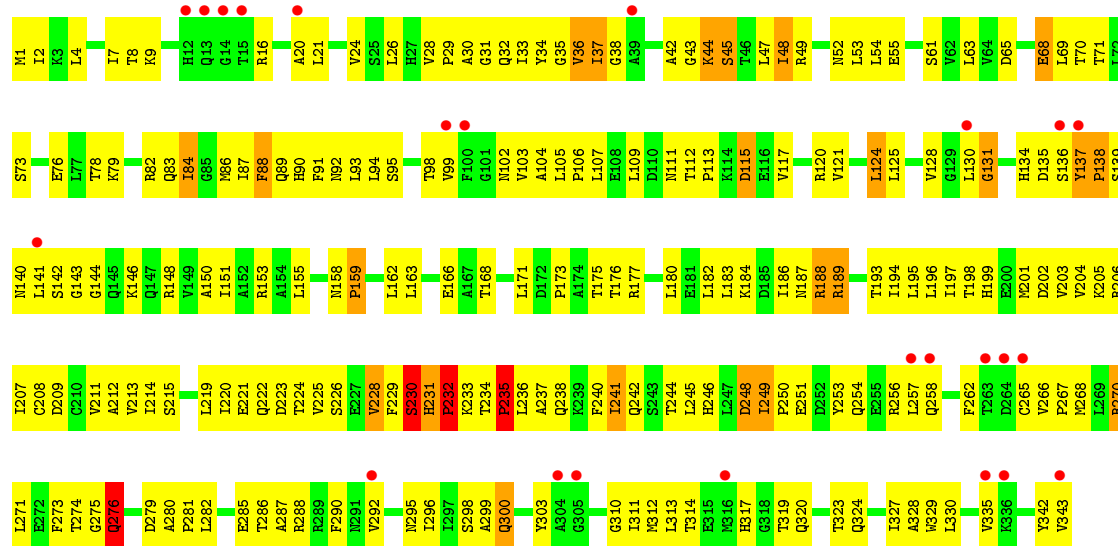
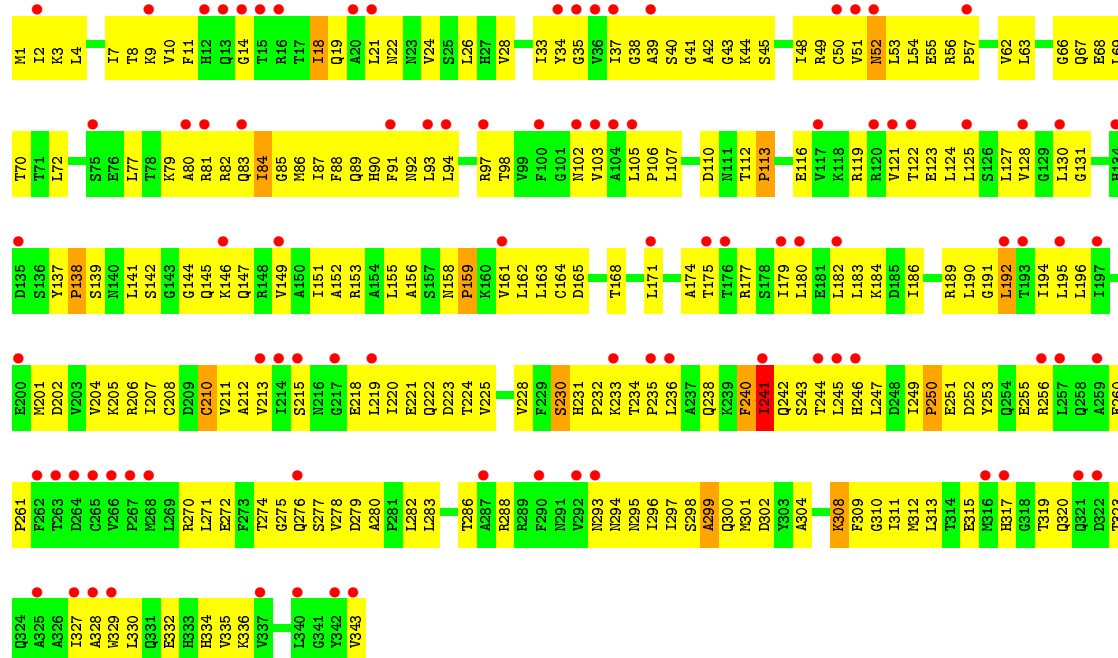
• Molecule 2: Methionine import ATP-binding protein metN

Chain C:

L330 K336 V337 L340 G341 Y342 V343

• Molecule 2: Methionine import ATP-binding protein metN

Chain D:

7%

38% 54% 7%

M1 I2 K3 L4 I7 T8 K9 H12 Q13 G14 T15 R16 A20 L21 V24 S25 L26 H27 V28 P29 A30 G31 Q32 I33 Y34 G35 V36 I37 G38 A39 A42 G43 K44 S45 T46 L47 I48 R49 N52 L53 L54 E55 S61 V62 L63 V64 D65 E68 L69 T70 T71 L72

S73 E76 L77 T78 K79 R82 Q83 I84 G85 M86 I87 F88 Q89 H90 F91 N92 L93 L94 S95 T98 V99 F100 G101 N102 V103 A104 L105 P106 L107 E108 L109 D110 N111 T112 P113 K114 D115 E116 V117 R120 V121 L124 L125 V128 G129 L130 G131 H134 D135 S136 Y137 P138 S139

N140 L141 S142 G143 G144 Q145 K146 Q147 R148 V149 A150 I151 A152 R153 A154 L155 M158 P159 L162 L163 E166 A167 T168 L171 D172 P173 A174 T175 R176 R177 L180 E181 L182 L183 K184 D185 I186 N187 R188 R189 T193 I194 L195 L196 I197 T198 H199 E200 M201 D202 V203 V204 K205 R206

I207 C208 D209 C210 V211 A212 V213 I214 S215 L219 I220 E221 Q222 D223 T224 V225 S226 E227 V228 F229 S230 H231 I232 K233 T234 I235 L236 A237 Q238 K239 F240 I241 Q242 S243 T244 L245 H246 D248 I249 P250 E251 D252 Y253 Q254 E255 R256 L257 Q258 F262 T263 D264 C265 V266 P267 M268 L269 R270

L271 E272 F273 T274 G275 Q276 D279 A280 P281 L282 E285 T286 A287 R288 R289 F290 N291 V292 N295 I296 I297 S298 A299 Q300 Y303 A304 G305 G310 I311 M312 L313 T314 E315 M316 H317 G318 T319 Q320 T323 Q324 I327 A328 W329 L330 V335 K336 Y342 V343

• Molecule 2: Methionine import ATP-binding protein metN

Chain G:

27%

37% 59%

M1 I2 K3 L4 I7 T8 K9 V10 F11 H12 Q13 G14 T15 R16 T17 I18 Q19 A20 L21 N22 N23 V24 S25 L26 H27 V28 I33 Y34 G35 V36 I37 G38 A39 S40 G41 A42 G43 K44 S45 I48 R49 C50 V51 N52 L53 L54 E55 R56 P57 V62 L63 G66 Q67 E68 L69

T70 T71 L72 S75 E76 L77 T78 K79 A80 R81 R82 Q83 I84 G85 M86 I87 F88 Q89 H90 F91 N92 L93 L94 R97 T98 V99 F100 G101 N102 V103 A104 L105 P106 L107 D110 N111 T112 P113 E116 V117 K118 R119 R120 V121 T122 K123 L124 L125 S126 L127 V128 G129 L130 G131 H134

D135 S136 Y137 P138 S139 N140 L141 S142 G143 G144 Q145 K146 Q147 R148 V149 A150 I151 A152 R153 A154 L155 A156 S157 N158 P159 K160 V161 L162 L163 C164 D165 T168 L171 A174 T175 R176 R177 S178 I179 L180 E181 L182 L183 K184 D185 I186 R189 L190 G191 L192 T193 I194 L195 L196 I197

E200 M201 D202 V203 V204 K205 R206 I207 C208 D209 C210 V211 A212 V213 I214 S215 N216 G217 L219 I220 E221 Q222 D223 T224 V225 V228 F229 S230 H231 P232 K233 T234 P235 L236 A237 Q238 K239 F240 I241 Q242 S243 T244 L245 H246 L247 D248 I249 P250 E251 D252 Y253 Q254 E255 R256 L257 Q258 A259 E260

F261 F262 T263 D264 C265 V266 P267 M268 L269 R270 L271 E272 F273 T274 G275 Q276 S277 V278 D279 A280 P281 L282 L283 T286 A287 R288 R289 F290 N291 V292 N293 N294 N295 I296 I297 S298 A299 Q300 M301 D302 Y303 A304 K308 F309 G310 I311 M312 L313 T314 E315 M316 H317 G318 T319 Q320 Q321 D322 T323

Q324 A325 A326 I327 A328 W329 L330 Q331 E332 H333 H334 V335 K336 V337 L340 G341 Y342 V343

• Molecule 2: Methionine import ATP-binding protein metN

Chain H:

14%

38% 55% 6%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.70Å 165.40Å 289.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 3.70 43.57 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.90-3.70) 99.6 (43.57-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.310 , 0.347 0.319 , 0.354	Depositor DCC
R_{free} test set	5070 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	153.5	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 95.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Outliers	0 of 50643 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16688	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	1.08	2/1552 (0.1%)	1.33	16/2122 (0.8%)
1	B	0.88	0/1552	1.21	7/2122 (0.3%)
1	E	0.79	0/1552	1.22	9/2122 (0.4%)
1	F	1.12	1/1552 (0.1%)	1.36	10/2122 (0.5%)
2	C	1.40	13/2691 (0.5%)	1.50	35/3647 (1.0%)
2	D	1.01	1/2691 (0.0%)	1.27	18/3647 (0.5%)
2	G	0.70	0/2691	1.08	7/3647 (0.2%)
2	H	0.93	0/2691	1.24	13/3647 (0.4%)
All	All	1.02	17/16972 (0.1%)	1.28	115/23076 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	E	0	2
2	C	0	2
All	All	0	8

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	309	PHE	CD2-CE2	12.45	1.64	1.39
2	C	309	PHE	CD1-CE1	12.23	1.63	1.39
2	C	229	PHE	CG-CD2	9.48	1.52	1.38
2	C	228	VAL	C-O	9.44	1.41	1.23
2	D	205	LYS	CD-CE	7.57	1.70	1.51

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	116	PRO	N-CA-C	9.67	137.25	112.10
2	D	205	LYS	CD-CE-NZ	9.19	132.83	111.70
2	H	125	LEU	CB-CG-CD2	-9.11	95.52	111.00
1	F	115	ILE	C-N-CD	-9.07	100.66	120.60
2	C	239	LYS	CA-C-N	-8.79	97.87	117.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	TYR	Sidechain
1	A	184	TYR	Sidechain
1	A	205	PHE	Sidechain
1	B	177	TYR	Sidechain
2	C	198	THR	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	1520	0	1622	240	0
1	B	1520	0	1622	259	0
1	E	1520	0	1622	258	0
1	F	1520	0	1622	301	0
2	C	2652	0	2705	375	0
2	D	2652	0	2705	310	0
2	G	2652	0	2705	280	0
2	H	2652	0	2705	344	0
All	All	16688	0	17308	2189	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 64.

The worst 5 of 2189 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:MET:SD	2:C:201:MET:CE	2.14	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:VAL:HG23	1:E:95:PRO:HD3	1.22	1.15
1:F:126:MET:SD	1:F:129:THR:HA	1.87	1.13
2:D:31:GLY:H	2:D:193:THR:HG22	1.08	1.12
1:B:72:LEU:HD22	1:B:95:PRO:HB2	1.28	1.08

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	201/217 (93%)	178 (89%)	9 (4%)	14 (7%)	1	22
1	B	201/217 (93%)	187 (93%)	3 (2%)	11 (6%)	2	29
1	E	201/217 (93%)	180 (90%)	11 (6%)	10 (5%)	3	31
1	F	201/217 (93%)	177 (88%)	10 (5%)	14 (7%)	1	22
2	C	341/343 (99%)	307 (90%)	19 (6%)	15 (4%)	3	35
2	D	341/343 (99%)	323 (95%)	8 (2%)	10 (3%)	6	46
2	G	341/343 (99%)	317 (93%)	14 (4%)	10 (3%)	6	46
2	H	341/343 (99%)	316 (93%)	14 (4%)	11 (3%)	5	44
All	All	2168/2240 (97%)	1985 (92%)	88 (4%)	95 (4%)	3	35

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	47	ILE
1	A	48	ALA
1	A	83	VAL
1	A	117	THR

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	158/172 (92%)	140 (89%)	18 (11%)	7	38
1	B	158/172 (92%)	145 (92%)	13 (8%)	14	53
1	E	158/172 (92%)	149 (94%)	9 (6%)	25	68
1	F	158/172 (92%)	146 (92%)	12 (8%)	16	57
2	C	298/298 (100%)	269 (90%)	29 (10%)	10	46
2	D	298/298 (100%)	281 (94%)	17 (6%)	25	68
2	G	298/298 (100%)	290 (97%)	8 (3%)	52	83
2	H	298/298 (100%)	289 (97%)	9 (3%)	48	81
All	All	1824/1880 (97%)	1709 (94%)	115 (6%)	22	64

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	232	PRO
2	D	84	ILE
2	H	2	ILE
2	C	240	PHE
2	C	276	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	242	GLN
1	F	110	ASN
2	H	158	ASN
2	D	334	HIS
1	F	190	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	203/217 (93%)	0.03	7 (3%)	49	34	113, 166, 210, 234	0
1	B	203/217 (93%)	0.26	16 (7%)	15	9	135, 195, 245, 259	0
1	E	203/217 (93%)	0.30	16 (7%)	15	9	136, 202, 249, 260	0
1	F	203/217 (93%)	-0.03	5 (2%)	61	45	106, 166, 222, 244	0
2	C	343/343 (100%)	0.07	11 (3%)	51	35	74, 133, 194, 241	0
2	D	343/343 (100%)	0.30	24 (6%)	19	11	105, 170, 214, 229	0
2	G	343/343 (100%)	1.19	93 (27%)	1	1	157, 209, 249, 265	0
2	H	343/343 (100%)	0.67	49 (14%)	4	3	94, 186, 234, 253	0
All	All	2184/2240 (97%)	0.40	221 (10%)	9	6	74, 179, 238, 265	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	214	ILE	8.7
2	H	17	THR	8.4
1	E	44	GLY	6.6
2	G	91	PHE	6.5
1	B	52	LEU	6.3

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.