wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 03:16 PM EDT

PDB ID	:	3NL2
Title	:	The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosyhthesis of Eukaryotes
Authors	:	Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.
Deposited on	:	2010-06-21
Resolution	:	3.08 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
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:

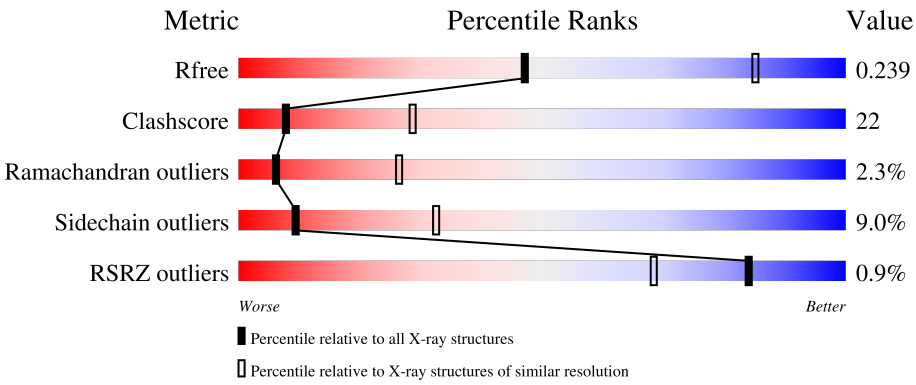
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	540	% 58% 29% 6% • 6%
1	B	540	% 56% 31% 6% • 6%
1	C	540	% 56% 30% 6% 8%
1	D	540	57% 29% 6% 7%
1	E	540	% 58% 29% 5% 7%

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Mol	Chain	Length	Quality of chain
1	F	540	2% 59% 28% 5% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22460 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 Thiamine biosynthetic bifunctional enzyme.

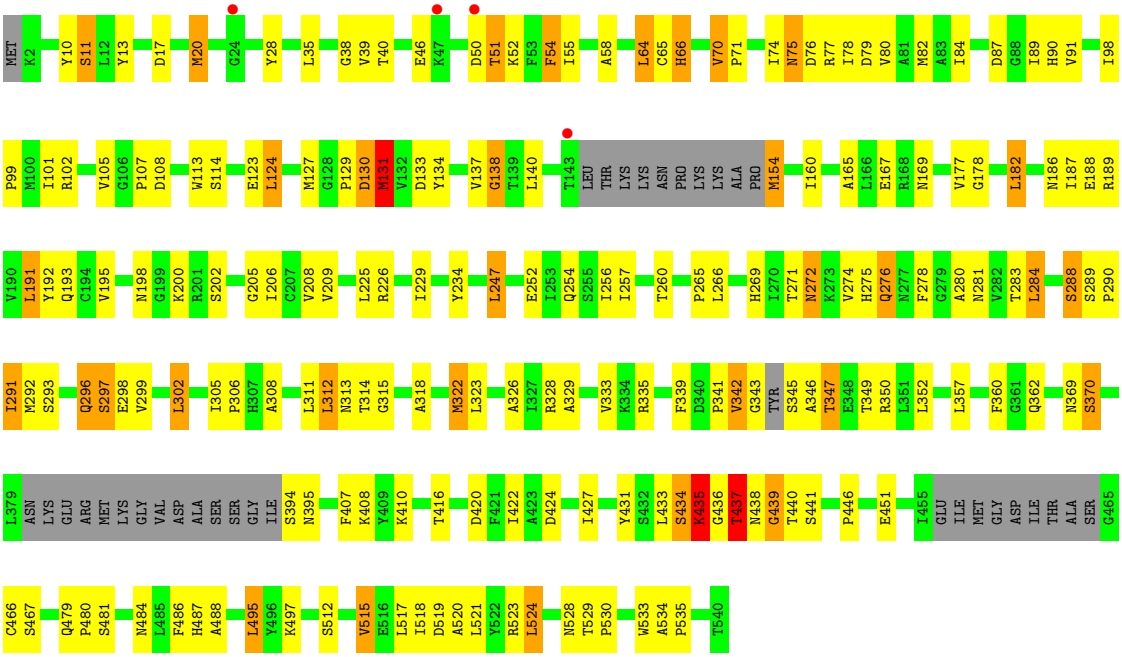
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	3764	2376	634	733	21	0	0	0
1	B	505	3766	2382	635	728	21	0	0	0
1	C	498	3727	2356	626	724	21	0	0	0
1	D	501	3739	2360	630	727	22	0	0	0
1	E	503	3767	2383	634	728	22	0	0	0
1	F	494	3697	2342	623	711	21	0	0	0

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.

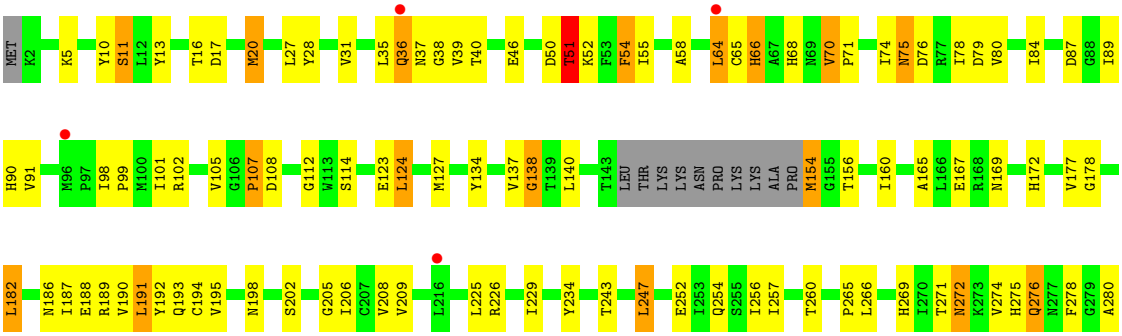
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

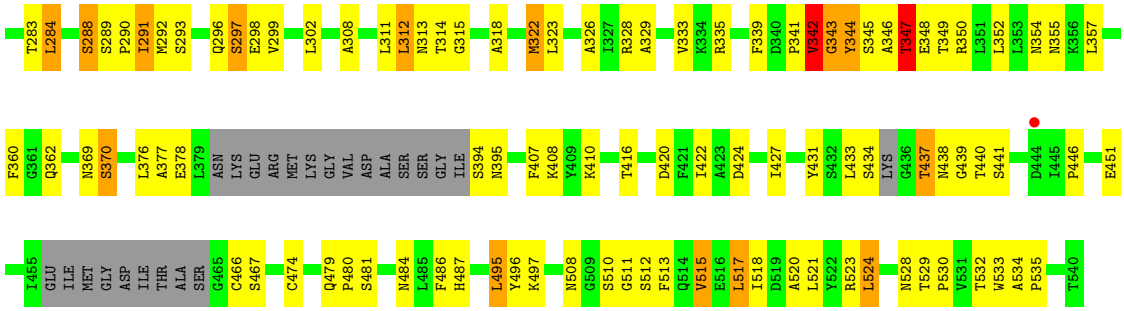
Chain A:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

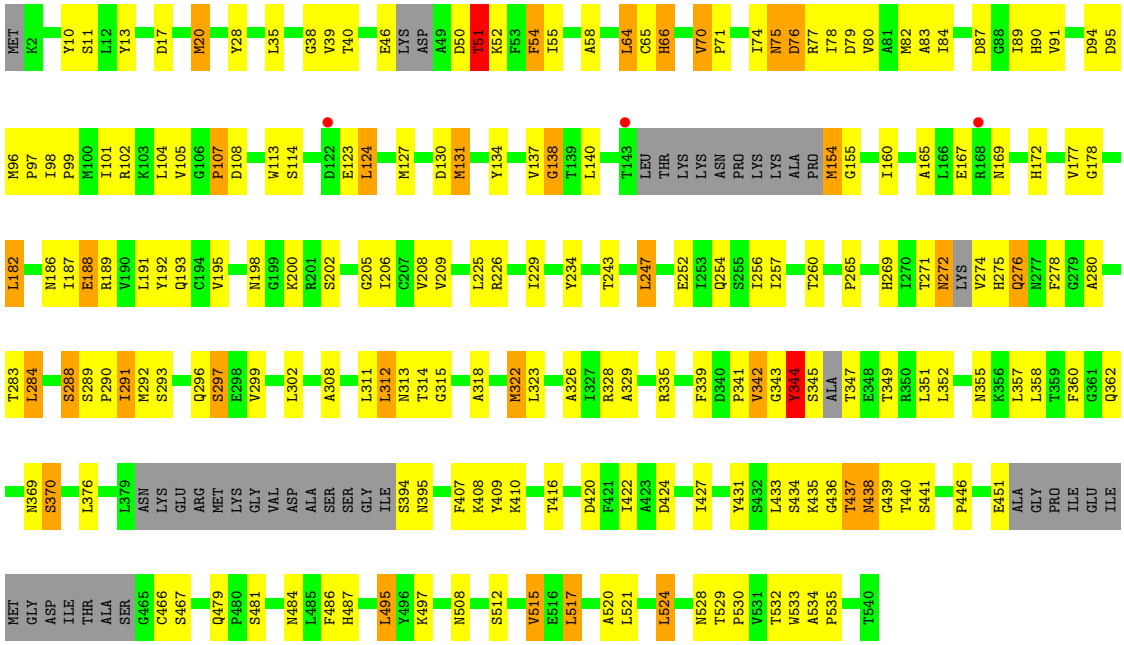
Chain B:





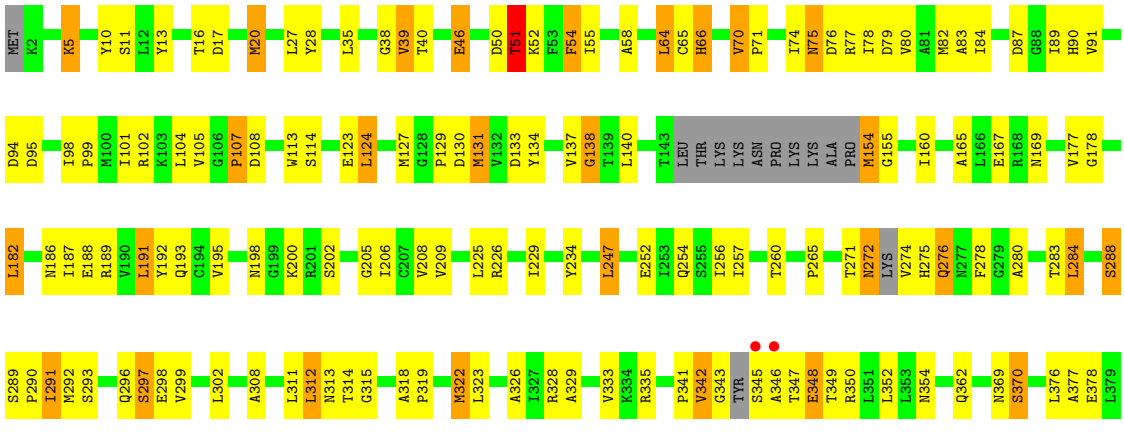
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

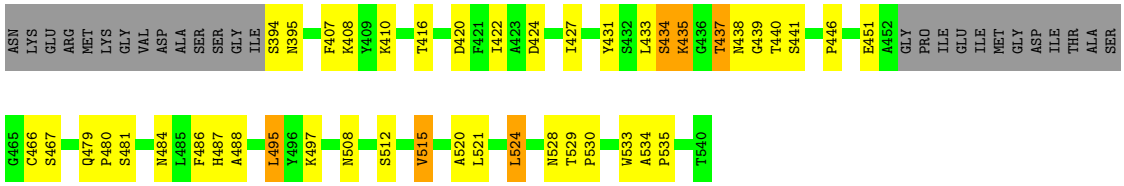
Chain C:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

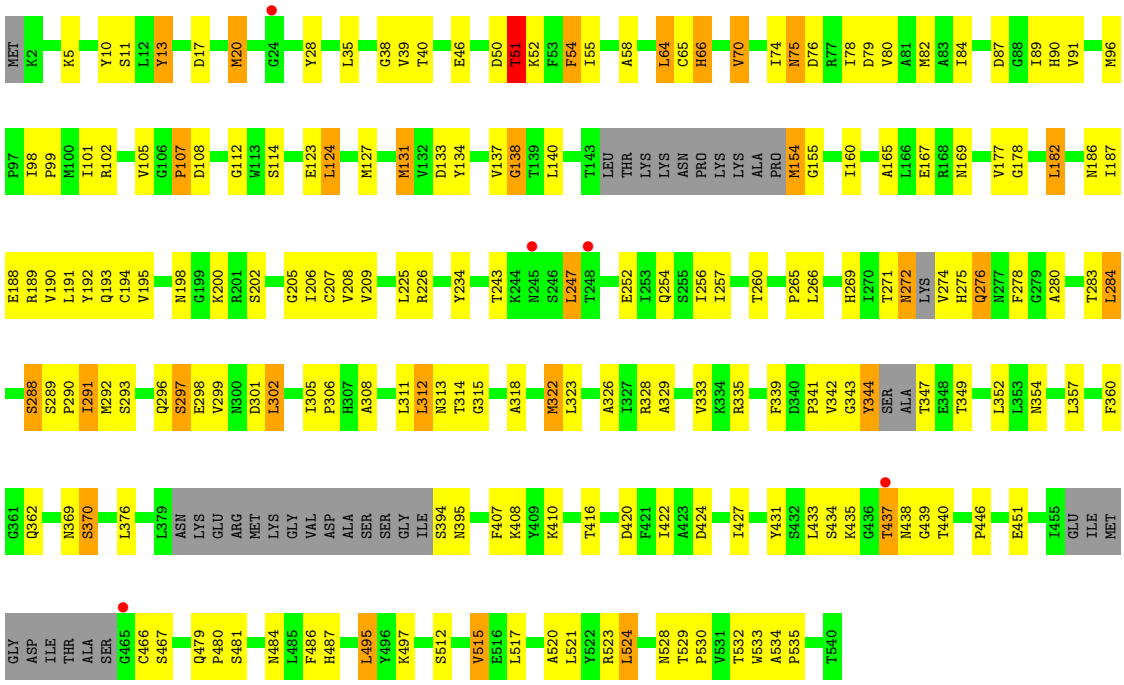
Chain D:





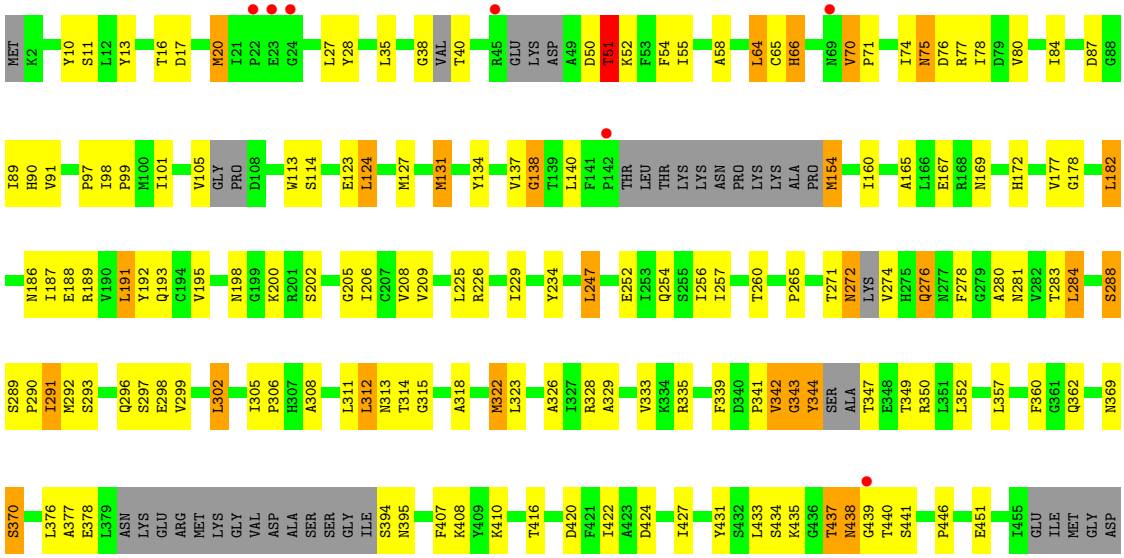
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

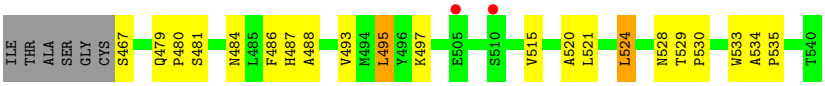
Chain E:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain F:




ILE
THR
ALA
SER
GLY
CYS
S467
Q479
P480
S481
N484
L485
F486
H487
A488
V493
M494
L495
Y496
K497
E505
S510
V515
A520
L521
L524
N528
T529
P530
W533
A534
P535
T540

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.47Å 153.01Å 146.75Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	37.00 – 3.08 49.64 – 3.08	Depositor EDS
% Data completeness (in resolution range)	85.8 (37.00-3.08) 93.1 (49.64-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.244 0.213 , 0.239	Depositor DCC
R_{free} test set	3826 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.9	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22460	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% 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 (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	0.41	0/3823	0.63	4/5189 (0.1%)
1	B	0.43	0/3826	0.60	0/5192
1	C	0.41	0/3784	0.58	1/5131 (0.0%)
1	D	0.42	0/3796	0.63	3/5149 (0.1%)
1	E	0.42	0/3826	0.60	0/5188
1	F	0.41	0/3752	0.59	1/5083 (0.0%)
All	All	0.42	0/22807	0.61	9/30932 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	D	0	1
1	E	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	345	SER	N-CA-CB	-10.62	94.57	110.50
1	A	434	SER	CB-CA-C	-9.02	92.96	110.10
1	A	437	THR	N-CA-C	8.15	133.02	111.00
1	D	434	SER	CB-CA-C	-7.64	95.58	110.10
1	A	435	LYS	N-CA-CB	6.20	121.75	110.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	PRO	Peptide
1	A	435	LYS	Peptide
1	A	436	GLY	Peptide
1	A	438	ASN	Peptide
1	B	347	THR	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	3764	0	3745	165	0
1	B	3766	0	3751	186	0
1	C	3727	0	3706	181	0
1	D	3739	0	3715	186	0
1	E	3767	0	3765	159	0
1	F	3697	0	3690	150	0
All	All	22460	0	22372	973	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 22.

The worst 5 of 973 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:339:PHE:CE2	1:F:341:PRO:HG3	1.66	1.27
1:A:339:PHE:CE2	1:A:341:PRO:HG3	1.76	1.19
1:C:265:PRO:HD2	1:C:288:SER:HB3	1.39	1.04
1:B:345:SER:HA	1:B:347:THR:N	1.73	1.03
1:D:274:VAL:HG13	1:E:292:MET:HG3	1.42	1.01

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	495/540 (92%)	445 (90%)	41 (8%)	9 (2%)	8	32
1	B	495/540 (92%)	439 (89%)	41 (8%)	15 (3%)	4	21
1	C	484/540 (90%)	434 (90%)	38 (8%)	12 (2%)	5	25
1	D	489/540 (91%)	440 (90%)	36 (7%)	13 (3%)	5	23
1	E	491/540 (91%)	444 (90%)	38 (8%)	9 (2%)	8	32
1	F	476/540 (88%)	434 (91%)	32 (7%)	10 (2%)	7	28
All	All	2930/3240 (90%)	2636 (90%)	226 (8%)	68 (2%)	6	26

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	MET
1	A	347	THR
1	A	370	SER
1	B	370	SER
1	C	344	TYR

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	408/449 (91%)	370 (91%)	38 (9%)	9	31
1	B	406/449 (90%)	369 (91%)	37 (9%)	9	31
1	C	404/449 (90%)	367 (91%)	37 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/449 (90%)	369 (91%)	35 (9%)	10	35
1	E	409/449 (91%)	374 (91%)	35 (9%)	10	36
1	F	399/449 (89%)	363 (91%)	36 (9%)	9	32
All	All	2430/2694 (90%)	2212 (91%)	218 (9%)	9	32

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	64	LEU
1	D	481	SER
1	F	288	SER
1	D	124	LEU
1	D	289	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	93	GLN
1	F	193	GLN
1	E	276	GLN
1	E	514	GLN
1	F	313	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 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 (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(Å^2)	Q<0.9
1	A	505/540 (93%)	-0.18	4 (0%)	86	71	51, 76, 110, 138	0
1	B	505/540 (93%)	-0.03	5 (0%)	82	66	39, 77, 112, 137	0
1	C	498/540 (92%)	-0.17	3 (0%)	89	77	52, 75, 108, 136	0
1	D	501/540 (92%)	-0.15	2 (0%)	92	84	20, 75, 108, 139	0
1	E	503/540 (93%)	-0.13	5 (0%)	82	66	39, 76, 111, 138	0
1	F	494/540 (91%)	-0.19	9 (1%)	68	46	37, 75, 106, 134	0
All	All	3006/3240 (92%)	-0.14	28 (0%)	84	68	20, 76, 110, 139	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	THR	6.6
1	E	245	ASN	3.1
1	A	24	GLY	2.9
1	C	122	ASP	2.9
1	E	248	THR	2.8

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 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.