wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 05:26 am BST

PDB ID	:	5GK0
Title	:	Crystal structure of selnomethionin-labeled ketosynthase StlD
Authors	:	Mori, T.; Saito, Y.; Morita, H.; Abe, I.
Deposited on	:	2016-07-03
Resolution	:	2.33 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 following versions of software and data (see references (i)) were used in the production of this report:

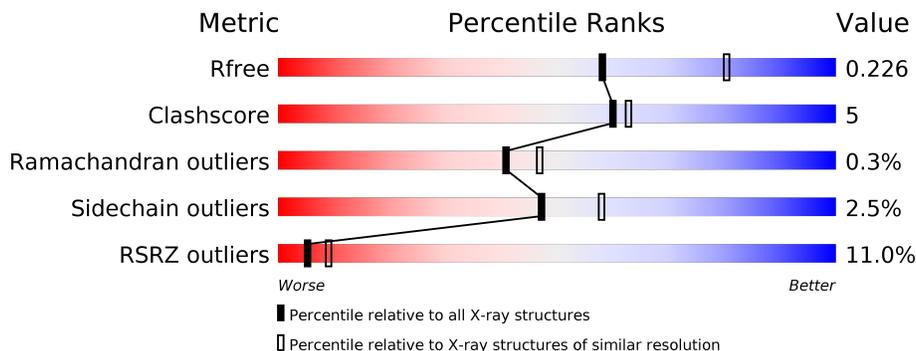|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.33 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		0.226
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		2.5%
RSRZ outliers		11.0%

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 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	402	4% / 85% 9% 5%
1	B	402	12% / 77% 14% 10%
1	C	402	18% / 77% 16% • 6%
1	D	402	6% / 85% 9% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12283 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 Ketosynthase StlD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	Se	0	0	0
			2974	1871	511	574	5	13			
1	B	363	Total	C	N	O	S	Se	0	0	0
			2843	1796	481	548	5	13			
1	C	379	Total	C	N	O	S	Se	0	0	0
			2966	1867	509	572	5	13			
1	D	380	Total	C	N	O	S	Se	0	0	0
			2974	1871	511	574	5	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP Q7N4Z6
A	-18	GLY	-	expression tag	UNP Q7N4Z6
A	-17	SER	-	expression tag	UNP Q7N4Z6
A	-16	SER	-	expression tag	UNP Q7N4Z6
A	-15	HIS	-	expression tag	UNP Q7N4Z6
A	-14	HIS	-	expression tag	UNP Q7N4Z6
A	-13	HIS	-	expression tag	UNP Q7N4Z6
A	-12	HIS	-	expression tag	UNP Q7N4Z6
A	-11	HIS	-	expression tag	UNP Q7N4Z6
A	-10	HIS	-	expression tag	UNP Q7N4Z6
A	-9	SER	-	expression tag	UNP Q7N4Z6
A	-8	SER	-	expression tag	UNP Q7N4Z6
A	-7	GLY	-	expression tag	UNP Q7N4Z6
A	-6	LEU	-	expression tag	UNP Q7N4Z6
A	-5	VAL	-	expression tag	UNP Q7N4Z6
A	-4	PRO	-	expression tag	UNP Q7N4Z6
A	-3	ARG	-	expression tag	UNP Q7N4Z6
A	-2	GLY	-	expression tag	UNP Q7N4Z6
A	-1	SER	-	expression tag	UNP Q7N4Z6
A	0	HIS	-	expression tag	UNP Q7N4Z6
B	-19	MSE	-	expression tag	UNP Q7N4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q7N4Z6
B	-17	SER	-	expression tag	UNP Q7N4Z6
B	-16	SER	-	expression tag	UNP Q7N4Z6
B	-15	HIS	-	expression tag	UNP Q7N4Z6
B	-14	HIS	-	expression tag	UNP Q7N4Z6
B	-13	HIS	-	expression tag	UNP Q7N4Z6
B	-12	HIS	-	expression tag	UNP Q7N4Z6
B	-11	HIS	-	expression tag	UNP Q7N4Z6
B	-10	HIS	-	expression tag	UNP Q7N4Z6
B	-9	SER	-	expression tag	UNP Q7N4Z6
B	-8	SER	-	expression tag	UNP Q7N4Z6
B	-7	GLY	-	expression tag	UNP Q7N4Z6
B	-6	LEU	-	expression tag	UNP Q7N4Z6
B	-5	VAL	-	expression tag	UNP Q7N4Z6
B	-4	PRO	-	expression tag	UNP Q7N4Z6
B	-3	ARG	-	expression tag	UNP Q7N4Z6
B	-2	GLY	-	expression tag	UNP Q7N4Z6
B	-1	SER	-	expression tag	UNP Q7N4Z6
B	0	HIS	-	expression tag	UNP Q7N4Z6
C	-19	MSE	-	expression tag	UNP Q7N4Z6
C	-18	GLY	-	expression tag	UNP Q7N4Z6
C	-17	SER	-	expression tag	UNP Q7N4Z6
C	-16	SER	-	expression tag	UNP Q7N4Z6
C	-15	HIS	-	expression tag	UNP Q7N4Z6
C	-14	HIS	-	expression tag	UNP Q7N4Z6
C	-13	HIS	-	expression tag	UNP Q7N4Z6
C	-12	HIS	-	expression tag	UNP Q7N4Z6
C	-11	HIS	-	expression tag	UNP Q7N4Z6
C	-10	HIS	-	expression tag	UNP Q7N4Z6
C	-9	SER	-	expression tag	UNP Q7N4Z6
C	-8	SER	-	expression tag	UNP Q7N4Z6
C	-7	GLY	-	expression tag	UNP Q7N4Z6
C	-6	LEU	-	expression tag	UNP Q7N4Z6
C	-5	VAL	-	expression tag	UNP Q7N4Z6
C	-4	PRO	-	expression tag	UNP Q7N4Z6
C	-3	ARG	-	expression tag	UNP Q7N4Z6
C	-2	GLY	-	expression tag	UNP Q7N4Z6
C	-1	SER	-	expression tag	UNP Q7N4Z6
C	0	HIS	-	expression tag	UNP Q7N4Z6
D	-19	MSE	-	expression tag	UNP Q7N4Z6
D	-18	GLY	-	expression tag	UNP Q7N4Z6
D	-17	SER	-	expression tag	UNP Q7N4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q7N4Z6
D	-15	HIS	-	expression tag	UNP Q7N4Z6
D	-14	HIS	-	expression tag	UNP Q7N4Z6
D	-13	HIS	-	expression tag	UNP Q7N4Z6
D	-12	HIS	-	expression tag	UNP Q7N4Z6
D	-11	HIS	-	expression tag	UNP Q7N4Z6
D	-10	HIS	-	expression tag	UNP Q7N4Z6
D	-9	SER	-	expression tag	UNP Q7N4Z6
D	-8	SER	-	expression tag	UNP Q7N4Z6
D	-7	GLY	-	expression tag	UNP Q7N4Z6
D	-6	LEU	-	expression tag	UNP Q7N4Z6
D	-5	VAL	-	expression tag	UNP Q7N4Z6
D	-4	PRO	-	expression tag	UNP Q7N4Z6
D	-3	ARG	-	expression tag	UNP Q7N4Z6
D	-2	GLY	-	expression tag	UNP Q7N4Z6
D	-1	SER	-	expression tag	UNP Q7N4Z6
D	0	HIS	-	expression tag	UNP Q7N4Z6

- Molecule 2 is water.

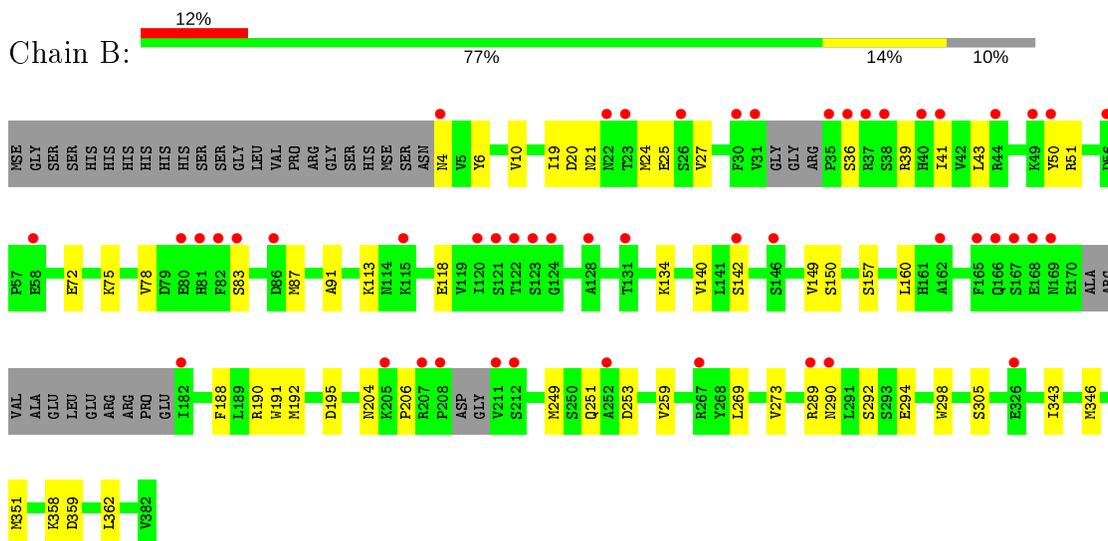| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	193	Total O 193 193	0	0
2	B	72	Total O 72 72	0	0
2	C	84	Total O 84 84	0	0
2	D	177	Total O 177 177	0	0

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 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.
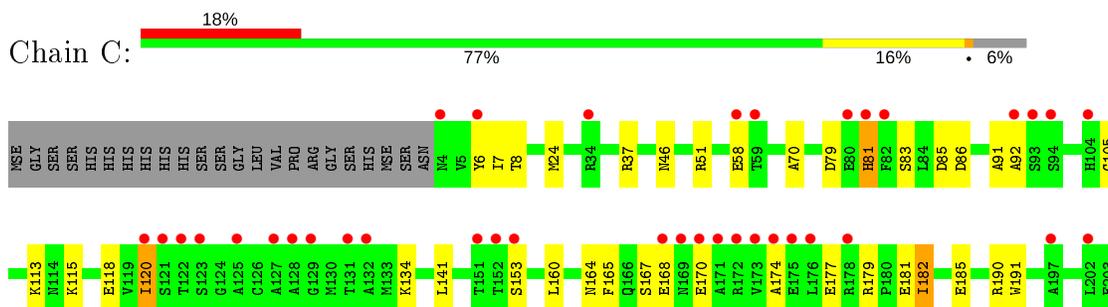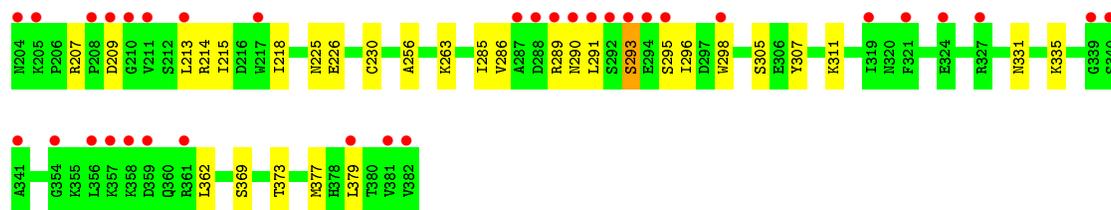
- Molecule 1: Ketosynthase StlD

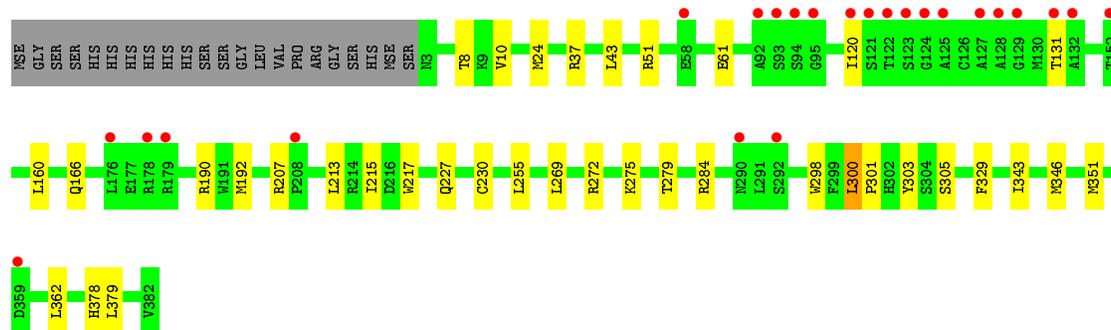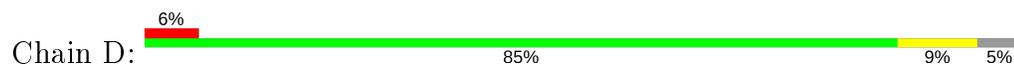
- Molecule 1: Ketosynthase StlD

- Molecule 1: Ketosynthase StlD

N204 K205 P206 R207 P208 D209 G210 V211 S212 L213 R214 I215 D216 W217 I218 N225 E226 C230 A256 K263 I285 V286 A287 D288 R289 N290 L291 S292 S293 E294 S295 I296 D297 W298 S305 E306 Y307 K311 I319 N320 F321 E324 R327 N331 K335 G339 S340

A341 G354 K355 L356 K357 K358 D359 Q360 R361 L362 S369 T373 M377 H378 L379 T380 V381 V382

• Molecule 1: Ketosynthase StlD

Chain D:

6%

85%   9%   5%

MSE GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MSE SER N3 T8 K9 V10 M24 R37 L43 R51 E58 E61 A92 S93 S94 G95 I120 S121 T122 S123 G124 A125 C126 A127 A128 G129 M130 T131 A132 T152

L160 Q166 L176 E177 R178 R179 R190 W191 M192 R207 P208 I213 R214 I215 D216 W217 Q227 C230 L255 I269 R272 K275 T279 R284 N290 L291 S292 W298 F299 L300 P301 H302 Y303 S304 S305 F329 I343 M346 M351

D359 L362 H378 L379 V382

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.22Å 127.71Å 108.02Å 90.00° 91.39° 90.00°	Depositor
Resolution (Å)	41.73 – 2.33 41.73 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.73-2.33) 99.6 (41.73-2.33)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.22 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.186 , 0.227 0.186 , 0.226	Depositor DCC
R_{free} test set	3637 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12283	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 0.333 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: CSD

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	0.44	0/3015	0.62	1/4056 (0.0%)
1	B	0.38	0/2880	0.56	0/3870
1	C	0.40	0/3007	0.55	0/4045
1	D	0.43	0/3015	0.58	0/4056
All	All	0.41	0/11917	0.58	1/16027 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	ARG	NE-CZ-NH2	-6.43	117.09	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2974	0	2906	24	0
1	B	2843	0	2778	32	0
1	C	2966	0	2900	39	0
1	D	2974	0	2906	18	0
2	A	193	0	0	2	0
2	B	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	0	0	0
2	D	177	0	0	0	0
All	All	12283	0	11490	107	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 5.

The worst 5 of 107 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:C:218:ILE:HG12	1:C:377:MSE:HG3	1.53	0.88
1:B:249:MSE:HE1	1:B:259:VAL:HG21	1.67	0.76
1:B:24:MSE:HE3	1:B:191:TRP:CE3	2.24	0.73
1:B:251:GLN:HG3	1:C:164:ASN:ND2	2.07	0.69
1:B:87:MSE:HE2	1:B:149:VAL:HG21	1.76	0.67

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	377/402 (94%)	363 (96%)	13 (3%)	1 (0%)	41	47
1	B	354/402 (88%)	331 (94%)	21 (6%)	2 (1%)	25	26
1	C	376/402 (94%)	355 (94%)	21 (6%)	0	100	100
1	D	377/402 (94%)	366 (97%)	10 (3%)	1 (0%)	41	47
All	All	1484/1608 (92%)	1415 (95%)	65 (4%)	4 (0%)	41	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	ASN
1	B	113	LYS
1	A	210	GLY
1	D	301	PRO

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	321/325 (99%)	314 (98%)	7 (2%)	52	63
1	B	309/325 (95%)	304 (98%)	5 (2%)	62	74
1	C	320/325 (98%)	307 (96%)	13 (4%)	30	38
1	D	321/325 (99%)	314 (98%)	7 (2%)	52	63
All	All	1271/1300 (98%)	1239 (98%)	32 (2%)	47	58

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	58	GLU
1	C	120	ILE
1	D	255	LEU
1	C	113	LYS
1	C	182	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	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)

4 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	CSD	C	126	1	3,7,8	0.73	0	1,8,10	0.50	0
1	CSD	D	126	1	3,7,8	0.66	0	1,8,10	2.49	1 (100%)
1	CSD	A	126	1	3,7,8	0.58	0	1,8,10	1.50	0
1	CSD	B	126	1	3,7,8	0.65	0	1,8,10	0.32	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	C	126	1	-	1/2/6/8	-
1	CSD	D	126	1	-	1/2/6/8	-
1	CSD	A	126	1	-	1/2/6/8	-
1	CSD	B	126	1	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	126	CSD	OD1-SG-CB	2.49	110.27	105.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	126	CSD	CA-CB-SG-OD1
1	D	126	CSD	CA-CB-SG-OD1
1	A	126	CSD	CA-CB-SG-OD1
1	B	126	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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(Å^2)	Q<0.9
1	A	366/402 (91%)	-0.03	15 (4%)	37	48	14, 25, 44, 68	0
1	B	349/402 (86%)	0.72	49 (14%)	2	4	20, 41, 62, 74	0
1	C	365/402 (90%)	0.96	71 (19%)	1	2	18, 41, 66, 78	0
1	D	366/402 (91%)	0.27	24 (6%)	18	26	12, 26, 47, 82	0
All	All	1446/1608 (89%)	0.48	159 (10%)	5	9	12, 32, 61, 82	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	TRP	6.7
1	B	37	ARG	6.6
1	C	209	ASP	5.5
1	D	178	ARG	5.4
1	B	40	HIS	5.2

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, 95th 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
1	CSD	C	126	8/9	0.97	0.23	28,31,33,44	0
1	CSD	D	126	8/9	0.97	0.22	18,18,25,37	0
1	CSD	A	126	8/9	0.98	0.18	14,18,22,25	0
1	CSD	B	126	8/9	0.98	0.17	21,24,31,40	0

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.