



wwPDB X-ray Structure Validation Summary Report

Jan 7, 2024 – 04:22 am GMT

PDB ID : 6GJV
Title : apo-structure of IMPDH from Pseudomonas aeruginosa
Authors : Labesse, G.; Haouz, A.; Alexandre, T.; Munier-Lehmann, H.
Deposited on : 2018-05-17
Resolution : 2.11 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  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](#) ) were used in the production of this report:

MolProbity : 4.02b-467
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

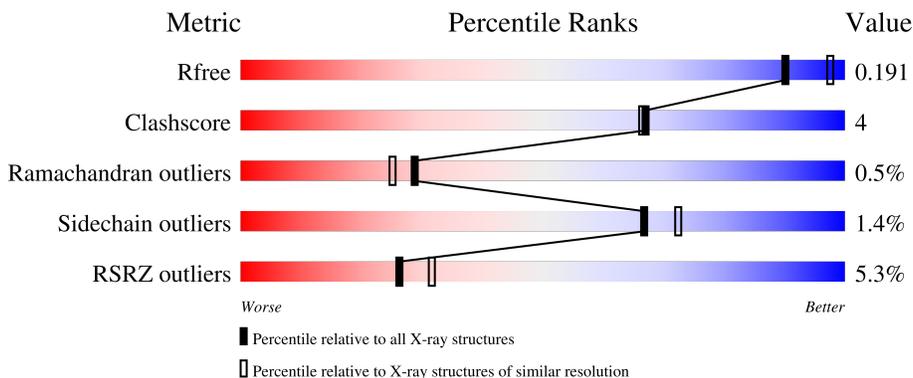
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 $\leq 5\%$. 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	509	 5% (poor fit), 73% (0-1 outliers), 10% (2 outliers), 17% (3+ outliers)
1	B	509	 14% (poor fit), 70% (0-1 outliers), 11% (2 outliers), 19% (3+ outliers)
1	C	509	 5% (poor fit), 76% (0-1 outliers), 8% (2 outliers), 16% (3+ outliers)
1	D	509	 2% (poor fit), 58% (0-1 outliers), 38% (2+ outliers)
1	E	509	 % (poor fit), 77% (0-1 outliers), 6% (2 outliers), 17% (3+ outliers)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	509	 <p>5% 75% 8% 16%</p>
1	G	509	 <p>% 77% 6% 17%</p>
1	H	509	 <p>% 57% 5% 38%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25755 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3150	1988	549	596	17	0	1	0
1	B	414	3038	1916	531	574	17	0	1	0
1	C	429	3182	2005	559	601	17	0	0	0
1	D	318	2315	1453	413	436	13	0	0	0
1	E	424	3183	2007	558	601	17	1	6	0
1	F	426	3178	2004	558	599	17	0	3	0
1	G	424	3172	1999	555	601	17	0	3	0
1	H	317	2314	1451	414	436	13	0	1	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9HXM5
A	-18	GLY	-	expression tag	UNP Q9HXM5
A	-17	SER	-	expression tag	UNP Q9HXM5
A	-16	SER	-	expression tag	UNP Q9HXM5
A	-15	HIS	-	expression tag	UNP Q9HXM5
A	-14	HIS	-	expression tag	UNP Q9HXM5
A	-13	HIS	-	expression tag	UNP Q9HXM5
A	-12	HIS	-	expression tag	UNP Q9HXM5
A	-11	HIS	-	expression tag	UNP Q9HXM5
A	-10	HIS	-	expression tag	UNP Q9HXM5
A	-9	SER	-	expression tag	UNP Q9HXM5
A	-8	SER	-	expression tag	UNP Q9HXM5
A	-7	GLY	-	expression tag	UNP Q9HXM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q9HXM5
A	-5	VAL	-	expression tag	UNP Q9HXM5
A	-4	PRO	-	expression tag	UNP Q9HXM5
A	-3	ARG	-	expression tag	UNP Q9HXM5
A	-2	GLY	-	expression tag	UNP Q9HXM5
A	-1	SER	-	expression tag	UNP Q9HXM5
A	0	HIS	-	expression tag	UNP Q9HXM5
B	-19	MET	-	initiating methionine	UNP Q9HXM5
B	-18	GLY	-	expression tag	UNP Q9HXM5
B	-17	SER	-	expression tag	UNP Q9HXM5
B	-16	SER	-	expression tag	UNP Q9HXM5
B	-15	HIS	-	expression tag	UNP Q9HXM5
B	-14	HIS	-	expression tag	UNP Q9HXM5
B	-13	HIS	-	expression tag	UNP Q9HXM5
B	-12	HIS	-	expression tag	UNP Q9HXM5
B	-11	HIS	-	expression tag	UNP Q9HXM5
B	-10	HIS	-	expression tag	UNP Q9HXM5
B	-9	SER	-	expression tag	UNP Q9HXM5
B	-8	SER	-	expression tag	UNP Q9HXM5
B	-7	GLY	-	expression tag	UNP Q9HXM5
B	-6	LEU	-	expression tag	UNP Q9HXM5
B	-5	VAL	-	expression tag	UNP Q9HXM5
B	-4	PRO	-	expression tag	UNP Q9HXM5
B	-3	ARG	-	expression tag	UNP Q9HXM5
B	-2	GLY	-	expression tag	UNP Q9HXM5
B	-1	SER	-	expression tag	UNP Q9HXM5
B	0	HIS	-	expression tag	UNP Q9HXM5
C	-19	MET	-	initiating methionine	UNP Q9HXM5
C	-18	GLY	-	expression tag	UNP Q9HXM5
C	-17	SER	-	expression tag	UNP Q9HXM5
C	-16	SER	-	expression tag	UNP Q9HXM5
C	-15	HIS	-	expression tag	UNP Q9HXM5
C	-14	HIS	-	expression tag	UNP Q9HXM5
C	-13	HIS	-	expression tag	UNP Q9HXM5
C	-12	HIS	-	expression tag	UNP Q9HXM5
C	-11	HIS	-	expression tag	UNP Q9HXM5
C	-10	HIS	-	expression tag	UNP Q9HXM5
C	-9	SER	-	expression tag	UNP Q9HXM5
C	-8	SER	-	expression tag	UNP Q9HXM5
C	-7	GLY	-	expression tag	UNP Q9HXM5
C	-6	LEU	-	expression tag	UNP Q9HXM5
C	-5	VAL	-	expression tag	UNP Q9HXM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q9HXM5
C	-3	ARG	-	expression tag	UNP Q9HXM5
C	-2	GLY	-	expression tag	UNP Q9HXM5
C	-1	SER	-	expression tag	UNP Q9HXM5
C	0	HIS	-	expression tag	UNP Q9HXM5
D	-19	MET	-	initiating methionine	UNP Q9HXM5
D	-18	GLY	-	expression tag	UNP Q9HXM5
D	-17	SER	-	expression tag	UNP Q9HXM5
D	-16	SER	-	expression tag	UNP Q9HXM5
D	-15	HIS	-	expression tag	UNP Q9HXM5
D	-14	HIS	-	expression tag	UNP Q9HXM5
D	-13	HIS	-	expression tag	UNP Q9HXM5
D	-12	HIS	-	expression tag	UNP Q9HXM5
D	-11	HIS	-	expression tag	UNP Q9HXM5
D	-10	HIS	-	expression tag	UNP Q9HXM5
D	-9	SER	-	expression tag	UNP Q9HXM5
D	-8	SER	-	expression tag	UNP Q9HXM5
D	-7	GLY	-	expression tag	UNP Q9HXM5
D	-6	LEU	-	expression tag	UNP Q9HXM5
D	-5	VAL	-	expression tag	UNP Q9HXM5
D	-4	PRO	-	expression tag	UNP Q9HXM5
D	-3	ARG	-	expression tag	UNP Q9HXM5
D	-2	GLY	-	expression tag	UNP Q9HXM5
D	-1	SER	-	expression tag	UNP Q9HXM5
D	0	HIS	-	expression tag	UNP Q9HXM5
E	-19	MET	-	initiating methionine	UNP Q9HXM5
E	-18	GLY	-	expression tag	UNP Q9HXM5
E	-17	SER	-	expression tag	UNP Q9HXM5
E	-16	SER	-	expression tag	UNP Q9HXM5
E	-15	HIS	-	expression tag	UNP Q9HXM5
E	-14	HIS	-	expression tag	UNP Q9HXM5
E	-13	HIS	-	expression tag	UNP Q9HXM5
E	-12	HIS	-	expression tag	UNP Q9HXM5
E	-11	HIS	-	expression tag	UNP Q9HXM5
E	-10	HIS	-	expression tag	UNP Q9HXM5
E	-9	SER	-	expression tag	UNP Q9HXM5
E	-8	SER	-	expression tag	UNP Q9HXM5
E	-7	GLY	-	expression tag	UNP Q9HXM5
E	-6	LEU	-	expression tag	UNP Q9HXM5
E	-5	VAL	-	expression tag	UNP Q9HXM5
E	-4	PRO	-	expression tag	UNP Q9HXM5
E	-3	ARG	-	expression tag	UNP Q9HXM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9HXM5
E	-1	SER	-	expression tag	UNP Q9HXM5
E	0	HIS	-	expression tag	UNP Q9HXM5
F	-19	MET	-	initiating methionine	UNP Q9HXM5
F	-18	GLY	-	expression tag	UNP Q9HXM5
F	-17	SER	-	expression tag	UNP Q9HXM5
F	-16	SER	-	expression tag	UNP Q9HXM5
F	-15	HIS	-	expression tag	UNP Q9HXM5
F	-14	HIS	-	expression tag	UNP Q9HXM5
F	-13	HIS	-	expression tag	UNP Q9HXM5
F	-12	HIS	-	expression tag	UNP Q9HXM5
F	-11	HIS	-	expression tag	UNP Q9HXM5
F	-10	HIS	-	expression tag	UNP Q9HXM5
F	-9	SER	-	expression tag	UNP Q9HXM5
F	-8	SER	-	expression tag	UNP Q9HXM5
F	-7	GLY	-	expression tag	UNP Q9HXM5
F	-6	LEU	-	expression tag	UNP Q9HXM5
F	-5	VAL	-	expression tag	UNP Q9HXM5
F	-4	PRO	-	expression tag	UNP Q9HXM5
F	-3	ARG	-	expression tag	UNP Q9HXM5
F	-2	GLY	-	expression tag	UNP Q9HXM5
F	-1	SER	-	expression tag	UNP Q9HXM5
F	0	HIS	-	expression tag	UNP Q9HXM5
G	-19	MET	-	initiating methionine	UNP Q9HXM5
G	-18	GLY	-	expression tag	UNP Q9HXM5
G	-17	SER	-	expression tag	UNP Q9HXM5
G	-16	SER	-	expression tag	UNP Q9HXM5
G	-15	HIS	-	expression tag	UNP Q9HXM5
G	-14	HIS	-	expression tag	UNP Q9HXM5
G	-13	HIS	-	expression tag	UNP Q9HXM5
G	-12	HIS	-	expression tag	UNP Q9HXM5
G	-11	HIS	-	expression tag	UNP Q9HXM5
G	-10	HIS	-	expression tag	UNP Q9HXM5
G	-9	SER	-	expression tag	UNP Q9HXM5
G	-8	SER	-	expression tag	UNP Q9HXM5
G	-7	GLY	-	expression tag	UNP Q9HXM5
G	-6	LEU	-	expression tag	UNP Q9HXM5
G	-5	VAL	-	expression tag	UNP Q9HXM5
G	-4	PRO	-	expression tag	UNP Q9HXM5
G	-3	ARG	-	expression tag	UNP Q9HXM5
G	-2	GLY	-	expression tag	UNP Q9HXM5
G	-1	SER	-	expression tag	UNP Q9HXM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q9HXM5
H	-19	MET	-	initiating methionine	UNP Q9HXM5
H	-18	GLY	-	expression tag	UNP Q9HXM5
H	-17	SER	-	expression tag	UNP Q9HXM5
H	-16	SER	-	expression tag	UNP Q9HXM5
H	-15	HIS	-	expression tag	UNP Q9HXM5
H	-14	HIS	-	expression tag	UNP Q9HXM5
H	-13	HIS	-	expression tag	UNP Q9HXM5
H	-12	HIS	-	expression tag	UNP Q9HXM5
H	-11	HIS	-	expression tag	UNP Q9HXM5
H	-10	HIS	-	expression tag	UNP Q9HXM5
H	-9	SER	-	expression tag	UNP Q9HXM5
H	-8	SER	-	expression tag	UNP Q9HXM5
H	-7	GLY	-	expression tag	UNP Q9HXM5
H	-6	LEU	-	expression tag	UNP Q9HXM5
H	-5	VAL	-	expression tag	UNP Q9HXM5
H	-4	PRO	-	expression tag	UNP Q9HXM5
H	-3	ARG	-	expression tag	UNP Q9HXM5
H	-2	GLY	-	expression tag	UNP Q9HXM5
H	-1	SER	-	expression tag	UNP Q9HXM5
H	0	HIS	-	expression tag	UNP Q9HXM5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	240	Total O 240 240	0	0
2	B	256	Total O 256 256	0	0
2	C	307	Total O 307 307	0	0
2	D	211	Total O 211 211	0	0
2	E	350	Total O 350 350	0	0
2	F	289	Total O 289 289	0	0
2	G	315	Total O 315 315	0	0
2	H	255	Total O 255 255	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.30Å 194.64Å 122.92Å 90.00° 117.75° 90.00°	Depositor
Resolution (Å)	44.63 – 2.11 49.35 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.63-2.11) 100.0 (49.35-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.160 , 0.191 0.159 , 0.191	Depositor DCC
R_{free} test set	13805 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25755	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0/3193	0.57	1/4319 (0.0%)
1	B	0.36	0/3078	0.56	1/4158 (0.0%)
1	C	0.38	1/3222 (0.0%)	0.57	0/4355
1	D	0.37	0/2343	0.55	0/3166
1	E	0.38	0/3246	0.57	0/4385
1	F	0.36	0/3227	0.55	1/4361 (0.0%)
1	G	0.40	0/3218	0.57	0/4348
1	H	0.41	0/2346	0.57	0/3169
All	All	0.38	1/23873 (0.0%)	0.57	3/32261 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	CYS	CB-SG	-5.09	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	MET	CA-CB-CG	5.56	122.76	113.30
1	B	102	PRO	N-CA-CB	5.52	109.93	103.30
1	F	358	MET	CG-SD-CE	5.48	108.96	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3150	0	3241	33	0
1	B	3038	0	3090	34	0
1	C	3182	0	3280	25	0
1	D	2315	0	2384	10	0
1	E	3183	0	3284	21	0
1	F	3178	0	3288	32	0
1	G	3172	0	3273	19	0
1	H	2314	0	2380	18	0
2	A	240	0	0	2	0
2	B	256	0	0	2	0
2	C	307	0	0	10	0
2	D	211	0	0	1	0
2	E	350	0	0	3	0
2	F	289	0	0	6	0
2	G	315	0	0	2	0
2	H	255	0	0	5	0
All	All	25755	0	24220	186	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 4.

The worst 5 of 186 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:A:455:MET:HE3	1:A:459:PRO:HG2	1.48	0.92
1:B:7:GLU:OE2	1:B:463:ARG:NH2	2.09	0.86
1:F:350:MET:HE3	1:F:357:VAL:HG23	1.60	0.84
1:C:425:TYR:O	2:C:501:HOH:O	1.96	0.83
1:A:455:MET:CE	1:A:459:PRO:HG2	2.09	0.82

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	420/509 (82%)	404 (96%)	13 (3%)	3 (1%)	22	17
1	B	405/509 (80%)	386 (95%)	13 (3%)	6 (2%)	10	5
1	C	423/509 (83%)	410 (97%)	10 (2%)	3 (1%)	22	17
1	D	312/509 (61%)	304 (97%)	8 (3%)	0	100	100
1	E	424/509 (83%)	415 (98%)	9 (2%)	0	100	100
1	F	423/509 (83%)	411 (97%)	11 (3%)	1 (0%)	47	48
1	G	421/509 (83%)	410 (97%)	10 (2%)	1 (0%)	47	48
1	H	312/509 (61%)	304 (97%)	7 (2%)	1 (0%)	41	40
All	All	3140/4072 (77%)	3044 (97%)	81 (3%)	15 (0%)	29	25

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	B	327	LEU
1	C	146	ASP
1	A	92	ALA
1	B	328	GLU

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	324/390 (83%)	320 (99%)	4 (1%)	71	77
1	B	305/390 (78%)	301 (99%)	4 (1%)	69	74
1	C	327/390 (84%)	322 (98%)	5 (2%)	65	70
1	D	233/390 (60%)	229 (98%)	4 (2%)	60	66
1	E	331/390 (85%)	326 (98%)	5 (2%)	65	70
1	F	329/390 (84%)	324 (98%)	5 (2%)	65	70
1	G	328/390 (84%)	323 (98%)	5 (2%)	65	70
1	H	233/390 (60%)	230 (99%)	3 (1%)	69	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2410/3120 (77%)	2375 (98%)	35 (2%)	67 70

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	189	PHE
1	G	334	LEU
1	H	1	MET
1	C	334	LEU
1	C	187	GLU

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

Mol	Chain	Res	Type
1	C	377	GLN

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

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	425/509 (83%)	0.21	27 (6%) 19 23	23, 36, 98, 133	22 (5%)
1	B	414/509 (81%)	0.61	71 (17%) 1 1	23, 40, 90, 108	107 (25%)
1	C	429/509 (84%)	0.07	25 (5%) 23 28	24, 35, 78, 137	19 (4%)
1	D	318/509 (62%)	-0.19	11 (3%) 44 50	27, 38, 69, 113	19 (5%)
1	E	424/509 (83%)	-0.21	4 (0%) 84 86	21, 34, 61, 85	22 (5%)
1	F	426/509 (83%)	-0.03	23 (5%) 25 31	26, 41, 71, 102	24 (5%)
1	G	424/509 (83%)	-0.33	3 (0%) 87 89	24, 36, 66, 97	19 (4%)
1	H	317/509 (62%)	-0.07	4 (1%) 77 80	23, 33, 63, 97	20 (6%)
All	All	3177/4072 (78%)	0.02	168 (5%) 26 31	21, 37, 81, 137	252 (7%)

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	LEU	8.4
1	B	151	ILE	8.2
1	B	109	LEU	8.0
1	B	118	PHE	7.9
1	A	175	TYR	7.6

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.