



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:58 AM UTC

PDB ID : 8CN8 / pdb_00008cn8
Title : apo Pseudomonas aeruginosa FabF C164A mutant
Authors : Georgiou, C.; Brenk, R.; Espeland, L.O.
Deposited on : 2023-02-22
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

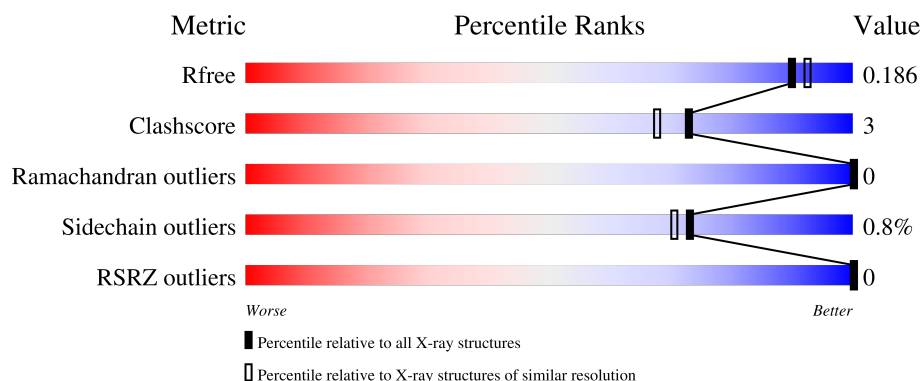
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	419	
1	B	419	
1	C	419	
1	D	419	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13761 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 3-oxoacyl-[acyl-carrier-protein] synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	6	0
			3110	1933	565	592	20			
1	B	419	Total	C	N	O	S	0	8	0
			3129	1946	568	595	20			
1	C	418	Total	C	N	O	S	0	5	0
			3106	1929	565	592	20			
1	D	419	Total	C	N	O	S	0	7	0
			3121	1941	565	595	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP G3XDA2
A	-3	HIS	-	expression tag	UNP G3XDA2
A	-2	MET	-	expression tag	UNP G3XDA2
A	-1	ALA	-	expression tag	UNP G3XDA2
A	0	SER	-	expression tag	UNP G3XDA2
A	164	ALA	CYS	engineered mutation	UNP G3XDA2
B	-4	GLY	-	expression tag	UNP G3XDA2
B	-3	HIS	-	expression tag	UNP G3XDA2
B	-2	MET	-	expression tag	UNP G3XDA2
B	-1	ALA	-	expression tag	UNP G3XDA2
B	0	SER	-	expression tag	UNP G3XDA2
B	164	ALA	CYS	engineered mutation	UNP G3XDA2
C	-4	GLY	-	expression tag	UNP G3XDA2
C	-3	HIS	-	expression tag	UNP G3XDA2
C	-2	MET	-	expression tag	UNP G3XDA2
C	-1	ALA	-	expression tag	UNP G3XDA2
C	0	SER	-	expression tag	UNP G3XDA2
C	164	ALA	CYS	engineered mutation	UNP G3XDA2
D	-4	GLY	-	expression tag	UNP G3XDA2
D	-3	HIS	-	expression tag	UNP G3XDA2
D	-2	MET	-	expression tag	UNP G3XDA2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP G3XDA2
D	0	SER	-	expression tag	UNP G3XDA2
D	164	ALA	CYS	engineered mutation	UNP G3XDA2

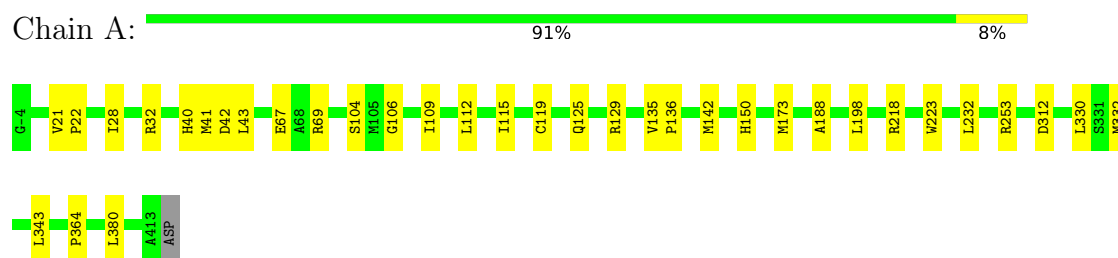
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	313	Total 313	O 313	0	0
2	B	333	Total 333	O 333	0	0
2	C	318	Total 318	O 318	0	0
2	D	331	Total 331	O 331	0	0

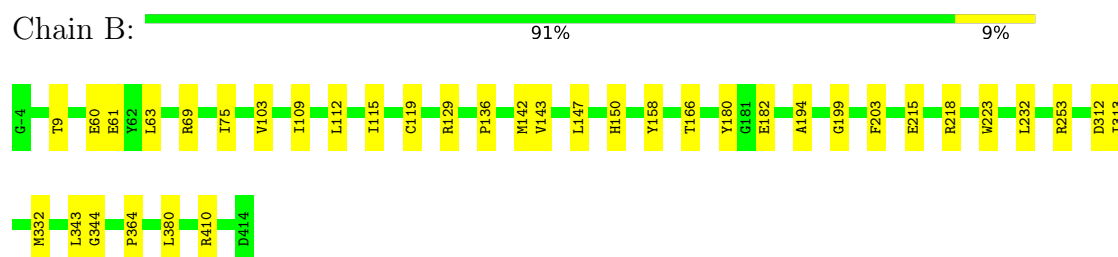
3 Residue-property plots

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 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.

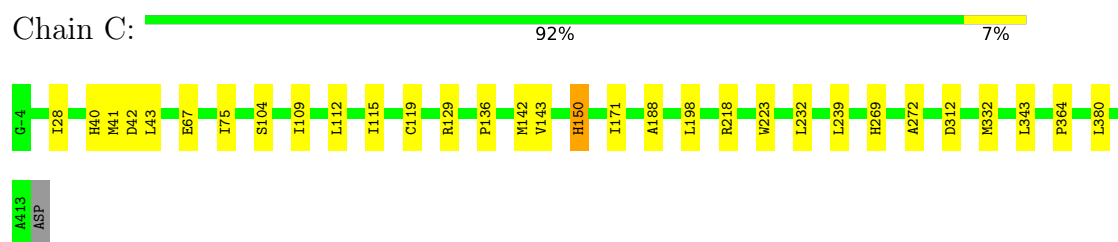
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



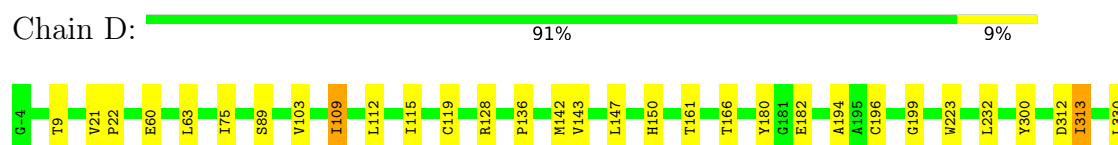
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



S331	M332	L343	G344	P364	L380	A393	R410	D414
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.84Å 72.50Å 139.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 1.80 47.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.67-1.80) 96.6 (47.67-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.141 , 0.175 0.156 , 0.186	Depositor DCC
R_{free} test set	6629 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l 0.016 for k,h,-l 0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13761	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [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	1.09	1/3182 (0.0%)	1.25	1/4297 (0.0%)
1	B	1.09	0/3208	1.23	1/4333 (0.0%)
1	C	1.11	1/3174 (0.0%)	1.26	1/4286 (0.0%)
1	D	1.10	0/3197	1.23	3/4319 (0.1%)
All	All	1.10	2/12761 (0.0%)	1.24	6/17235 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	HIS	CE1-NE2	5.18	1.37	1.32
1	A	106	GLY	N-CA	5.05	1.49	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	364	PRO	CB-CA-C	-7.41	104.42	111.39
1	B	364	PRO	CB-CA-C	-6.61	105.17	111.39
1	A	41	MET	CA-C-O	-5.43	115.60	121.36
1	D	109	ILE	CB-CA-C	5.28	115.82	110.65
1	D	313	ILE	CA-C-O	-5.06	115.49	120.85
1	C	41	MET	CA-C-O	-5.00	116.06	121.36

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	3110	0	3073	20	0
1	B	3129	0	3093	23	0
1	C	3106	0	3066	18	0
1	D	3121	0	3080	25	0
2	A	313	0	0	3	0
2	B	333	0	0	2	0
2	C	318	0	0	2	0
2	D	331	0	0	2	0
All	All	13761	0	12312	79	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 3.

All (79) 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:198:LEU:HD11	1:D:119:CYS:SG	2.22	0.80
1:A:198:LEU:HD11	1:B:119:CYS:SG	2.25	0.77
1:C:136:PRO:O	1:C:142:MET:HG3	1.96	0.66
1:C:332:MET:O	1:C:380:LEU:HA	2.00	0.62
1:A:332:MET:O	1:A:380:LEU:HA	2.02	0.59
1:A:136:PRO:O	1:A:142:MET:HG3	2.03	0.58
1:D:332:MET:O	1:D:380:LEU:HA	2.05	0.56
1:C:42:ASP:OD1	1:C:43:LEU:N	2.39	0.55
1:A:218:ARG:NH2	2:A:502:HOH:O	2.41	0.54
1:D:109:ILE:HG22	1:D:112:LEU:HG	1.89	0.54
1:C:115:ILE:HG21	1:D:115:ILE:HG21	1.90	0.54
1:A:125:GLN:HB3	1:A:129:ARG:HG3	1.92	0.52
1:B:332:MET:O	1:B:380:LEU:HA	2.09	0.52
1:C:218:ARG:NH2	2:C:505:HOH:O	2.42	0.51
1:D:109:ILE:CG2	1:D:112:LEU:HG	2.41	0.51
1:D:223:TRP:CD1	1:D:312:ASP:HB3	2.46	0.51
1:B:232:LEU:CD1	1:B:343[A]:LEU:HD11	2.41	0.51
1:C:42:ASP:OD1	1:C:42:ASP:C	2.54	0.50
1:C:67:GLU:OE2	1:C:150:HIS:HE1	1.95	0.50
1:B:60:GLU:HA	1:B:63:LEU:O	2.11	0.50
1:B:109:ILE:CG2	1:B:112:LEU:HG	2.42	0.50
1:B:215:GLU:OE1	1:B:218:ARG:NH1	2.45	0.50
1:A:223:TRP:CD1	1:A:312:ASP:HB3	2.47	0.49
1:D:60:GLU:HA	1:D:63:LEU:O	2.12	0.49
1:D:150:HIS:CD2	2:D:792:HOH:O	2.65	0.49
1:B:150:HIS:CD2	2:B:793:HOH:O	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:PRO:O	1:D:142:MET:HG3	2.12	0.49
1:B:109:ILE:HG22	1:B:112:LEU:HG	1.95	0.49
1:B:136:PRO:O	1:B:142:MET:HG3	2.12	0.48
1:B:150:HIS:HD2	2:B:793:HOH:O	1.97	0.47
1:A:109:ILE:HG21	1:A:112:LEU:HD22	1.96	0.47
1:C:223:TRP:CD1	1:C:312:ASP:HB3	2.50	0.47
1:C:40:HIS:HE1	2:C:531:HOH:O	1.99	0.46
1:C:109:ILE:HG21	1:C:112:LEU:HD22	1.97	0.46
1:D:75:ILE:HA	1:D:143:VAL:HG22	1.98	0.46
1:D:180:TYR:HD2	1:D:182:GLU:HG3	1.81	0.46
1:B:75:ILE:HA	1:B:143:VAL:HG22	1.98	0.45
1:D:232:LEU:CD1	1:D:343[A]:LEU:HD11	2.46	0.45
1:B:223:TRP:CD1	1:B:312:ASP:HB3	2.52	0.45
1:D:103[B]:VAL:HG11	1:D:147:LEU:HD23	1.99	0.45
1:A:115:ILE:HG21	1:B:115:ILE:HG21	1.99	0.44
1:B:103[B]:VAL:HG11	1:B:147:LEU:HD23	1.99	0.44
1:A:135:VAL:HG11	1:B:203:PHE:CE1	2.53	0.44
1:A:21:VAL:HB	1:A:22[B]:PRO:HD3	1.99	0.44
1:A:40:HIS:HE1	2:A:554:HOH:O	2.01	0.44
1:D:103[B]:VAL:CG1	1:D:147:LEU:HD23	2.47	0.44
1:B:166:THR:HB	1:B:344:GLY:HA2	2.00	0.44
1:C:232:LEU:CD1	1:C:343[B]:LEU:HD11	2.46	0.44
1:D:112:LEU:HB3	1:D:196:CYS:SG	2.57	0.44
1:B:61:GLU:O	1:D:128:ARG:HD2	2.18	0.44
1:B:180:TYR:HD2	1:B:182:GLU:HG3	1.83	0.43
1:D:150:HIS:HD2	2:D:792:HOH:O	1.98	0.43
1:A:104:SER:O	1:A:188:ALA:HA	2.18	0.43
1:C:75:ILE:HA	1:C:143:VAL:HG22	2.01	0.43
1:D:166:THR:HB	1:D:344:GLY:HA2	2.01	0.43
1:A:173:MET:HE1	1:B:158:TYR:CG	2.53	0.43
1:B:194:ALA:O	1:B:199:GLY:HA3	2.19	0.42
1:C:269:HIS:HB3	1:C:272:ALA:O	2.20	0.42
1:D:9:THR:O	1:D:89:SER:HA	2.19	0.42
1:D:300:TYR:O	1:D:393:ALA:HA	2.20	0.42
1:A:32[B]:ARG:NH2	2:A:515:HOH:O	2.52	0.42
1:C:198:LEU:HD23	1:C:198:LEU:HA	1.88	0.42
1:C:104:SER:O	1:C:188:ALA:HA	2.20	0.41
1:C:28:ILE:CG2	1:C:364:PRO:HB3	2.50	0.41
1:B:103[B]:VAL:CG1	1:B:147:LEU:HD23	2.50	0.41
1:A:28:ILE:CG2	1:A:364:PRO:HB3	2.50	0.41
1:C:171:ILE:HD11	1:C:239:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ALA:O	1:D:199:GLY:HA3	2.21	0.41
1:D:330:LEU:HD12	1:D:330:LEU:C	2.46	0.41
1:A:67:GLU:OE2	1:A:150:HIS:HE1	2.03	0.41
1:D:343[B]:LEU:HD12	1:D:343[B]:LEU:HA	1.94	0.41
1:A:232:LEU:CD1	1:A:343[B]:LEU:HD11	2.51	0.40
1:A:330:LEU:HD12	1:A:330:LEU:C	2.45	0.40
1:D:21:VAL:HB	1:D:22[B]:PRO:HD3	2.03	0.40
1:B:9:THR:O	1:B:253:ARG:NH1	2.55	0.40
1:A:42:ASP:OD1	1:A:43:LEU:N	2.54	0.40
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.83	0.40
1:D:161:THR:HG23	1:D:161:THR:O	2.20	0.40

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	422/419 (101%)	403 (96%)	19 (4%)	0	100	100
1	B	425/419 (101%)	408 (96%)	17 (4%)	0	100	100
1	C	421/419 (100%)	401 (95%)	20 (5%)	0	100	100
1	D	424/419 (101%)	409 (96%)	15 (4%)	0	100	100
All	All	1692/1676 (101%)	1621 (96%)	71 (4%)	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	318/313 (102%)	316 (99%)	2 (1%)	78	77
1	B	321/313 (103%)	317 (99%)	4 (1%)	63	57
1	C	317/313 (101%)	315 (99%)	2 (1%)	78	77
1	D	320/313 (102%)	318 (99%)	2 (1%)	78	77
All	All	1276/1252 (102%)	1266 (99%)	10 (1%)	73	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	119	CYS
1	B	69	ARG
1	B	129	ARG
1	B	313	ILE
1	B	410	ARG
1	C	119	CYS
1	C	129	ARG
1	D	313	ILE
1	D	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	150	HIS
1	A	177	ASN
1	A	304	HIS
1	B	150	HIS
1	B	154	GLN
1	C	125	GLN
1	C	177	ASN
1	C	286	ASN
1	C	304	HIS
1	D	40	HIS
1	D	150	HIS
1	D	154	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 oligosaccharides 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	418/419 (99%)	-1.42	0 100 100	8, 17, 35, 60	6 (1%)
1	B	419/419 (100%)	-1.45	0 100 100	8, 16, 34, 55	8 (1%)
1	C	418/419 (99%)	-1.43	0 100 100	8, 17, 35, 59	5 (1%)
1	D	419/419 (100%)	-1.45	0 100 100	8, 16, 33, 55	7 (1%)
All	All	1674/1676 (99%)	-1.44	0 100 100	8, 16, 35, 60	26 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.