



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:15 am GMT

PDB ID : 2GER
Title : Crystal Structure and Oxidative Mechanism of Human Pyrroline-5-carboxylate Reductase
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-03-20
Resolution : 3.10 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.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

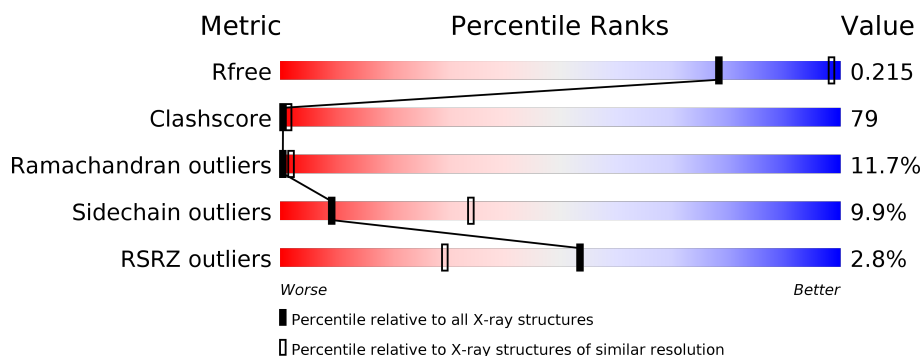
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 $\leq 5\%$. 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	321	<div> <div>21%</div> <div>49%</div> <div>15%</div> <div>•</div> <div>14%</div> </div>
1	B	321	<div> <div>5%</div> <div>19%</div> <div>54%</div> <div>13%</div> <div>•</div> <div>14%</div> </div>
1	C	321	<div> <div>5%</div> <div>20%</div> <div>55%</div> <div>11%</div> <div>14%</div> </div>
1	D	321	<div> <div>22%</div> <div>50%</div> <div>14%</div> <div>14%</div> </div>
1	E	321	<div> <div>22%</div> <div>51%</div> <div>12%</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10768 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 Pyrroline-5-carboxylate reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	B	276	Total	C	N	O	S	0	0	0
			2025	1271	359	382	13			
1	C	277	Total	C	N	O	S	0	0	0
			2032	1276	360	383	13			
1	D	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	E	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	CLONING ARTIFACT	UNP P32322
A	0	ALA	-	CLONING ARTIFACT	UNP P32322
B	-1	ARG	-	CLONING ARTIFACT	UNP P32322
B	0	ALA	-	CLONING ARTIFACT	UNP P32322
C	-1	ARG	-	CLONING ARTIFACT	UNP P32322
C	0	ALA	-	CLONING ARTIFACT	UNP P32322
D	-1	ARG	-	CLONING ARTIFACT	UNP P32322
D	0	ALA	-	CLONING ARTIFACT	UNP P32322
E	-1	ARG	-	CLONING ARTIFACT	UNP P32322
E	0	ALA	-	CLONING ARTIFACT	UNP P32322

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	118	Total	O	0	0
			118	118		

Continued on next page...

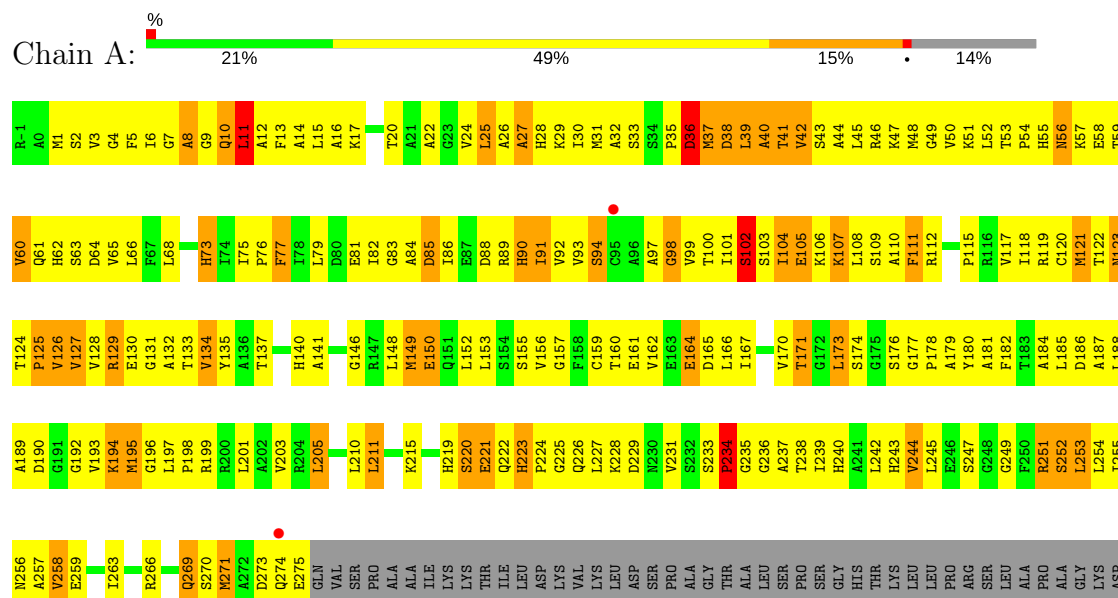
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	119	Total 119	O 119	0	0
2	D	126	Total 126	O 126	0	0
2	E	128	Total 128	O 128	0	0

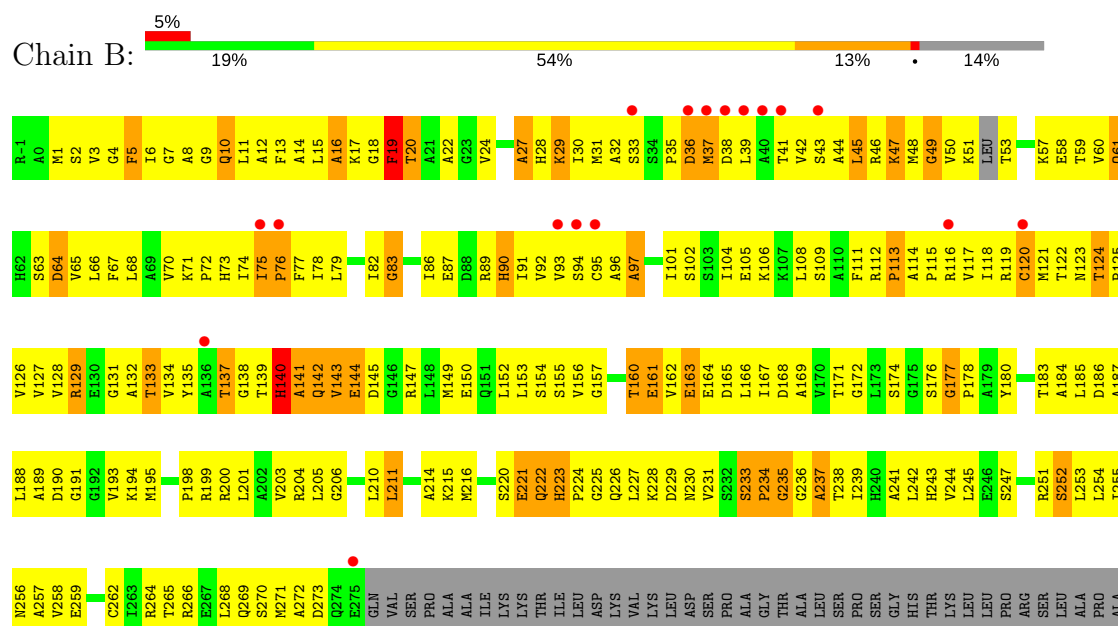
3 Residue-property plots

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: Pyrroline-5-carboxylate reductase 1

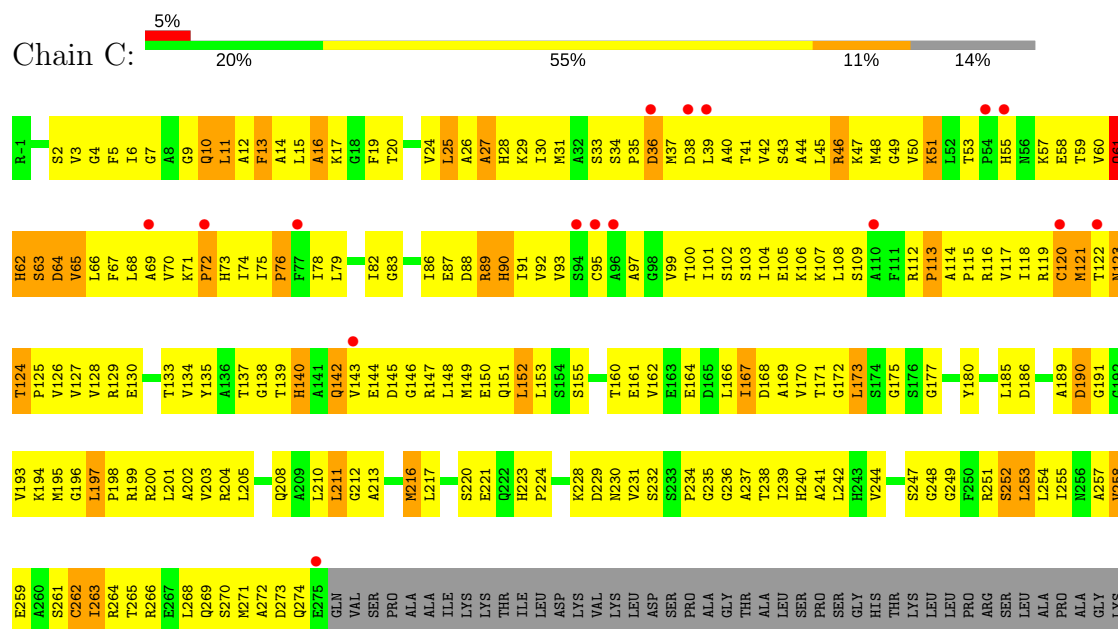


• Molecule 1: Pyrroline-5-carboxylate reductase 1



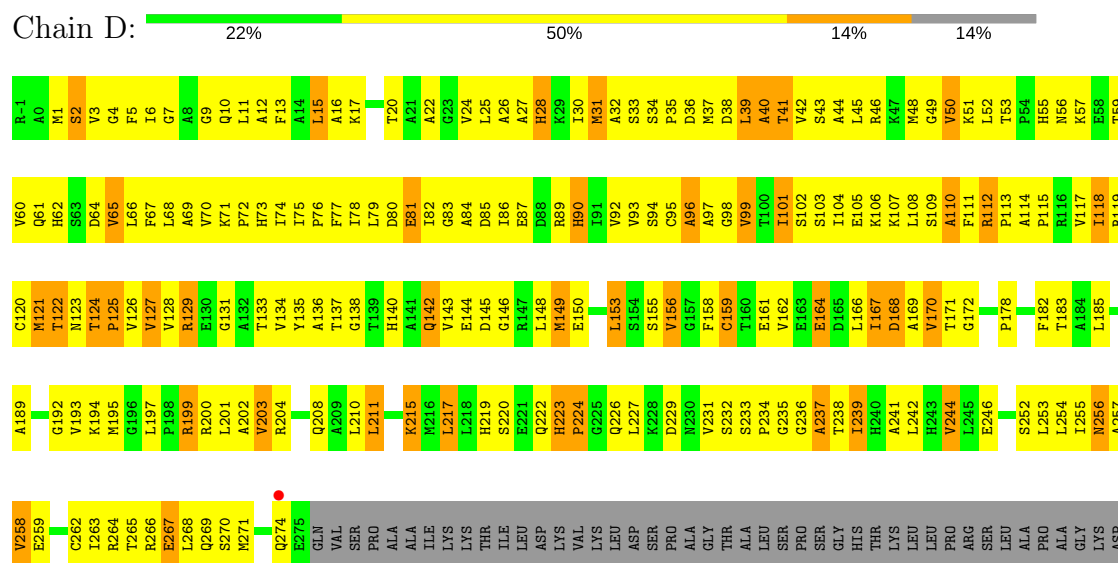
GLY
LYS
ASP

• Molecule 1: Pyrroline-5-carboxylate reductase 1

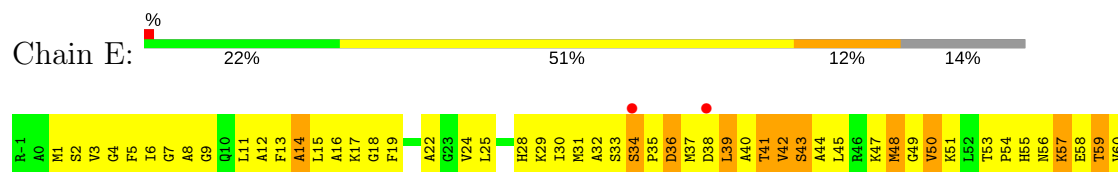


ASP

• Molecule 1: Pyrroline-5-carboxylate reductase 1



• Molecule 1: Pyrroline-5-carboxylate reductase 1



V258	D190	V126	G61
S261	V193	V127	H62
C262	K194	V128	
I263	M195	R129	V65
R264	G196	E130	L66
T265	L197	G131	F67
R266	P198	A132	L68
E267	R199	T133	A69
L268	R200	V134	V70
Q269	L201	Y135	K71
S270	A202	A136	P72
Q274	V203	T137	H73
E275	R204	G138	I74
G1N	L205	T139	I75
VAL	G206	H140	P76
SER	A207	A141	F77
PRO	Q208	Q142	I78
ALA	A209	V143	L79
ALA	L210	E144	D80
ILE	L211	D145	E81
LYS	M216	G146	L82
LYS	L217	R147	G83
THR	L218	L148	
ILE	H219	M149	T86
LEU	S220	E150	E87
ASP	E221	Q151	D88
LYS	Q222	L152	R89
VAL	H223	L153	H90
LYS	P224	S154	
LEU	L227	S155	S94
ASP	K228	V156	C95
SER		G157	A96
PRO	V231	T160	A97
ALA	S232	E161	G98
GLY	S233	V162	V99
THR	P234	E163	T100
ALA	G235	L166	I101
LEU	G236	I167	S102
SER	A237	D168	S103
PRO	T238	A169	I104
SER	I239	V170	K106
GLY	H240	T171	K107
HIS	A241	G172	L108
THR	L242		F111
LYS	H243	G175	R112
LEU	V244	S176	P113
LEU	L245	G177	A114
PRO		P178	P115
PRO		A179	P116
ARG	G249	Y180	V117
SER	F250	A181	I118
LEU	R251		R119
ALA	S252	A184	C120
PRO	L253	L185	M121
ALA	L254	D186	T122
GLY	L255	A187	N123
LYS	T256	L188	T124
ASP	N256	A189	P125
	A257		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.61Å 123.81Å 120.79Å 90.00° 121.76° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 28.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 98.7 (28.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.11Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.261 0.221 , 0.215	Depositor DCC
R_{free} test set	2326 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 123.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.036 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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	0.68	0/2069	0.90	0/2800
1	B	0.58	0/2055	0.85	2/2781 (0.1%)
1	C	0.62	0/2063	0.86	2/2793 (0.1%)
1	D	0.68	0/2069	0.88	0/2800
1	E	0.65	0/2069	0.89	1/2800 (0.0%)
All	All	0.64	0/10325	0.88	5/13974 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	GLY	N-CA-C	-6.07	97.94	113.10
1	C	120	CYS	CA-CB-SG	5.82	124.48	114.00
1	B	45	LEU	CA-CB-CG	5.27	127.43	115.30
1	E	39	LEU	N-CA-C	-5.04	97.39	111.00
1	B	49	GLY	N-CA-C	-5.02	100.55	113.10

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	2038	0	2082	320	0
1	B	2025	0	2063	352	0
1	C	2032	0	2071	359	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2038	0	2082	291	0
1	E	2038	0	2082	311	0
2	A	106	0	0	48	0
2	B	118	0	0	54	0
2	C	119	0	0	55	0
2	D	126	0	0	49	0
2	E	128	0	0	60	0
All	All	10768	0	10380	1614	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 79.

The worst 5 of 1614 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:D:239:ILE:H	1:D:239:ILE:HD12	1.08	1.16
1:C:75:ILE:HD12	1:C:99:VAL:HG21	1.27	1.16
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.22	1.14
1:E:101:ILE:HD11	1:E:138:GLY:HA2	1.28	1.14
1:C:86:ILE:HD11	1:C:108:LEU:HD22	1.34	1.09

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	275/321 (86%)	182 (66%)	60 (22%)	33 (12%)	0	2
1	B	272/321 (85%)	168 (62%)	68 (25%)	36 (13%)	0	1
1	C	275/321 (86%)	183 (66%)	60 (22%)	32 (12%)	0	2
1	D	275/321 (86%)	183 (66%)	68 (25%)	24 (9%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	275/321 (86%)	183 (66%)	57 (21%)	35 (13%)	0	1
All	All	1372/1605 (86%)	899 (66%)	313 (23%)	160 (12%)	0	2

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	GLN
1	A	11	LEU
1	A	36	ASP
1	A	37	MET

5.3.2 Protein sidechains ⓘ

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	215/250 (86%)	185 (86%)	30 (14%)	4	18
1	B	213/250 (85%)	197 (92%)	16 (8%)	16	49
1	C	214/250 (86%)	196 (92%)	18 (8%)	13	44
1	D	215/250 (86%)	185 (86%)	30 (14%)	4	18
1	E	215/250 (86%)	203 (94%)	12 (6%)	25	61
All	All	1072/1250 (86%)	966 (90%)	106 (10%)	9	34

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	LYS
1	C	211	LEU
1	E	120	CYS
1	C	89	ARG
1	C	123	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	HIS
1	C	90	HIS
1	D	140	HIS
1	B	240	HIS
1	D	240	HIS

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(Å ²)	Q<0.9
1	A	277/321 (86%)	-0.38	2 (0%) 87 75	27, 79, 115, 154	0
1	B	276/321 (85%)	0.01	17 (6%) 21 8	26, 120, 172, 187	0
1	C	277/321 (86%)	0.04	16 (5%) 24 10	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.46	1 (0%) 92 84	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.43	3 (1%) 80 65	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.25	39 (2%) 53 29	23, 82, 160, 187	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	CYS	3.8
1	B	39	LEU	3.7
1	B	38	ASP	3.6
1	C	96	ALA	3.6
1	C	95	CYS	3.6

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 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.