



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 05:53 pm 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

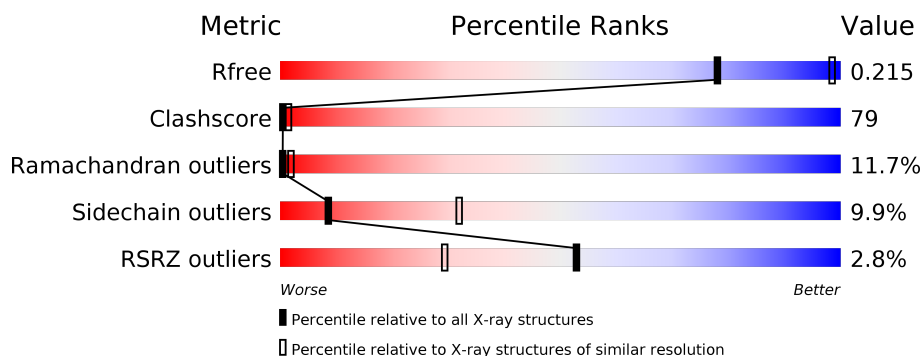
1 Overall quality at a glance

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}	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (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 style="width: 21%; background-color: red;"></div> <div style="width: 49%; background-color: yellow;"></div> <div style="width: 15%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>21% 49% 15% 14%</div>
1	B	321	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 19%; background-color: green;"></div> <div style="width: 54%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>5% 19% 54% 13% 14%</div>
1	C	321	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 20%; background-color: green;"></div> <div style="width: 55%; background-color: yellow;"></div> <div style="width: 11%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>5% 20% 55% 11% 14%</div>
1	D	321	<div> <div style="width: 22%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>22% 50% 14% 14%</div>
1	E	321	<div> <div style="width: 22%; background-color: green;"></div> <div style="width: 51%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>22% 51% 12% 14%</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		

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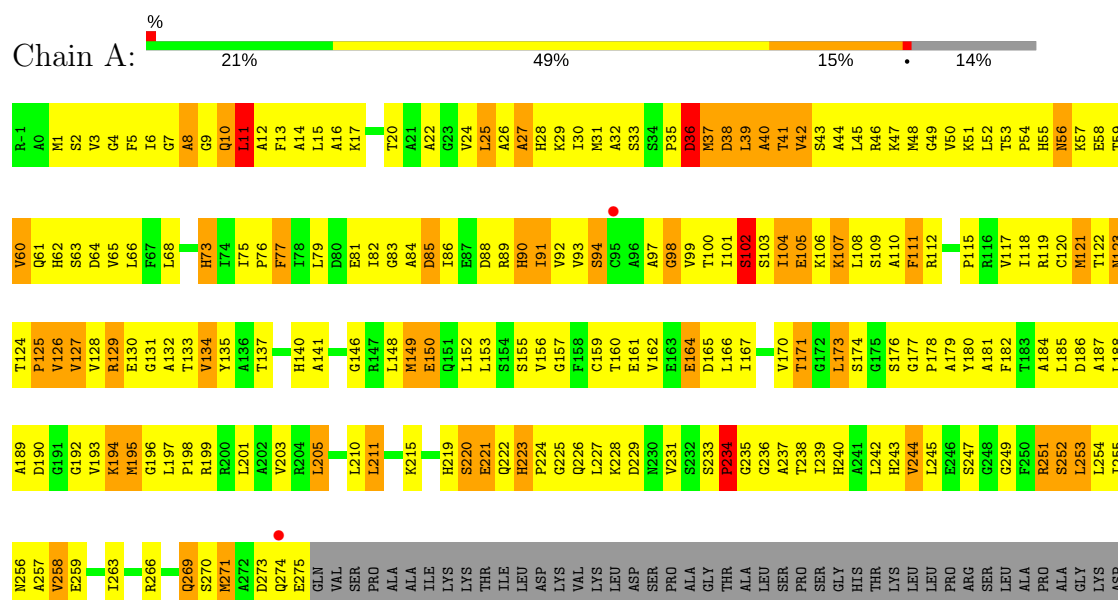
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	119	Total 119	O 119	0	0
2	D	126	Total 126	O 126	0	0
2	E	128	Total 128	O 128	0	0

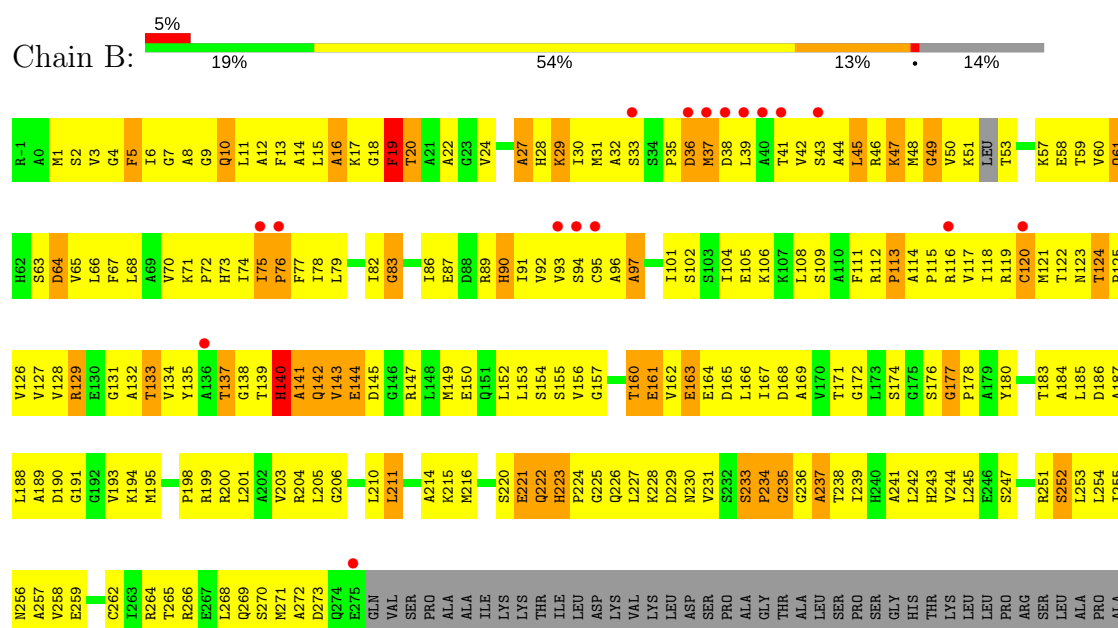
3 Residue-property plots

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

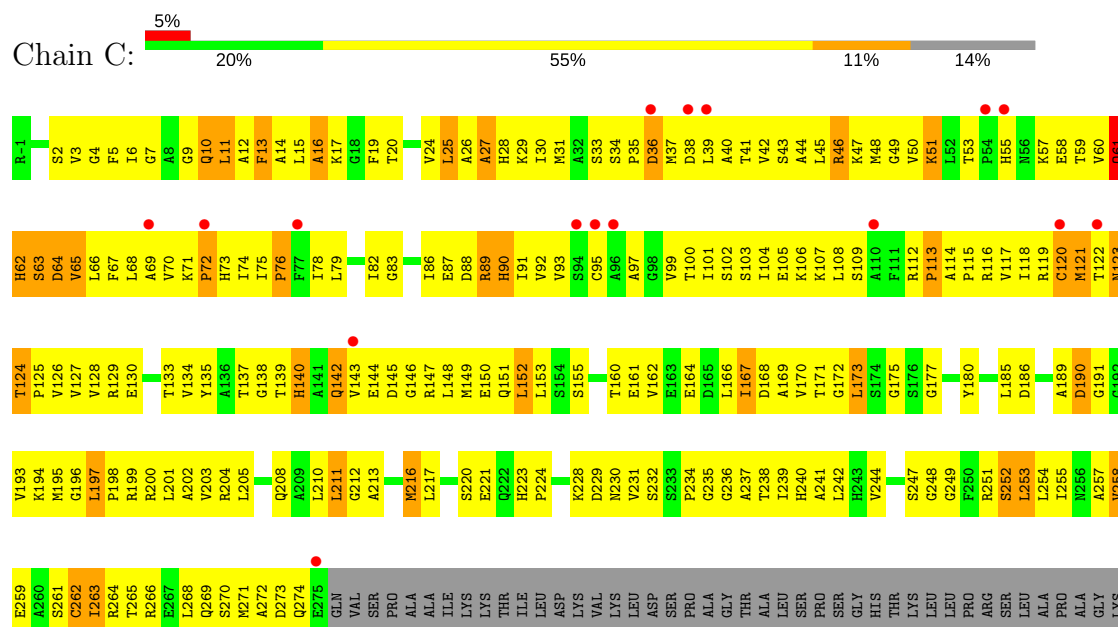


• Molecule 1: Pyrroline-5-carboxylate reductase 1



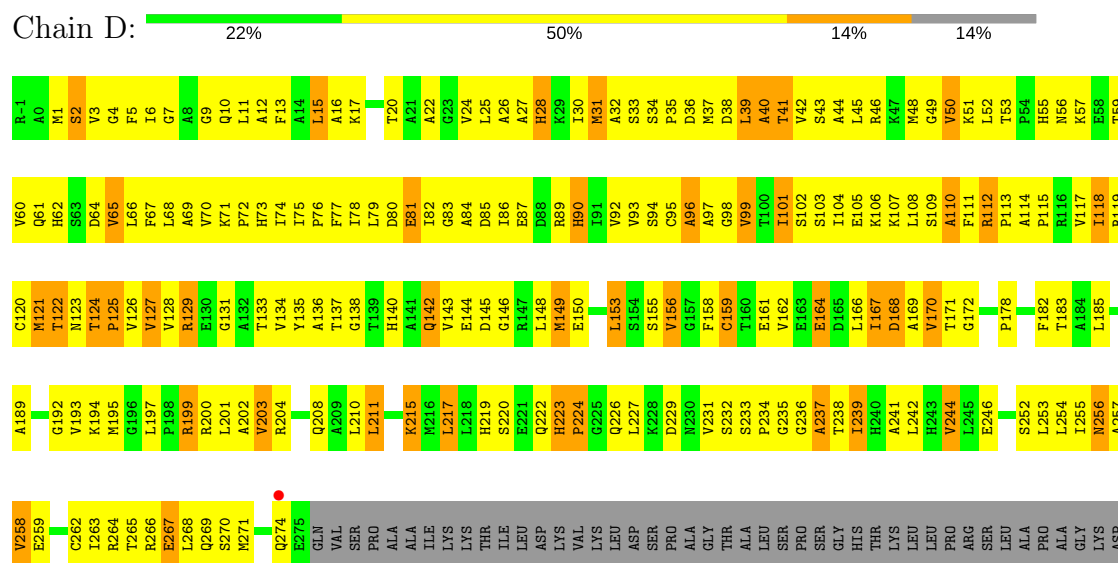
GLY
LYS
ASP

• Molecule 1: Pyrroline-5-carboxylate reductase 1

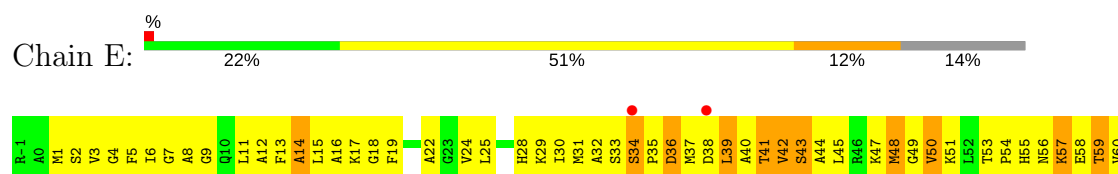


ASP

• Molecule 1: Pyrroline-5-carboxylate reductase 1



• Molecule 1: Pyrroline-5-carboxylate reductase 1



V258	S261	C262	I263	R264	T265	R266	E267	L268	Q269	S270	Q274	E275	GLN	VAL	SER	PRO	ALA	ALA	ALA	ILE	LYS	LYS	THR	ILE	LEU	ASP	LYS	VAL	LYS	LEU	ASP	SER	PRO	ALA	GLY	THR	ALA	LEU	SER	PRO	SER	THR	GLY	HIS	THR	LYS	LEU	LEU	PRO	ARG	SER	SER	ALA	ALA	PRO	ALA	GLY	LYS	ASP
D190	V193	K194	M195	G196	L197	P198	R199	R200	L201	A202	V203	R204	L205	G206	Q208	A209	L210	L211	M216	L217	L218	H219	S220	E221	Q222	H223	P224	L227	K228	V231	S232	S233	P234	G235	G236	A237	T238	I239	H240	A241	L242	H243	V244	L245	G249	F250	R251	S252	L253	L254	I255	N256	A257						
V126	V127	V128	R129	E130	G131	A132	T133	V134	Y135	A136	T137	G138	T139	H140	A141	Q142	V143	E144	D145	G146	R147	L148	M149	E150	Q151	L152	L153	S154	S155	V156	G157	T160	E161	V162	E163	L166	I167	D168	E169	V170	T171	G172	G175	S176	G177	P178	A179	Y180	A181	A184	L185	D186	A187	L188	A189				
G61	H62					A69	V70	K71	P72	H73	I74	I75	F76	F77	I78	L79	D80	E81	L82	G83			T86	E87	D88	R89	H90		S94	C95	A96	A97	G98	V99	T100	I101	S102	S103	I104	E105	K106	K107	L108		F111	R112	P113	A114	P115	R116	V117	I118	R119	C120	M121	T122	N123	T124	P125

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	2346 reflections (4.99%)	wwPDB-VP
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

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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

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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	17
1	B	213/250 (85%)	197 (92%)	16 (8%)	15	46
1	C	214/250 (86%)	196 (92%)	18 (8%)	12	41
1	D	215/250 (86%)	185 (86%)	30 (14%)	4	17
1	E	215/250 (86%)	203 (94%)	12 (6%)	23	57
All	All	1072/1250 (86%)	966 (90%)	106 (10%)	8	32

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%) 20 8	26, 120, 172, 187	0
1	C	277/321 (86%)	0.04	16 (5%) 23 10	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.46	1 (0%) 92 85	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.43	3 (1%) 80 64	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.24	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	3.7
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.