



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:21 AM GMT

PDB ID : 2GR9  
Title : Crystal structure of P5CR complexed with NADH  
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.  
Deposited on : 2006-04-23  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

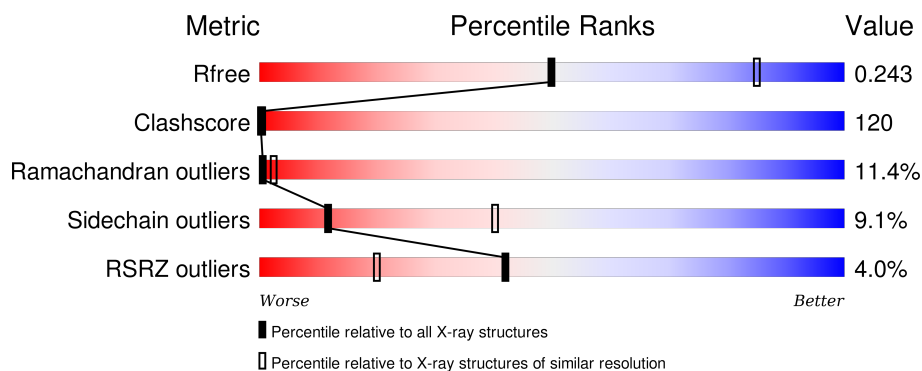
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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	277	<div> <div>19%</div> <div>63%</div> <div>16%</div> <div>.</div> </div>
1	B	277	<div> <div>9%</div> <div>18%</div> <div>65%</div> <div>14%</div> <div>.</div> </div>
1	C	277	<div> <div>8%</div> <div>19%</div> <div>68%</div> <div>13%</div> </div>
1	D	277	<div> <div>%</div> <div>21%</div> <div>67%</div> <div>11%</div> <div>.</div> </div>
1	E	277	<div> <div>2%</div> <div>17%</div> <div>67%</div> <div>15%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAI	A	1300	X	-	X	X
2	NAI	B	2300	X	-	X	X
2	NAI	C	3300	X	-	X	X
2	NAI	D	4300	X	-	X	X
2	NAI	E	5300	X	-	X	X
3	GLU	A	1301	-	-	X	-
3	GLU	B	2301	-	-	X	-
3	GLU	C	3301	-	-	X	-
3	GLU	D	4301	-	-	X	-
3	GLU	E	5301	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11077 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.

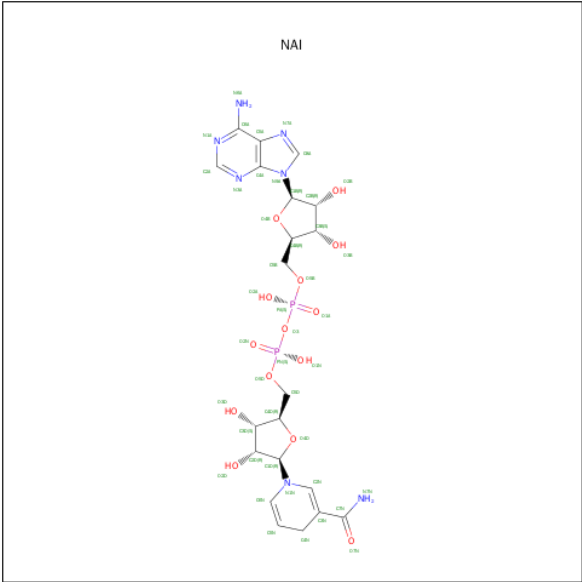
- Molecule 1 is a protein called Pyrroline-5-carboxylate reductase 1.

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
			2023	1270	358	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:

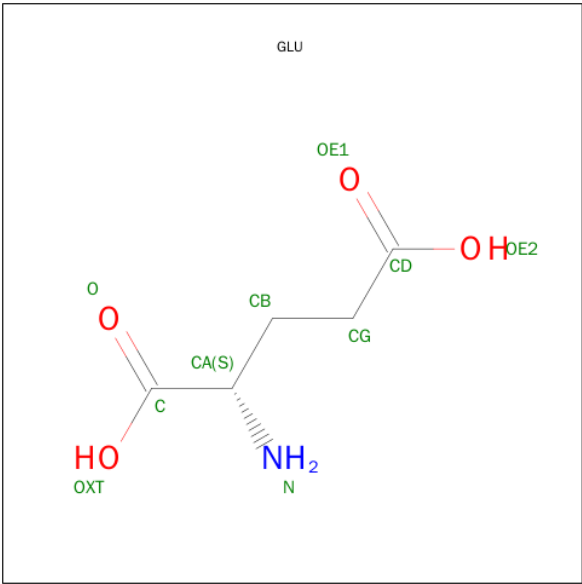
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	CLONING ARTIFACT	UNP P32322
A	0	GLY	-	CLONING ARTIFACT	UNP P32322
B	-1	ARG	-	CLONING ARTIFACT	UNP P32322
B	0	GLY	-	CLONING ARTIFACT	UNP P32322
C	-1	ARG	-	CLONING ARTIFACT	UNP P32322
C	0	GLY	-	CLONING ARTIFACT	UNP P32322
D	-1	ARG	-	CLONING ARTIFACT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

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			43	21	6	14	2		
2	B	1	Total	C	N	O	P	0	0
			43	21	6	14	2		
2	C	1	Total	C	N	O	P	0	0
			43	21	6	14	2		
2	D	1	Total	C	N	O	P	0	0
			43	21	6	14	2		
2	E	1	Total	C	N	O	P	0	0
			43	21	6	14	2		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		
3	E	1	Total	C	N	O	0	0
			10	5	1	4		

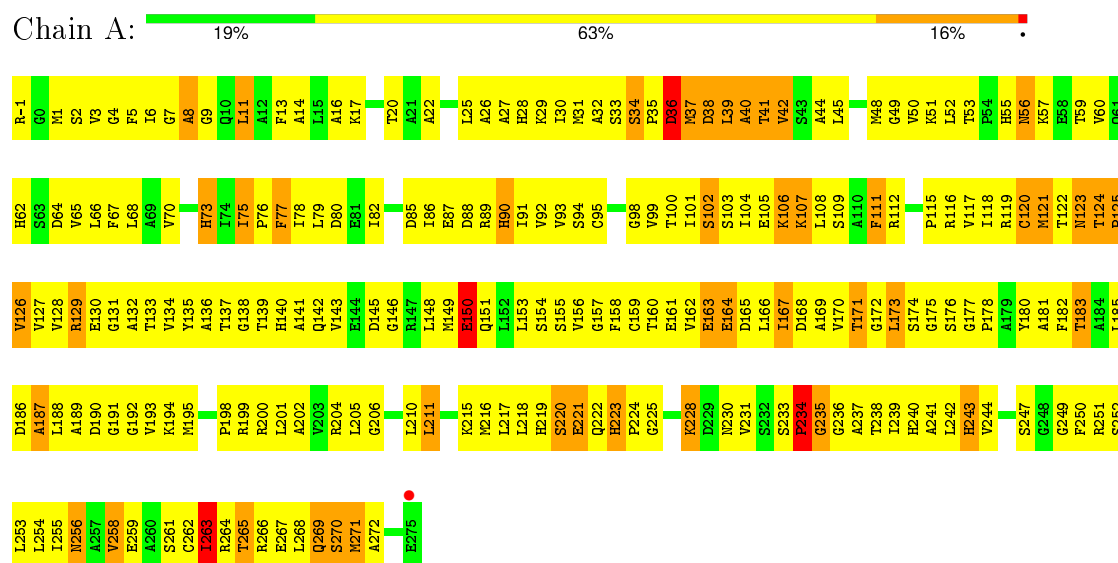
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	93	Total	O	0	0
			93	93		
4	C	116	Total	O	0	0
			116	116		
4	D	155	Total	O	0	0
			155	155		
4	E	138	Total	O	0	0
			138	138		

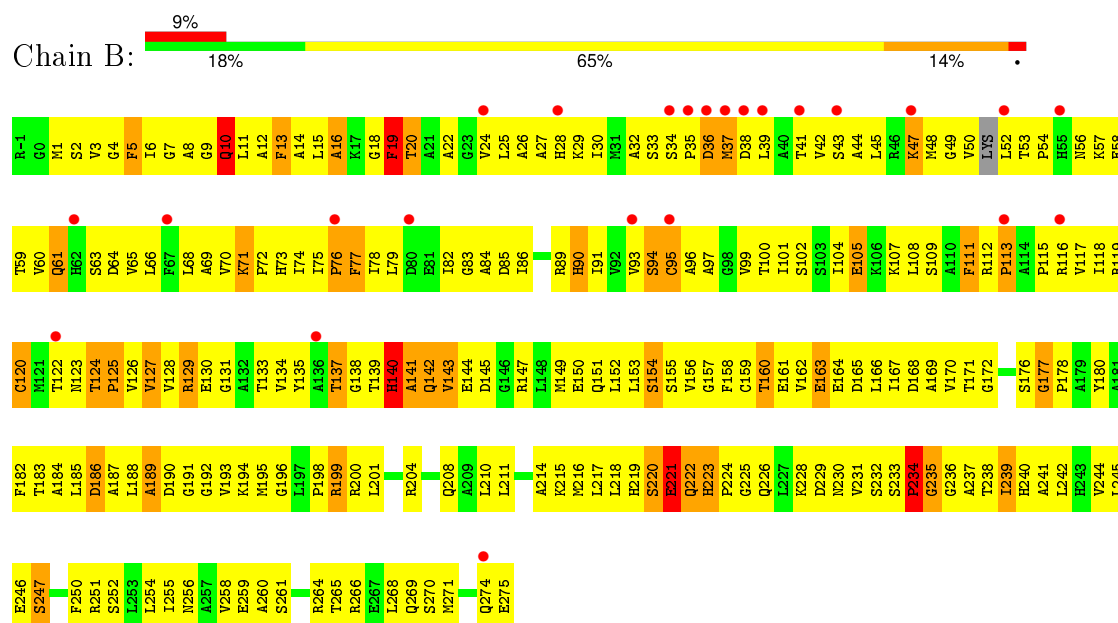
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

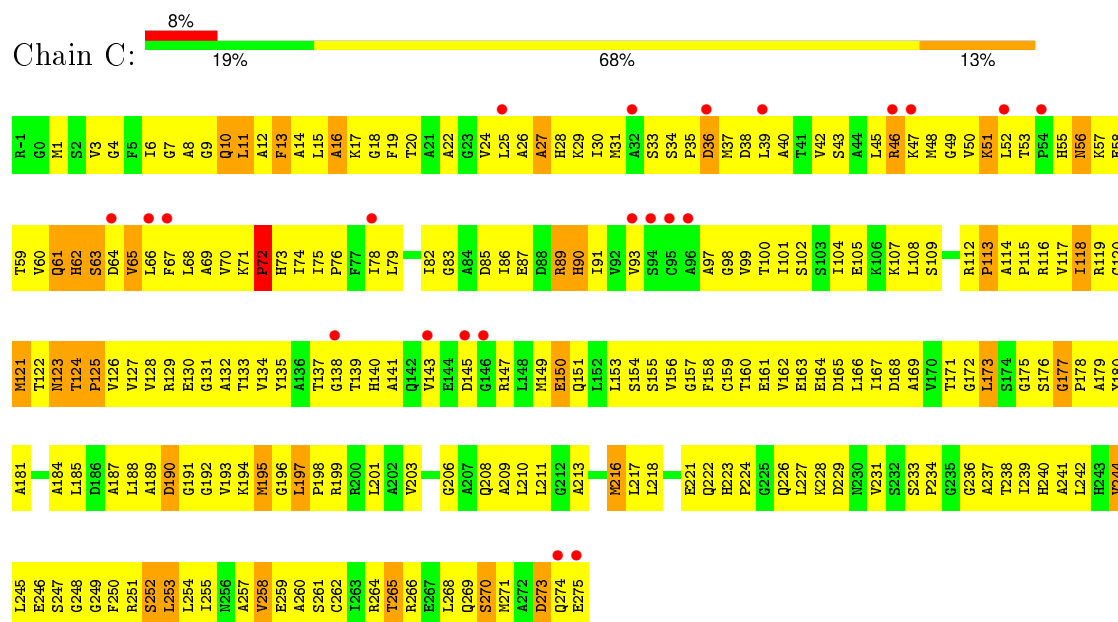
#### ● Molecule 1: Pyrroline-5-carboxylate reductase 1



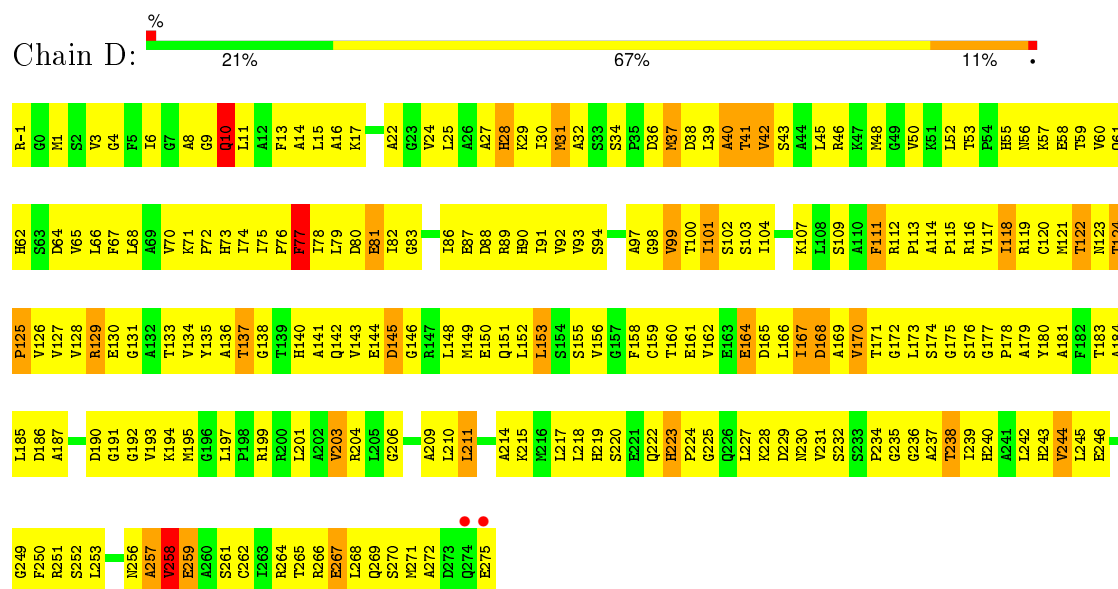
#### ● Molecule 1: Pyrroline-5-carboxylate reductase 1



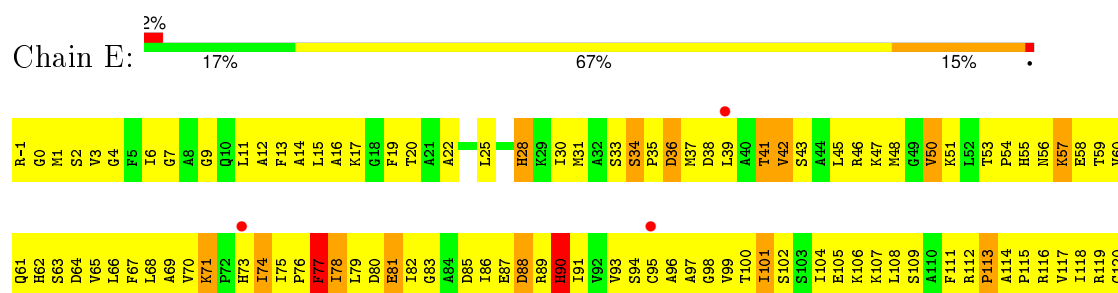
• Molecule 1: Pyrroline-5-carboxylate reductase 1



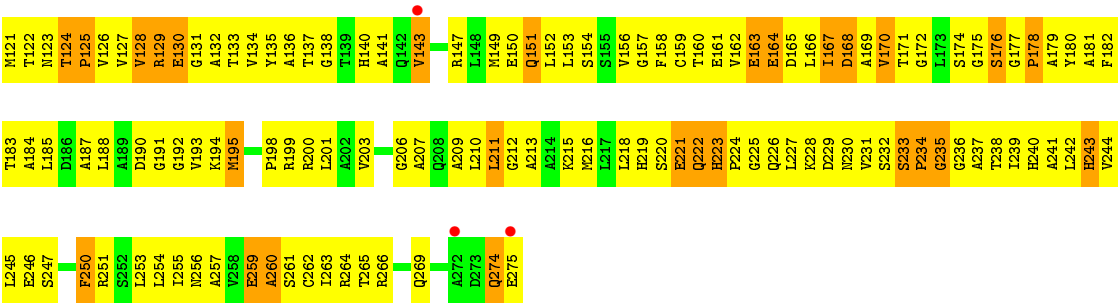
• Molecule 1: Pyrroline-5-carboxylate reductase 1



• Molecule 1: Pyrroline-5-carboxylate reductase 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.18Å 122.64Å 120.71Å 90.00° 122.03° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 28.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 94.9 (28.96-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.278 0.239 , 0.243	Depositor DCC
$R_{free}$ test set	2279 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 96.4	EDS
Estimated twinning fraction	0.017 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.026 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 62185 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAI

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	0.41	0/2069	0.72	1/2800 (0.0%)
1	B	0.37	0/2053	0.71	1/2779 (0.0%)
1	C	0.38	0/2063	0.70	1/2793 (0.0%)
1	D	0.42	0/2069	0.69	0/2800
1	E	0.49	2/2069 (0.1%)	0.86	6/2800 (0.2%)
All	All	0.41	2/10323 (0.0%)	0.74	9/13972 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	ARG	C-N	11.03	1.59	1.34
1	E	128	VAL	C-N	-5.02	1.22	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	VAL	O-C-N	14.89	146.53	122.70
1	E	128	VAL	CA-C-N	-11.74	91.36	117.20
1	E	129	ARG	O-C-N	-10.77	105.48	122.70
1	E	128	VAL	C-N-CA	-8.96	99.30	121.70
1	E	129	ARG	CA-C-N	6.87	132.32	117.20

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	2038	0	2084	489	6
1	B	2023	0	2059	491	5
1	C	2032	0	2072	530	2
1	D	2038	0	2084	436	2
1	E	2038	0	2084	492	1
2	A	43	0	23	26	0
2	B	43	0	24	67	5
2	C	43	0	23	39	4
2	D	43	0	24	40	0
2	E	43	0	21	32	1
3	A	10	0	5	8	0
3	B	10	0	5	17	0
3	C	10	0	5	12	0
3	D	10	0	5	21	0
3	E	10	0	5	11	0
4	A	141	0	0	262	6
4	B	93	0	0	169	3
4	C	116	0	0	256	4
4	D	155	0	0	247	2
4	E	138	0	0	298	1
All	All	11077	0	10523	2520	22

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 120.

The worst 5 of 2520 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)
2:A:1300:NAI:C1D	2:A:1300:NAI:N1N	1.68	1.55
2:E:5300:NAI:O3	2:E:5300:NAI:PN	1.13	1.50
1:B:129:ARG:CZ	2:B:2300:NAI:H2N	1.48	1.40
2:E:5300:NAI:O5B	2:E:5300:NAI:C5B	1.71	1.36
2:D:4300:NAI:H1D	3:D:4301:GLU:N	1.41	1.36

The worst 5 of 22 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH1	2:B:2300:NAI:N7A[2_555]	1.66	0.54
1:A:204:ARG:CB	2:C:3300:NAI:C3B[2_555]	1.75	0.45
1:B:204:ARG:CB	2:B:2300:NAI:C3B[2_555]	1.76	0.44
2:B:2300:NAI:O5B	4:B:2359:HOH:O[2_555]	1.88	0.32
1:D:204:ARG:CB	2:E:5300:NAI:C2B[2_555]	1.94	0.26

## 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	275/277 (99%)	189 (69%)	54 (20%)	32 (12%)	0	2
1	B	272/277 (98%)	168 (62%)	62 (23%)	42 (15%)	0	0
1	C	275/277 (99%)	198 (72%)	49 (18%)	28 (10%)	1	4
1	D	275/277 (99%)	190 (69%)	64 (23%)	21 (8%)	1	7
1	E	275/277 (99%)	178 (65%)	64 (23%)	33 (12%)	0	2
All	All	1372/1385 (99%)	923 (67%)	293 (21%)	156 (11%)	0	2

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	36	ASP
1	A	39	LEU
1	A	107	LYS
1	A	129	ARG

### 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	215/215 (100%)	188 (87%)	27 (13%)	5	22
1	B	213/215 (99%)	197 (92%)	16 (8%)	17	51
1	C	214/215 (100%)	197 (92%)	17 (8%)	15	49
1	D	215/215 (100%)	195 (91%)	20 (9%)	11	39
1	E	215/215 (100%)	200 (93%)	15 (7%)	19	54
All	All	1072/1075 (100%)	977 (91%)	95 (9%)	12	42

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	265	THR
1	C	124	THR
1	E	160	THR
1	C	51	LYS
1	C	90	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	HIS
1	C	243	HIS
1	E	28	HIS
1	C	73	HIS
1	E	142	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 ligands 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$
2	NAI	A	1300	-	37,47,48	5.85	23 (62%)	48,71,73	5.96	25 (52%)
3	GLU	A	1301	-	3,9,9	1.32	1 (33%)	2,11,11	7.51	1 (50%)
2	NAI	B	2300	-	37,47,48	5.45	22 (59%)	48,71,73	4.91	25 (52%)
3	GLU	B	2301	-	3,9,9	1.32	1 (33%)	2,11,11	7.52	1 (50%)
2	NAI	C	3300	-	37,47,48	5.45	22 (59%)	48,71,73	4.92	25 (52%)
3	GLU	C	3301	-	3,9,9	1.32	1 (33%)	2,11,11	7.52	1 (50%)
2	NAI	D	4300	-	37,47,48	5.46	23 (62%)	48,71,73	4.92	25 (52%)
3	GLU	D	4301	-	3,9,9	0.38	0	2,11,11	0.07	0
2	NAI	E	5300	-	37,47,48	5.83	26 (70%)	48,71,73	6.70	33 (68%)
3	GLU	E	5301	-	3,9,9	0.38	0	2,11,11	0.08	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
2	NAI	A	1300	-	2/2/13/16	0/25/72/72	0/5/5/5
3	GLU	A	1301	-	-	0/3/9/9	0/0/0/0
2	NAI	B	2300	-	1/1/13/16	0/25/72/72	0/5/5/5
3	GLU	B	2301	-	-	0/3/9/9	0/0/0/0
2	NAI	C	3300	-	1/1/13/16	0/25/72/72	0/5/5/5
3	GLU	C	3301	-	-	0/3/9/9	0/0/0/0
2	NAI	D	4300	-	1/1/13/16	0/25/72/72	0/5/5/5
3	GLU	D	4301	-	-	0/3/9/9	0/0/0/0
2	NAI	E	5300	-	3/3/13/16	1/25/72/72	0/5/5/5
3	GLU	E	5301	-	-	0/3/9/9	0/0/0/0

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NAI	O4D-C4D	-13.96	1.12	1.45
2	D	4300	NAI	O4D-C4D	-13.95	1.12	1.45
2	C	3300	NAI	O4D-C4D	-13.95	1.12	1.45
2	B	2300	NAI	O4D-C4D	-13.94	1.12	1.45
2	E	5300	NAI	C3D-C4D	-11.84	1.21	1.53

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5300	NAI	C1D-N1N-C6N	-18.51	79.40	120.81
2	D	4300	NAI	C4B-O4B-C1B	-15.88	92.27	109.72
2	C	3300	NAI	C4B-O4B-C1B	-15.87	92.28	109.72
2	B	2300	NAI	C4B-O4B-C1B	-15.86	92.29	109.72
2	E	5300	NAI	C4B-O4B-C1B	-15.86	92.29	109.72

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1300	NAI	C1D
2	A	1300	NAI	C4D
2	D	4300	NAI	C4D
2	E	5300	NAI	C1D
2	E	5300	NAI	C4D

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5300	NAI	PA-O5B-C5B-C4B

There are no ring outliers.

10 monomers are involved in 231 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1300	NAI	26	0
3	A	1301	GLU	8	0
2	B	2300	NAI	67	5
3	B	2301	GLU	17	0
2	C	3300	NAI	39	4
3	C	3301	GLU	12	0
2	D	4300	NAI	40	0
3	D	4301	GLU	21	0
2	E	5300	NAI	32	1

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5301	GLU	11	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/277 (100%)	-0.35	1 (0%) 93 85	32, 82, 117, 153	0
1	B	276/277 (99%)	0.14	24 (8%) 13 4	39, 129, 183, 200	0
1	C	277/277 (100%)	0.15	22 (7%) 15 5	31, 125, 181, 195	0
1	D	277/277 (100%)	-0.41	2 (0%) 89 78	34, 76, 118, 191	0
1	E	277/277 (100%)	-0.38	6 (2%) 65 42	24, 80, 128, 142	0
All	All	1384/1385 (99%)	-0.17	55 (3%) 42 20	24, 87, 168, 200	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	GLU	4.9
1	C	95	CYS	4.9
1	C	36	ASP	4.8
1	C	32	ALA	4.7
1	C	274	GLN	3.8

### 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](#)

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAI	B	2300	43/44	0.65	0.73	9.22	192,195,195,195	0
2	NAI	C	3300	43/44	0.54	0.97	8.48	189,195,195,195	0
2	NAI	D	4300	43/44	0.74	0.65	7.46	81,91,95,95	0
2	NAI	E	5300	43/44	0.81	0.54	6.15	69,94,95,95	0
2	NAI	A	1300	43/44	0.78	0.57	5.78	63,93,95,95	0
3	GLU	B	2301	10/10	0.42	0.87	-	192,200,200,200	0
3	GLU	E	5301	10/10	0.78	0.56	-	195,200,200,200	0
3	GLU	D	4301	10/10	0.58	0.73	-	182,193,196,198	0
3	GLU	C	3301	10/10	0.09	1.45	-	200,200,200,200	0
3	GLU	A	1301	10/10	0.63	0.61	-	120,131,140,140	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.