W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 11:40 AM EST

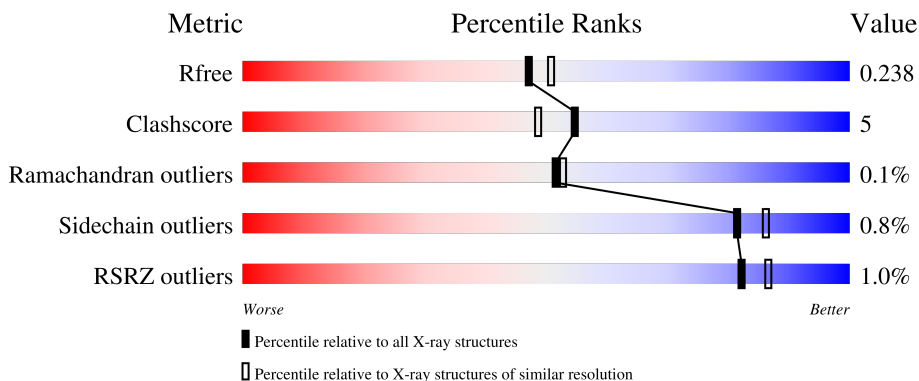|		
PDB ID	:	6NVA
Title	:	Crystal structure of Escherichia coli dihydrodipicolinate synthase and propionate covalently bound to K161.
Authors	:	Thomas, L.M.; Chooback, L.
Deposited on	:	2019-02-04
Resolution	:	2.16 Å(reported)

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 2.16 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.
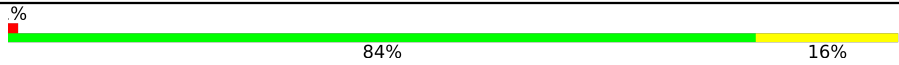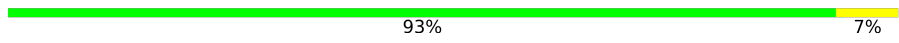
Metric	Percentile Ranks	Value
Rfree		0.238
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		0.8%
RSRZ outliers		1.0%

Worse .... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	294	.% 89% 11%
1	B	294	.% 87% 13% •
1	C	294	2% 89% 11%
1	D	294	.% 88% 12% •
1	E	294	.% 90% 10%

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Mol	Chain	Length	Quality of chain
1	F	294	.% 84% 16%
1	G	294	93% 7%
1	H	294	.% 88% 12%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 20204 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total 2210	C 1385	N 388	O 423	S 14	0	0	0
1	B	294	Total 2215	C 1388	N 390	O 423	S 14	0	0	0
1	C	294	Total 2221	C 1392	N 390	O 425	S 14	0	1	0
1	D	294	Total 2223	C 1393	N 393	O 423	S 14	0	1	0
1	E	294	Total 2215	C 1388	N 390	O 423	S 14	0	0	0
1	F	293	Total 2206	C 1383	N 385	O 424	S 14	0	1	0
1	G	293	Total 2206	C 1383	N 385	O 424	S 14	0	1	0
1	H	294	Total 2215	C 1388	N 390	O 423	S 14	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP A0A066Q637
A	0	HIS	-	expression tag	UNP A0A066Q637
A	161	RF9	LYS	modified residue	UNP A0A066Q637
B	-1	HIS	-	expression tag	UNP A0A066Q637
B	0	HIS	-	expression tag	UNP A0A066Q637
B	161	RF9	LYS	modified residue	UNP A0A066Q637
C	-1	HIS	-	expression tag	UNP A0A066Q637
C	0	HIS	-	expression tag	UNP A0A066Q637
C	161	RF9	LYS	modified residue	UNP A0A066Q637
D	-1	HIS	-	expression tag	UNP A0A066Q637
D	0	HIS	-	expression tag	UNP A0A066Q637
D	161	RF9	LYS	modified residue	UNP A0A066Q637
E	-1	HIS	-	expression tag	UNP A0A066Q637

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP A0A066Q637
E	161	RF9	LYS	modified residue	UNP A0A066Q637
F	-1	HIS	-	expression tag	UNP A0A066Q637
F	0	HIS	-	expression tag	UNP A0A066Q637
F	161	RF9	LYS	modified residue	UNP A0A066Q637
G	-1	HIS	-	expression tag	UNP A0A066Q637
G	0	HIS	-	expression tag	UNP A0A066Q637
G	161	RF9	LYS	modified residue	UNP A0A066Q637
H	-1	HIS	-	expression tag	UNP A0A066Q637
H	0	HIS	-	expression tag	UNP A0A066Q637
H	161	RF9	LYS	modified residue	UNP A0A066Q637

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
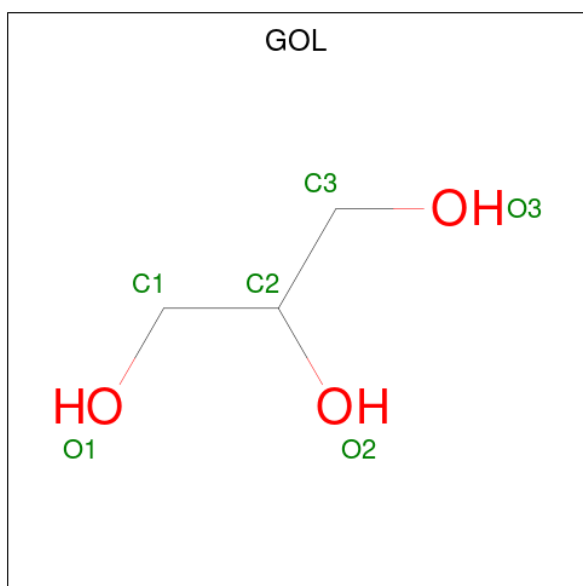
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	F	1	Total 6	C 3	O 3	0	0
2	G	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total 6	C 3	O 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total 278	O 278	0	0
4	B	335	Total 335	O 335	0	0
4	C	300	Total 300	O 300	0	0
4	D	305	Total 305	O 305	0	0
4	E	308	Total 308	O 308	0	0
4	F	303	Total 303	O 303	0	0
4	G	321	Total 321	O 321	0	0
4	H	299	Total 299	O 299	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 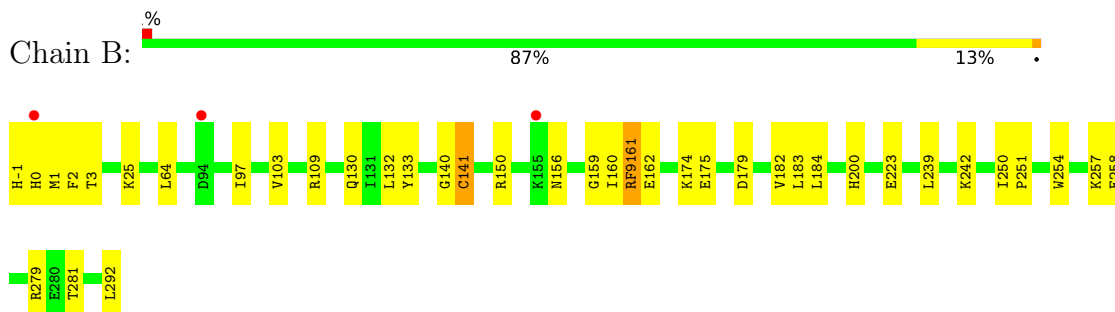the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to 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: 4-hydroxy-tetrahydrodipicolinate synthase
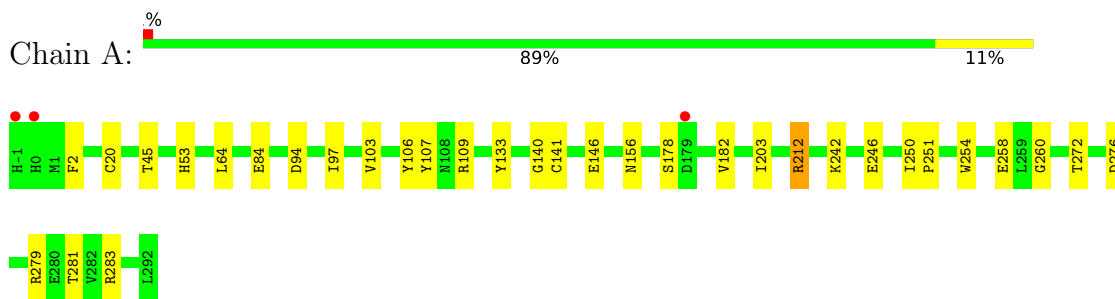
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

E280 R283 L292

● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:

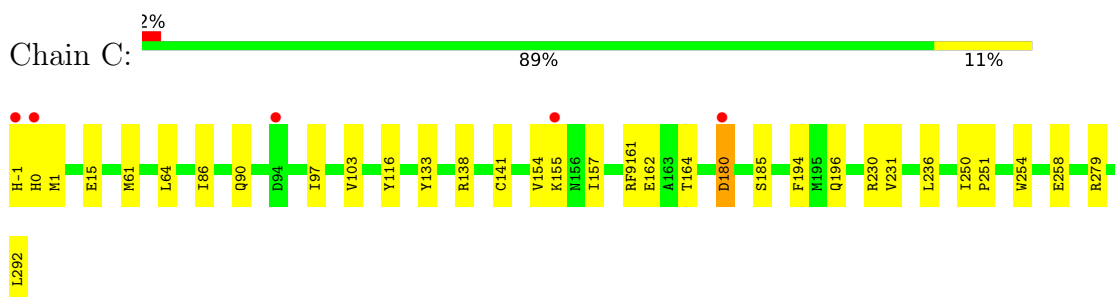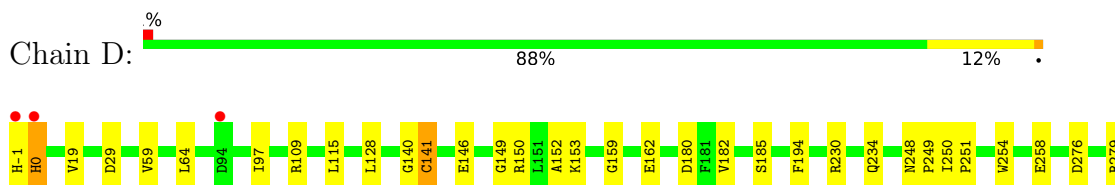● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:

● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain G:

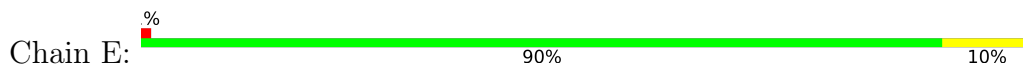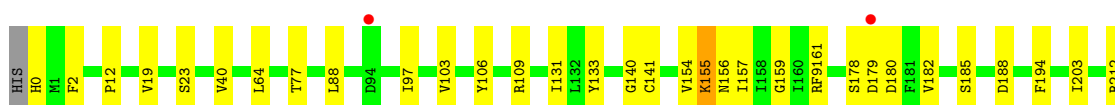

● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain H:
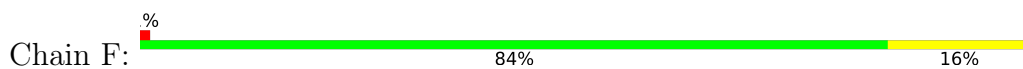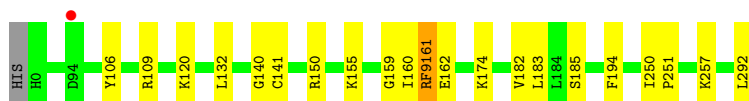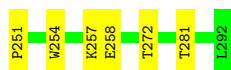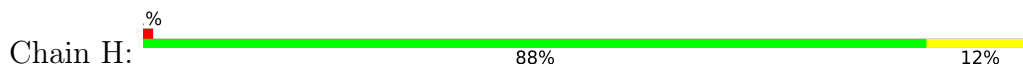
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.14Å 86.33Å 107.00Å 109.72° 104.24° 99.18°	Depositor
Resolution (Å)	25.17 – 2.16 23.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	85.4 (25.17-2.16) 74.0 (23.84-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 2.15Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.183 , 0.239 0.183 , 0.238	Depositor DCC
R_{free} test set	1732 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20204	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, RF9

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	0.40	0/2231	0.58	0/3030
1	B	0.41	1/2237 (0.0%)	0.59	1/3038 (0.0%)
1	C	0.40	1/2246 (0.0%)	0.56	0/3050
1	D	0.43	1/2248 (0.0%)	0.57	0/3053
1	E	0.42	1/2237 (0.0%)	0.56	0/3038
1	F	0.40	1/2229 (0.0%)	0.56	0/3027
1	G	0.42	1/2229 (0.0%)	0.56	0/3027
1	H	0.41	1/2237 (0.0%)	0.58	0/3038
All	All	0.41	7/17894 (0.0%)	0.57	1/24301 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	CYS	CB-SG	-7.74	1.69	1.82
1	G	141	CYS	CB-SG	-7.49	1.69	1.82
1	B	141	CYS	CB-SG	-6.04	1.72	1.82
1	H	141	CYS	CB-SG	-5.84	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	CYS	CB-SG	-5.64	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	LEU	CA-CB-CG	5.89	128.84	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ILE	Peptide
1	B	161	RF9	Mainchain
1	C	161	RF9	Mainchain
1	F	161	RF9	Mainchain
1	G	160	ILE	Mainchain

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	2210	0	2221	24	0
1	B	2215	0	2226	26	0
1	C	2221	0	2232	25	0
1	D	2223	0	2239	28	0
1	E	2215	0	2226	19	0
1	F	2206	0	2220	32	0
1	G	2206	0	2220	12	0
1	H	2215	0	2226	24	0
2	A	6	0	8	2	0
2	B	6	0	8	1	0
2	C	6	0	8	0	0
2	E	6	0	8	1	0
2	F	6	0	8	1	0
2	G	6	0	8	2	0
2	H	6	0	8	2	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
4	A	278	0	0	8	1
4	B	335	0	0	9	0
4	C	300	0	0	3	0
4	D	305	0	0	8	0
4	E	308	0	0	6	1
4	F	303	0	0	5	0
4	G	321	0	0	4	0
4	H	299	0	0	7	0
All	All	20204	0	17866	186	1

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 5.

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:D:149:GLY:O	4:D:301:HOH:O	1.90	0.88
1:A:212:ARG:NH1	4:A:402:HOH:O	2.15	0.78
1:F:0:HIS:N	4:F:401:HOH:O	2.11	0.74
1:A:246:GLU:OE1	4:A:401:HOH:O	2.05	0.74
1:B:1:MET:SD	4:B:719:HOH:O	2.49	0.71

All (1) 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)
4:A:599:HOH:O	4:E:615:HOH:O[1_544]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	291/294 (99%)	287 (99%)	4 (1%)	0	100	100
1	B	291/294 (99%)	285 (98%)	6 (2%)	0	100	100
1	C	292/294 (99%)	285 (98%)	6 (2%)	1 (0%)	41	37
1	D	292/294 (99%)	287 (98%)	4 (1%)	1 (0%)	41	37
1	E	291/294 (99%)	285 (98%)	6 (2%)	0	100	100
1	F	291/294 (99%)	286 (98%)	5 (2%)	0	100	100
1	G	291/294 (99%)	285 (98%)	6 (2%)	0	100	100
1	H	291/294 (99%)	288 (99%)	3 (1%)	0	100	100
All	All	2330/2352 (99%)	2288 (98%)	40 (2%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	0	HIS
1	D	0	HIS

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	238/239 (100%)	235 (99%)	3 (1%)	69	74
1	B	239/239 (100%)	237 (99%)	2 (1%)	81	86
1	C	240/239 (100%)	238 (99%)	2 (1%)	81	86
1	D	240/239 (100%)	239 (100%)	1 (0%)	91	93
1	E	239/239 (100%)	237 (99%)	2 (1%)	81	86
1	F	238/239 (100%)	235 (99%)	3 (1%)	69	74
1	G	238/239 (100%)	235 (99%)	3 (1%)	69	74
1	H	239/239 (100%)	238 (100%)	1 (0%)	91	93
All	All	1911/1912 (100%)	1894 (99%)	17 (1%)	81	83

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	162[A]	GLU
1	H	127	ASP
1	D	162	GLU
1	E	230	ARG
1	E	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	RF9	B	161	1	11,13,14	0.76	0	8,15,17	0.70	0
1	RF9	A	161	1	11,13,14	0.87	0	8,15,17	0.66	0
1	RF9	D	161	1	11,13,14	0.85	0	8,15,17	1.06	0
1	RF9	C	161	1	11,13,14	0.74	0	8,15,17	0.87	0
1	RF9	F	161	1	11,13,14	0.85	0	8,15,17	0.85	0
1	RF9	E	161	1	11,13,14	0.69	0	8,15,17	0.93	0
1	RF9	G	161	1	11,13,14	0.75	0	8,15,17	0.71	0
1	RF9	H	161	1	11,13,14	0.79	0	8,15,17	0.75	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
1	RF9	B	161	1	-	10/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	RF9	A	161	1	-	8/13/14/16	-
1	RF9	D	161	1	-	5/13/14/16	-
1	RF9	C	161	1	-	11/13/14/16	-
1	RF9	F	161	1	-	8/13/14/16	-
1	RF9	E	161	1	-	8/13/14/16	-
1	RF9	G	161	1	-	11/13/14/16	-
1	RF9	H	161	1	-	11/13/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	161	RF9	C1-CX1-NZ-CE
1	A	161	RF9	NZ-CX1-CX2-O3
1	A	161	RF9	NZ-CX1-CX2-O2
1	B	161	RF9	C-CA-CB-CG
1	B	161	RF9	C1-CX1-NZ-CE

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	161	RF9	1	0
1	G	161	RF9	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	GOL	G	301	-	5,5,5	1.00	0	5,5,5	0.94	0
2	GOL	E	301	-	5,5,5	1.07	0	5,5,5	1.02	0
2	GOL	F	301	-	5,5,5	1.16	0	5,5,5	1.04	0
2	GOL	C	301	-	5,5,5	0.81	0	5,5,5	1.21	1 (20%)
2	GOL	B	301	-	5,5,5	1.06	0	5,5,5	1.01	1 (20%)
2	GOL	A	301	-	5,5,5	1.03	0	5,5,5	1.12	1 (20%)
2	GOL	H	301	-	5,5,5	1.14	0	5,5,5	1.12	1 (20%)

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	GOL	G	301	-	-	2/4/4/4	-
2	GOL	E	301	-	-	1/4/4/4	-
2	GOL	F	301	-	-	4/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	B	301	-	-	1/4/4/4	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	H	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	GOL	C3-C2-C1	-2.37	102.49	111.70
2	A	301	GOL	C3-C2-C1	-2.12	103.48	111.70
2	H	301	GOL	C3-C2-C1	-2.11	103.50	111.70
2	B	301	GOL	C3-C2-C1	-2.09	103.58	111.70

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	GOL	O1-C1-C2-C3
2	G	301	GOL	C1-C2-C3-O3
2	H	301	GOL	O1-C1-C2-C3
2	G	301	GOL	O2-C2-C3-O3
2	F	301	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	GOL	2	0
2	E	301	GOL	1	0
2	F	301	GOL	1	0
2	B	301	GOL	1	0
2	A	301	GOL	2	0
2	H	301	GOL	2	0

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	293/294 (99%)	-0.26	3 (1%)	82	86	14, 21, 35, 55	0
1	B	293/294 (99%)	-0.30	3 (1%)	82	86	14, 20, 33, 62	0
1	C	293/294 (99%)	-0.21	5 (1%)	70	76	14, 22, 37, 73	0
1	D	293/294 (99%)	-0.25	3 (1%)	82	86	14, 22, 34, 78	0
1	E	293/294 (99%)	-0.30	3 (1%)	82	86	14, 21, 34, 68	0
1	F	292/294 (99%)	-0.27	2 (0%)	87	91	14, 22, 34, 56	0
1	G	292/294 (99%)	-0.29	1 (0%)	94	95	14, 21, 35, 50	0
1	H	293/294 (99%)	-0.23	4 (1%)	75	80	15, 23, 36, 67	0
All	All	2342/2352 (99%)	-0.26	24 (1%)	82	86	14, 22, 35, 78	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	HIS	7.0
1	C	0	HIS	6.5
1	E	0	HIS	4.9
1	H	0	HIS	3.6
1	C	-1	HIS	3.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
1	RF9	C	161	14/15	0.92	0.14	13,22,30,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	RF9	G	161	14/15	0.92	0.12	16,20,32,36	0
1	RF9	E	161	14/15	0.94	0.14	13,19,37,43	0
1	RF9	D	161	14/15	0.95	0.13	12,20,35,41	0
1	RF9	B	161	14/15	0.95	0.10	11,20,31,31	0
1	RF9	F	161	14/15	0.95	0.12	15,20,33,34	0
1	RF9	A	161	14/15	0.95	0.11	11,19,34,38	0
1	RF9	H	161	14/15	0.95	0.12	13,21,32,35	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
3	NA	C	302	1/1	0.85	0.10	36,36,36,36	0
2	GOL	F	301	6/6	0.93	0.12	21,24,30,34	0
2	GOL	H	301	6/6	0.94	0.11	23,25,28,34	0
2	GOL	A	301	6/6	0.94	0.13	21,22,27,30	0
2	GOL	G	301	6/6	0.95	0.10	24,25,26,27	0
2	GOL	C	301	6/6	0.95	0.09	21,22,27,31	0
2	GOL	B	301	6/6	0.95	0.13	21,23,26,29	0
2	GOL	E	301	6/6	0.97	0.11	19,23,25,27	0
3	NA	F	302	1/1	0.99	0.05	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.