



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 5, 2022 – 02:22 pm GMT

PDB ID : 7QF6
Title : N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF
Authors : Poonsiri, T.; Demitri, N.; Stefano, B.
Deposited on : 2021-12-03
Resolution : 1.87 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 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

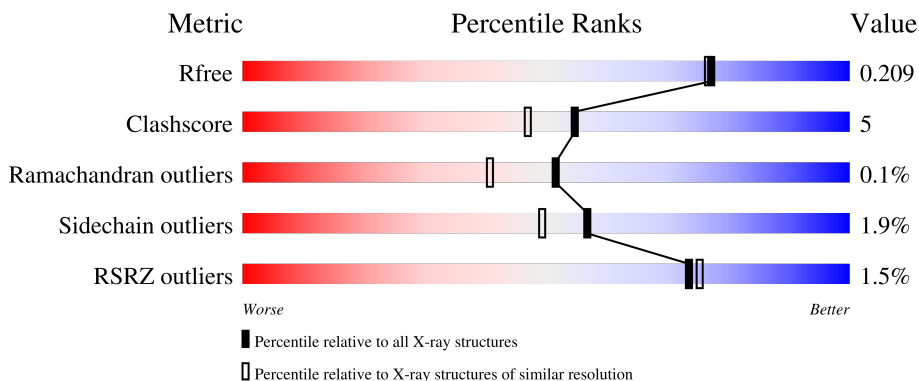
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	462	85% 10% 5%
1	B	462	2% 86% 8% 5%
1	C	462	2% 81% 13% 5%
1	D	462	2% 84% 10% 5%
1	E	462	2% 84% 10% 5%

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Mol	Chain	Length	Quality of chain
1	F	462	<p>3% 82% 10% • 6%</p>
1	G	462	<p>2% 84% 10% • 5%</p>
1	H	462	<p>% 81% 14% 5%</p>

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	GOL	A	502	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30901 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 N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	3	0
			3610	2307	646	648	9			
1	B	440	Total	C	N	O	S	0	1	0
			3621	2313	650	649	9			
1	C	438	Total	C	N	O	S	0	3	0
			3607	2306	644	648	9			
1	D	438	Total	C	N	O	S	0	1	0
			3598	2300	643	646	9			
1	E	439	Total	C	N	O	S	0	1	0
			3605	2303	646	647	9			
1	F	433	Total	C	N	O	S	0	1	0
			3553	2270	634	640	9			
1	G	439	Total	C	N	O	S	0	1	0
			3618	2312	651	646	9			
1	H	438	Total	C	N	O	S	0	1	0
			3600	2301	646	644	9			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



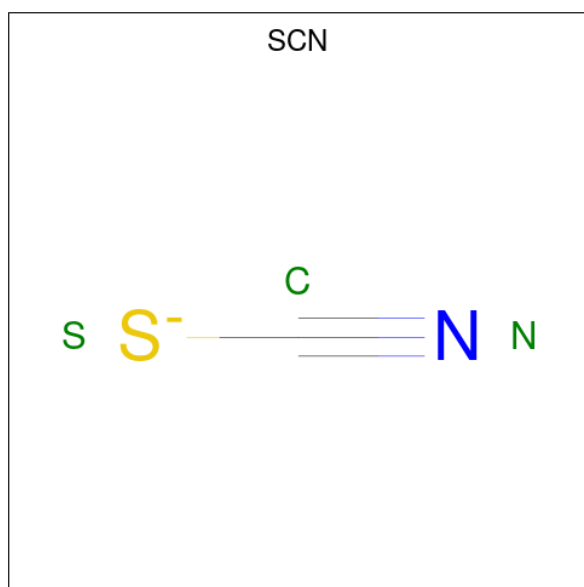
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

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

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	S	0	0
			3	1	1	1		
3	D	1	Total	C	N	S	0	0
			3	1	1	1		
3	G	1	Total	C	N	S	0	0
			3	1	1	1		
3	G	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		


- Molecule 5 is water.

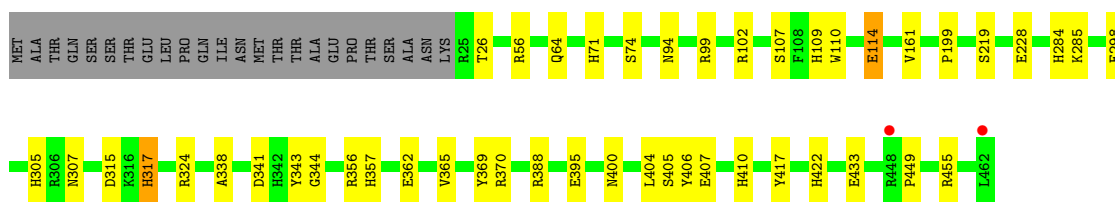
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	293	Total O 293 293	0	0
5	B	300	Total O 300 300	0	0
5	C	239	Total O 239 239	0	0
5	D	223	Total O 223 223	0	0
5	E	267	Total O 267 267	0	0
5	F	224	Total O 224 224	0	0
5	G	228	Total O 228 228	0	0
5	H	199	Total O 199 199	0	0

3 Residue-property plots [i](#)


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.

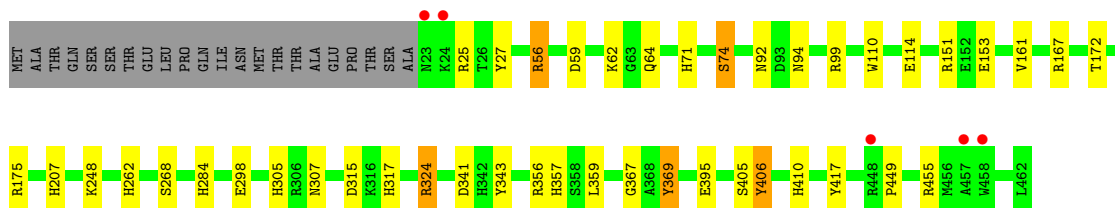
- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

Chain A: 




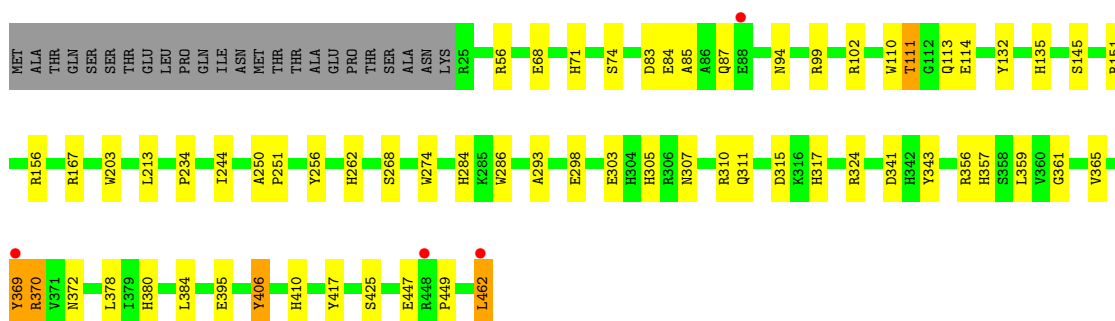
- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

Chain B: 



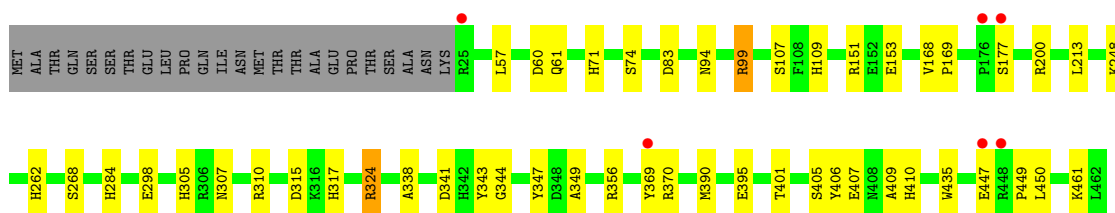
- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

Chain C: 



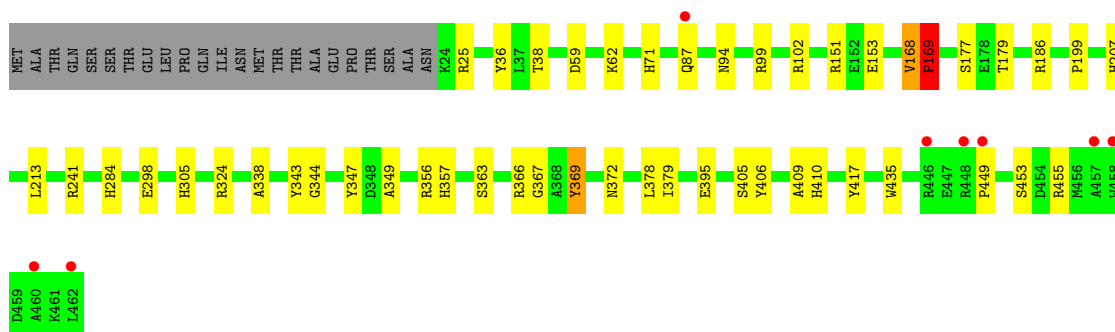
- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

Chain D: 84% 10% 5%



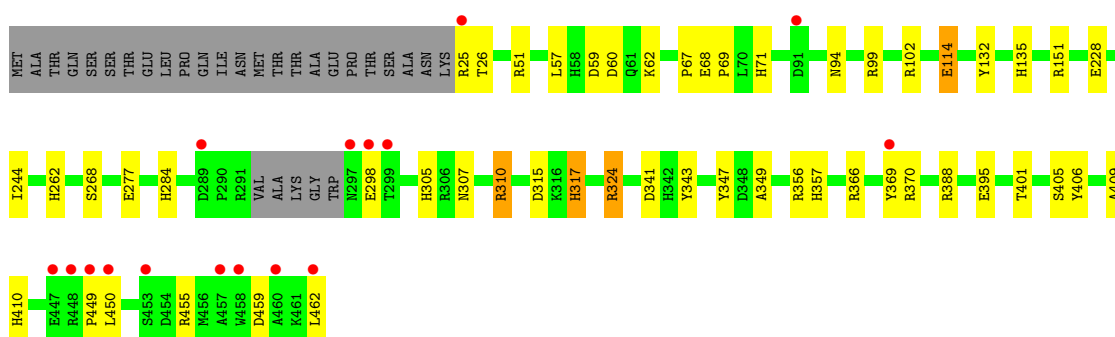
- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

Chain E: 84% 10% 5%



- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

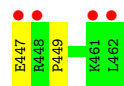
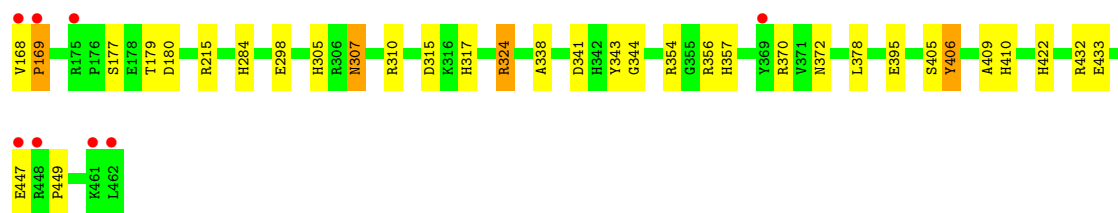
Chain F: 82% 10% 6%



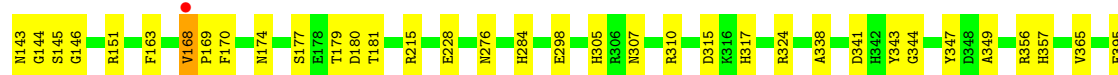
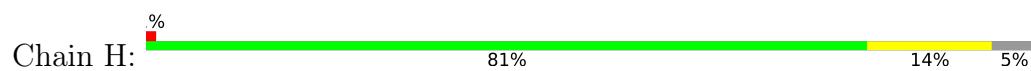
- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF

Chain G: 84% 10% 5%





- Molecule 1: N(5)-hydroxyornithine:cis-anhydromevalonyl coenzyme A-N(5)-transacylase sidF



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.27Å 80.84Å 179.84Å 101.17° 91.67° 117.25°	Depositor
Resolution (Å)	174.82 – 1.87 174.82 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.1 (174.82-1.87) 97.1 (174.82-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 1.87Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.209 0.172 , 0.209	Depositor DCC
R_{free} test set	15716 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	0.479	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-h-k-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	30901	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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](#)

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

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	0.79	3/3746 (0.1%)	1.02	5/5109 (0.1%)
1	B	0.79	1/3751 (0.0%)	1.03	7/5115 (0.1%)
1	C	0.76	3/3744 (0.1%)	1.04	12/5110 (0.2%)
1	D	0.70	0/3728	0.99	9/5086 (0.2%)
1	E	0.71	0/3735	1.04	10/5096 (0.2%)
1	F	0.75	3/3681 (0.1%)	1.02	7/5023 (0.1%)
1	G	0.73	1/3748 (0.0%)	1.02	13/5110 (0.3%)
1	H	0.74	1/3730 (0.0%)	1.03	1/5088 (0.0%)
All	All	0.75	12/29863 (0.0%)	1.02	64/40737 (0.2%)

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	E	0	1
1	G	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68[A]	GLU	CD-OE2	11.26	1.38	1.25
1	C	68[B]	GLU	CD-OE2	11.26	1.38	1.25
1	A	433	GLU	CD-OE2	-8.23	1.16	1.25
1	F	277	GLU	CD-OE1	8.01	1.34	1.25
1	G	433	GLU	CD-OE2	-7.31	1.17	1.25

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	PRO	N-CA-CB	-10.66	90.51	103.30
1	C	151	ARG	NE-CZ-NH1	-10.52	115.04	120.30
1	D	200	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	A	102	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	F	388	ARG	NE-CZ-NH1	-8.19	116.20	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	168	VAL	Peptide
1	G	168	VAL	Peptide

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	3610	0	3441	31	0
1	B	3621	0	3450	36	0
1	C	3607	0	3422	43	0
1	D	3598	0	3420	37	0
1	E	3605	0	3422	36	0
1	F	3553	0	3359	41	0
1	G	3618	0	3452	35	0
1	H	3600	0	3427	51	0
2	A	24	0	32	6	0
2	B	18	0	24	2	0
2	C	6	0	8	1	0
2	D	12	0	16	2	0
2	E	12	0	16	2	0
2	F	12	0	16	0	0
2	G	18	0	24	3	0
3	B	3	0	0	0	0
3	D	3	0	0	0	0
3	G	6	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	293	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	300	0	0	3	0
5	C	239	0	0	3	0
5	D	223	0	0	3	0
5	E	267	0	0	2	0
5	F	224	0	0	5	0
5	G	228	0	0	1	0
5	H	199	0	0	6	0
All	All	30901	0	27529	293	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 5.

The worst 5 of 293 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:F:307:ASN:ND2	1:F:310:ARG:HH22	1.16	1.40
1:F:307:ASN:ND2	1:F:310:ARG:NH2	1.76	1.33
1:F:307:ASN:HD22	1:F:310:ARG:NH2	1.30	1.26
1:H:215:ARG:NH1	5:H:501:HOH:O	1.87	1.06
1:E:284:HIS:CD2	1:E:305:HIS:HD2	1.79	0.99

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	439/462 (95%)	430 (98%)	9 (2%)	0	100	100
1	B	439/462 (95%)	431 (98%)	8 (2%)	0	100	100
1	C	439/462 (95%)	431 (98%)	8 (2%)	0	100	100
1	D	437/462 (95%)	429 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	438/462 (95%)	431 (98%)	6 (1%)	1 (0%)	47	37
1	F	430/462 (93%)	424 (99%)	6 (1%)	0	100	100
1	G	438/462 (95%)	431 (98%)	6 (1%)	1 (0%)	47	37
1	H	437/462 (95%)	427 (98%)	9 (2%)	1 (0%)	47	37
All	All	3497/3696 (95%)	3434 (98%)	60 (2%)	3 (0%)	51	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	169	PRO
1	G	169	PRO
1	H	168	VAL

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	389/407 (96%)	380 (98%)	9 (2%)	50	41
1	B	389/407 (96%)	384 (99%)	5 (1%)	69	64
1	C	387/407 (95%)	379 (98%)	8 (2%)	53	45
1	D	386/407 (95%)	381 (99%)	5 (1%)	69	64
1	E	386/407 (95%)	377 (98%)	9 (2%)	50	41
1	F	381/407 (94%)	372 (98%)	9 (2%)	49	39
1	G	388/407 (95%)	381 (98%)	7 (2%)	59	52
1	H	386/407 (95%)	379 (98%)	7 (2%)	59	52
All	All	3092/3256 (95%)	3033 (98%)	59 (2%)	57	49

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	38	THR

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Mol	Chain	Res	Type
1	H	343	TYR
1	E	395	GLU
1	H	324	ARG
1	G	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	262	HIS
1	F	305	HIS
1	H	317	HIS
1	E	305	HIS
1	F	71	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	A	504	-	5,5,5	0.17	0	5,5,5	0.54	0
2	GOL	E	502	-	5,5,5	0.30	0	5,5,5	0.37	0
2	GOL	B	504	-	5,5,5	0.34	0	5,5,5	0.71	0
2	GOL	E	501	-	5,5,5	0.24	0	5,5,5	0.39	0
2	GOL	D	502	-	5,5,5	0.30	0	5,5,5	1.08	0
3	SCN	G	501	-	1,2,2	0.39	0	0,1,1	-	-
2	GOL	C	501	-	5,5,5	0.22	0	5,5,5	0.34	0
2	GOL	B	503	-	5,5,5	0.53	0	5,5,5	0.42	0
2	GOL	D	501	-	5,5,5	0.38	0	5,5,5	1.15	0
2	GOL	F	501	-	5,5,5	0.30	0	5,5,5	0.80	0
3	SCN	B	501	-	1,2,2	2.67	1 (100%)	0,1,1	-	-
2	GOL	B	502	-	5,5,5	0.16	0	5,5,5	0.66	0
2	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.80	0
2	GOL	A	503	-	5,5,5	0.21	0	5,5,5	1.05	0
2	GOL	G	504	-	5,5,5	0.22	0	5,5,5	0.44	0
3	SCN	G	502	-	1,2,2	0.53	0	0,1,1	-	-
2	GOL	G	503	-	5,5,5	0.36	0	5,5,5	0.57	0
2	GOL	G	505	-	5,5,5	0.10	0	5,5,5	0.37	0
2	GOL	F	502	-	5,5,5	0.20	0	5,5,5	0.47	0
2	GOL	A	501	-	5,5,5	0.17	0	5,5,5	0.71	0
3	SCN	D	503	-	1,2,2	1.25	0	0,1,1	-	-

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	A	503	-	-	1/4/4/4	-
2	GOL	G	504	-	-	0/4/4/4	-
2	GOL	B	503	-	-	1/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-
2	GOL	F	501	-	-	3/4/4/4	-
2	GOL	A	504	-	-	2/4/4/4	-
2	GOL	E	502	-	-	0/4/4/4	-
2	GOL	G	503	-	-	2/4/4/4	-
2	GOL	B	504	-	-	4/4/4/4	-
2	GOL	E	501	-	-	0/4/4/4	-
2	GOL	D	502	-	-	2/4/4/4	-
2	GOL	F	502	-	-	3/4/4/4	-
2	GOL	G	505	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	502	-	-	4/4/4/4	-
2	GOL	A	501	-	-	3/4/4/4	-
2	GOL	C	501	-	-	0/4/4/4	-
2	GOL	A	502	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	SCN	C-N	-2.67	1.06	1.15

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	A	504	GOL	C1-C2-C3-O3
2	B	502	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3
2	B	504	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	502	GOL	1	0
2	B	504	GOL	1	0
2	E	501	GOL	1	0
2	C	501	GOL	1	0
2	B	503	GOL	1	0
2	D	501	GOL	2	0
2	A	502	GOL	5	0
2	G	504	GOL	1	0
2	G	503	GOL	2	0
2	A	501	GOL	1	0

5.7 Other polymers [i](#)

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 [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	438/462 (94%)	-0.39	2 (0%) 91 91	18, 27, 51, 79	0
1	B	440/462 (95%)	-0.35	5 (1%) 80 82	17, 26, 54, 101	0
1	C	438/462 (94%)	-0.28	4 (0%) 84 85	18, 30, 54, 93	0
1	D	438/462 (94%)	-0.32	6 (1%) 75 77	19, 31, 56, 80	0
1	E	439/462 (95%)	-0.28	8 (1%) 68 70	18, 29, 58, 82	0
1	F	433/462 (93%)	-0.18	16 (3%) 41 43	19, 29, 62, 88	0
1	G	439/462 (95%)	-0.24	9 (2%) 63 65	20, 31, 60, 87	0
1	H	438/462 (94%)	-0.08	4 (0%) 84 85	21, 35, 62, 92	0
All	All	3503/3696 (94%)	-0.27	54 (1%) 73 75	17, 30, 57, 101	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	168	VAL	6.0
1	E	458	TRP	4.9
1	F	297	ASN	4.8
1	F	460	ALA	4.7
1	C	462	LEU	4.7

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 monosaccharides 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. 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
2	GOL	B	504	6/6	0.90	0.15	31,43,45,49	0
4	K	B	505	1/1	0.91	0.08	75,75,75,75	0
2	GOL	A	502	6/6	0.92	0.13	38,45,52,65	0
2	GOL	F	501	6/6	0.92	0.12	41,49,57,60	0
2	GOL	A	504	6/6	0.92	0.15	40,57,65,77	0
2	GOL	F	502	6/6	0.93	0.13	37,45,46,55	0
2	GOL	G	504	6/6	0.93	0.10	36,44,45,49	0
2	GOL	A	503	6/6	0.93	0.10	34,41,50,56	0
2	GOL	B	502	6/6	0.94	0.11	31,40,48,50	0
2	GOL	A	501	6/6	0.94	0.09	32,42,46,47	0
2	GOL	C	501	6/6	0.94	0.11	37,41,42,54	0
2	GOL	D	502	6/6	0.94	0.10	35,45,50,52	0
2	GOL	E	502	6/6	0.95	0.07	35,37,39,40	0
3	SCN	G	501	3/3	0.95	0.18	20,20,26,62	0
2	GOL	G	503	6/6	0.95	0.09	34,49,54,54	0
4	K	E	503	1/1	0.95	0.12	45,45,45,45	0
2	GOL	E	501	6/6	0.96	0.09	30,37,39,41	0
2	GOL	D	501	6/6	0.96	0.13	26,36,38,45	0
3	SCN	B	501	3/3	0.96	0.11	17,17,24,55	0
2	GOL	G	505	6/6	0.97	0.08	36,46,49,50	0
3	SCN	G	502	3/3	0.97	0.08	38,38,39,42	0
2	GOL	B	503	6/6	0.97	0.11	23,27,36,37	0
3	SCN	D	503	3/3	0.97	0.09	41,41,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.