



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2026 – 06:58 pm BST

PDB ID : 5AA5 / pdb_00005aa5
Title : Actinobacterial-type NiFe-hydrogenase from Ralstonia eutropha H16 at 2.85 Angstrom resolution
Authors : Schaefer, C.; Bommer, M.; Hennig, S.; Jeoung, J.H.; Dobbek, H.; Lenz, O.
Deposited on : 2015-07-23
Resolution : 2.50 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

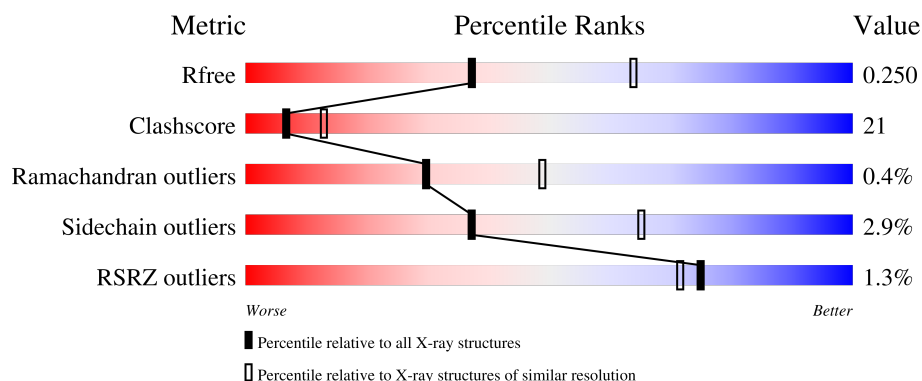
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	351	% 69% 28% ..
1	B	351	 64% 32% ..
1	D	351	% 65% 32% ..
1	F	351	% 62% 33% ..
1	H	351	% 58% 38% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	351	
2	C	579	
2	E	579	
2	G	579	
2	I	579	
2	K	579	
2	L	579	

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
3	SF4	M	702	-	-	X	-
5	FCO	C	580	-	-	X	-
5	FCO	E	580	-	-	X	-
5	FCO	I	580	-	-	X	-
5	FCO	L	580	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42867 atoms, of which 2 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.

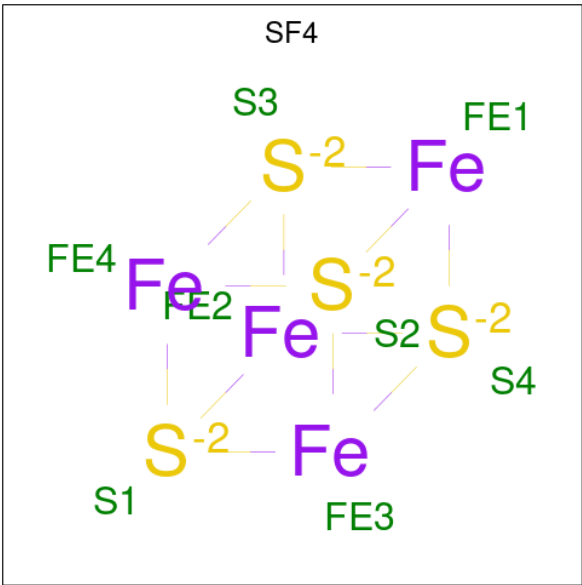
- Molecule 1 is a protein called NIFE-HYDROGENASE SMALL SUBUNIT, HOFK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	B	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	D	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	F	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	H	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	M	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			

- Molecule 2 is a protein called NIFE-HYDROGENASE LARGE SUBUNIT, HOFG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	561	Total	C	N	O	S	0	0	0
			4495	2875	775	819	26			
2	E	559	Total	C	N	O	S	0	0	0
			4478	2863	772	817	26			
2	G	561	Total	C	N	O	S	0	0	0
			4495	2875	775	819	26			
2	I	560	Total	C	N	O	S	0	0	0
			4486	2869	773	818	26			
2	K	561	Total	C	N	O	S	0	0	0
			4495	2875	775	819	26			
2	L	560	Total	C	N	O	S	0	0	0
			4486	2869	773	818	26			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



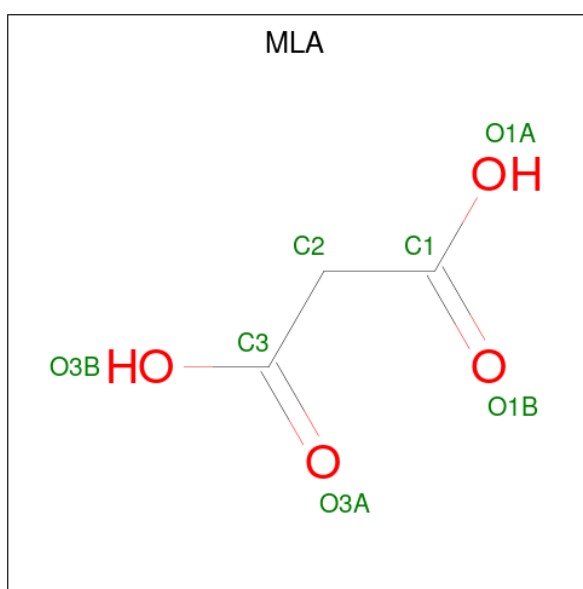
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	H	1	Total	Fe	S	0	0
			8	4	4		
3	H	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

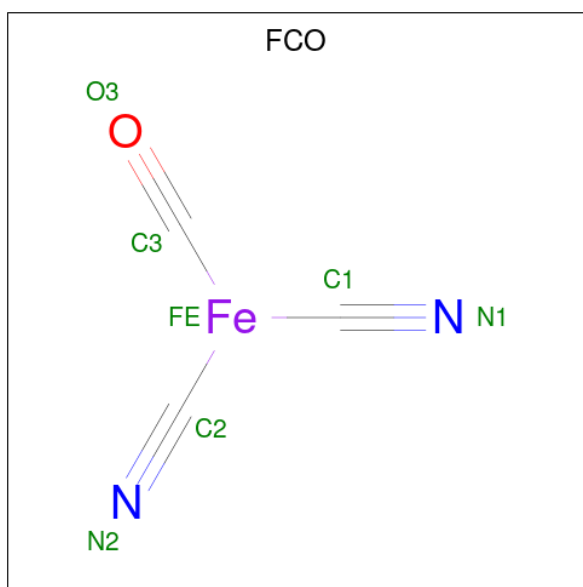
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			7	3	4			
4	A	1	Total	C	O		0	0
			7	3	4			
4	A	1	Total	C	H	O	0	0
			9	3	2	4		
4	D	1	Total	C	O		0	0
			7	3	4			
4	F	1	Total	C	O		0	0
			7	3	4			
4	M	1	Total	C	O		0	0
			7	3	4			

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	E	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	G	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	I	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	K	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
5	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

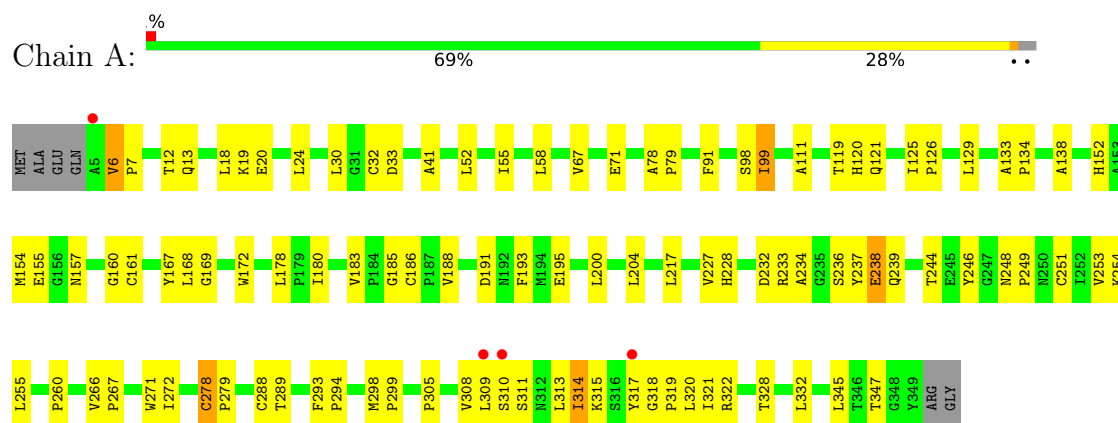
- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ni	0	0
			1	1		
6	E	1	Total	Ni	0	0
			1	1		
6	G	1	Total	Ni	0	0
			1	1		
6	I	1	Total	Ni	0	0
			1	1		
6	K	1	Total	Ni	0	0
			1	1		
6	L	1	Total	Ni	0	0
			1	1		

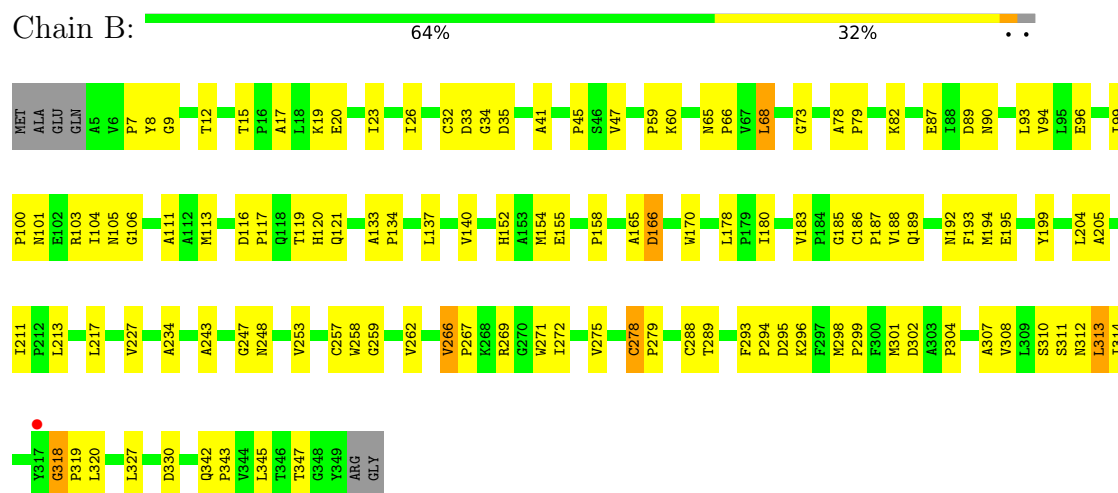
3 Residue-property plots [i](#)

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.

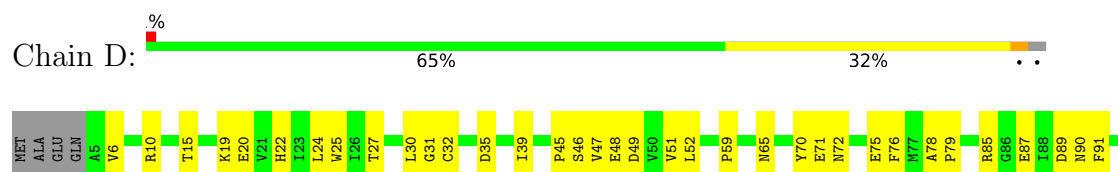
• Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK

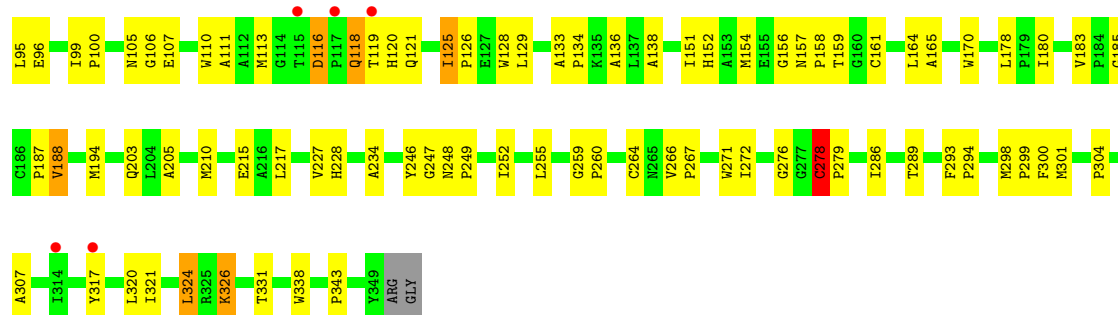


• Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK

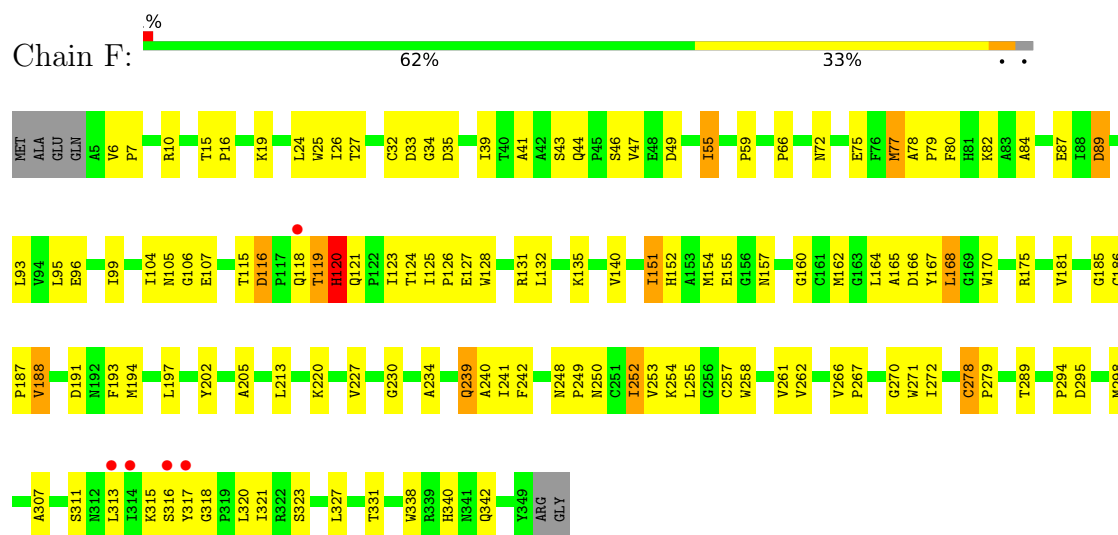


• Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK

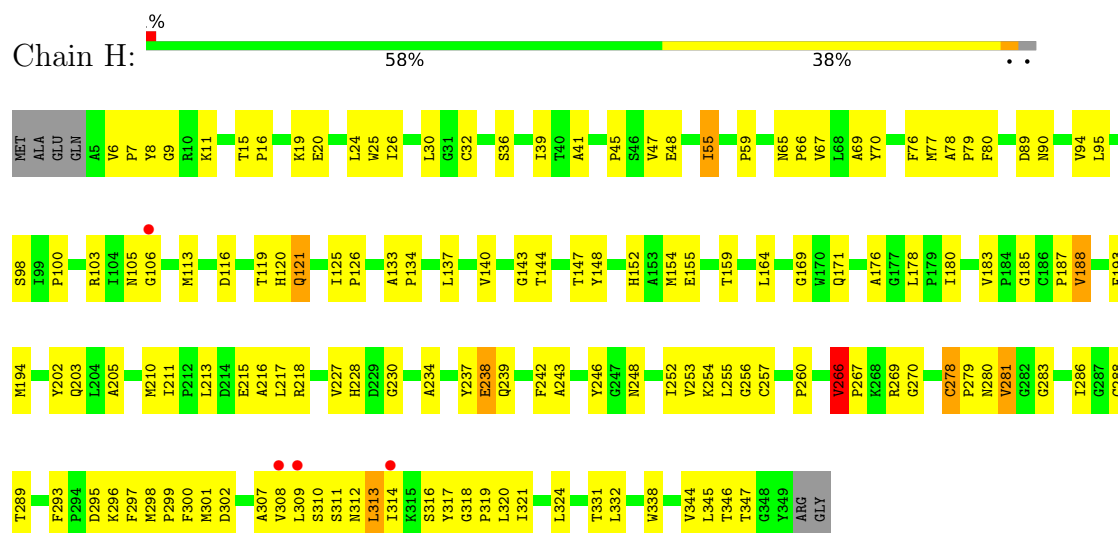




• Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK



• Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK



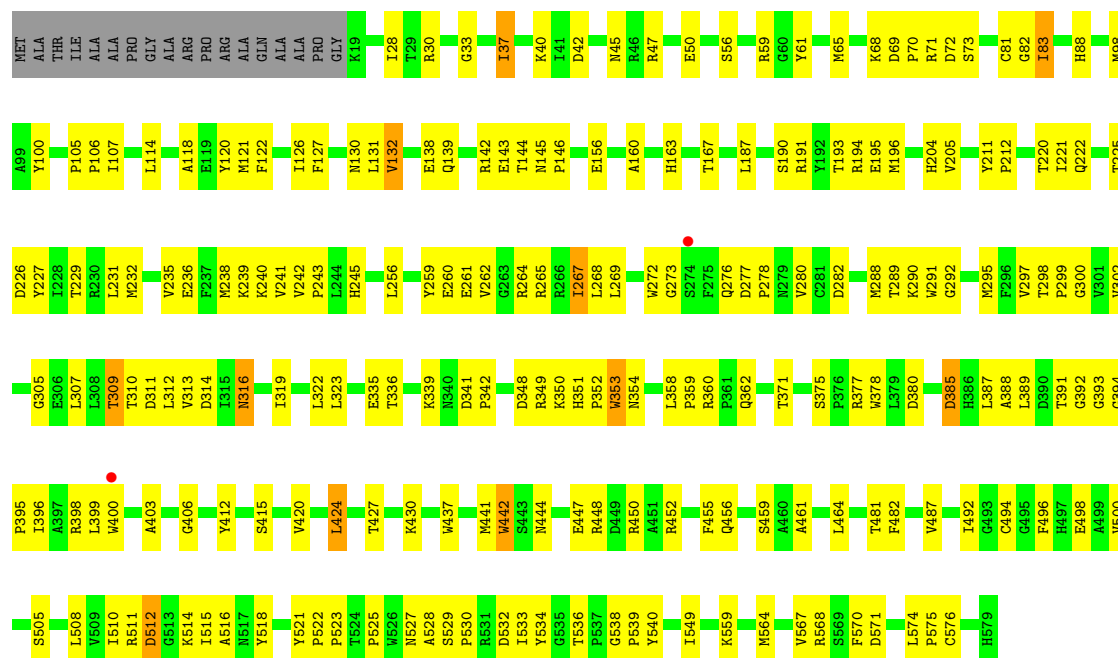
• Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK

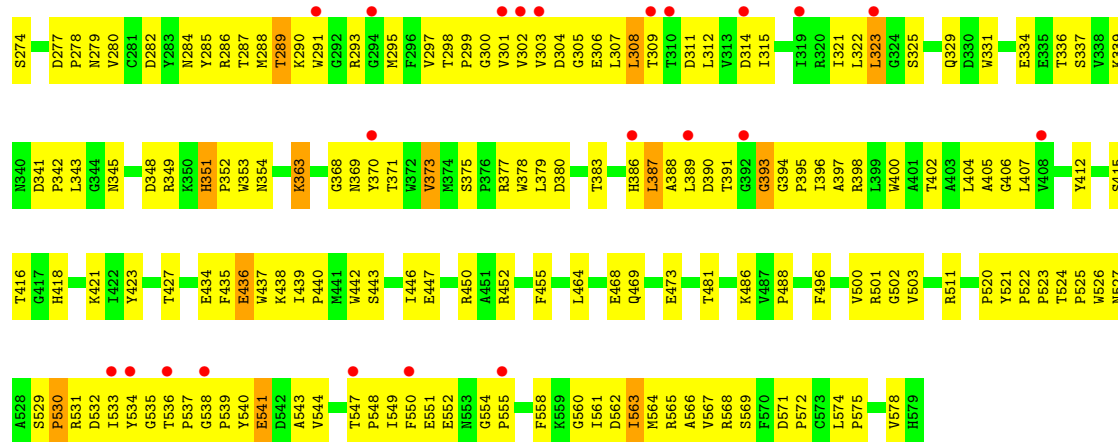




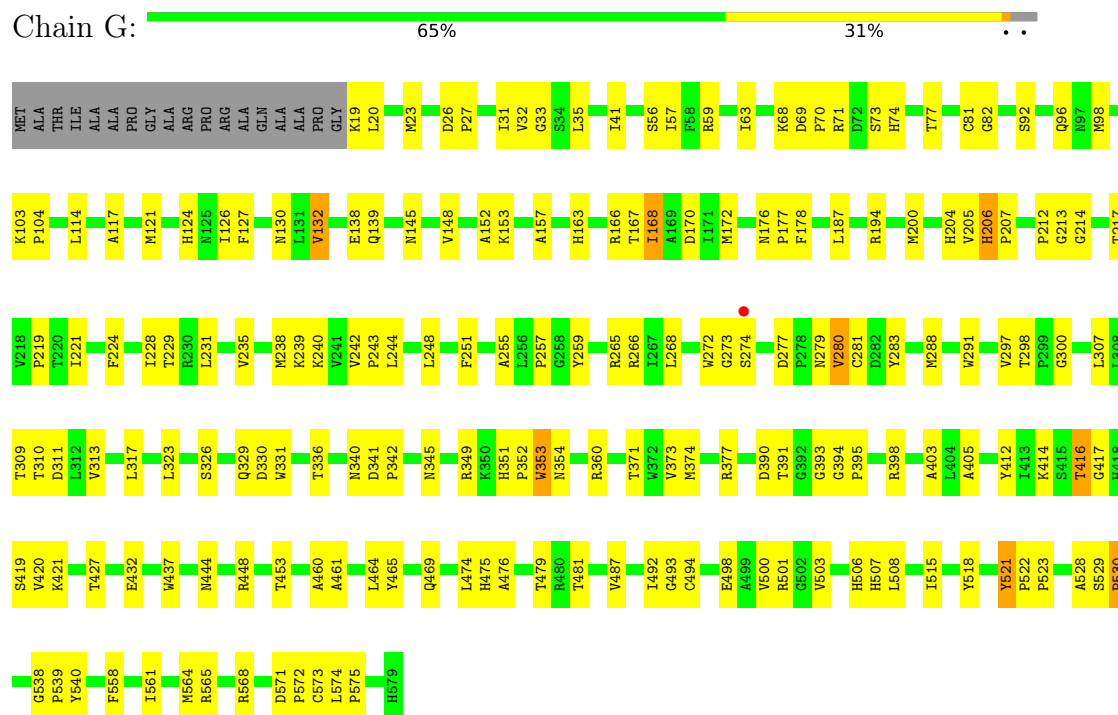
• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG

Chain C: 60% 35%



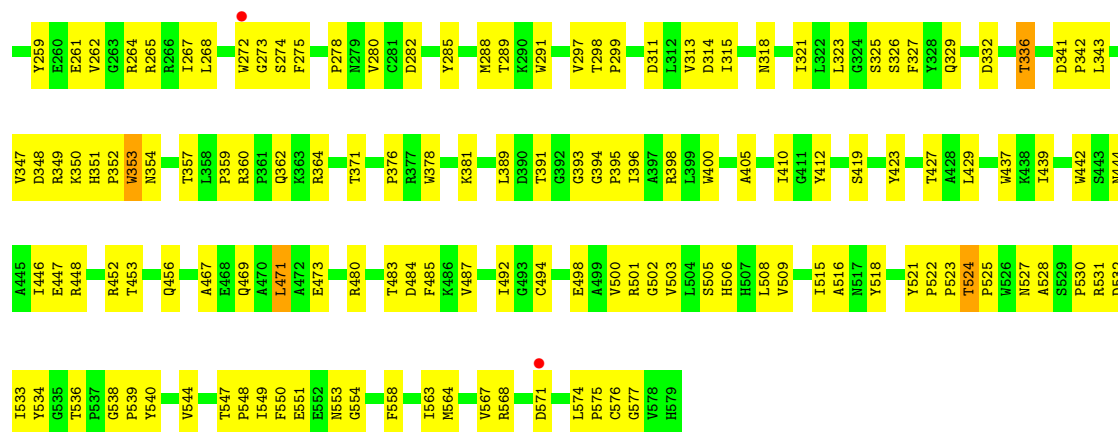


• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG

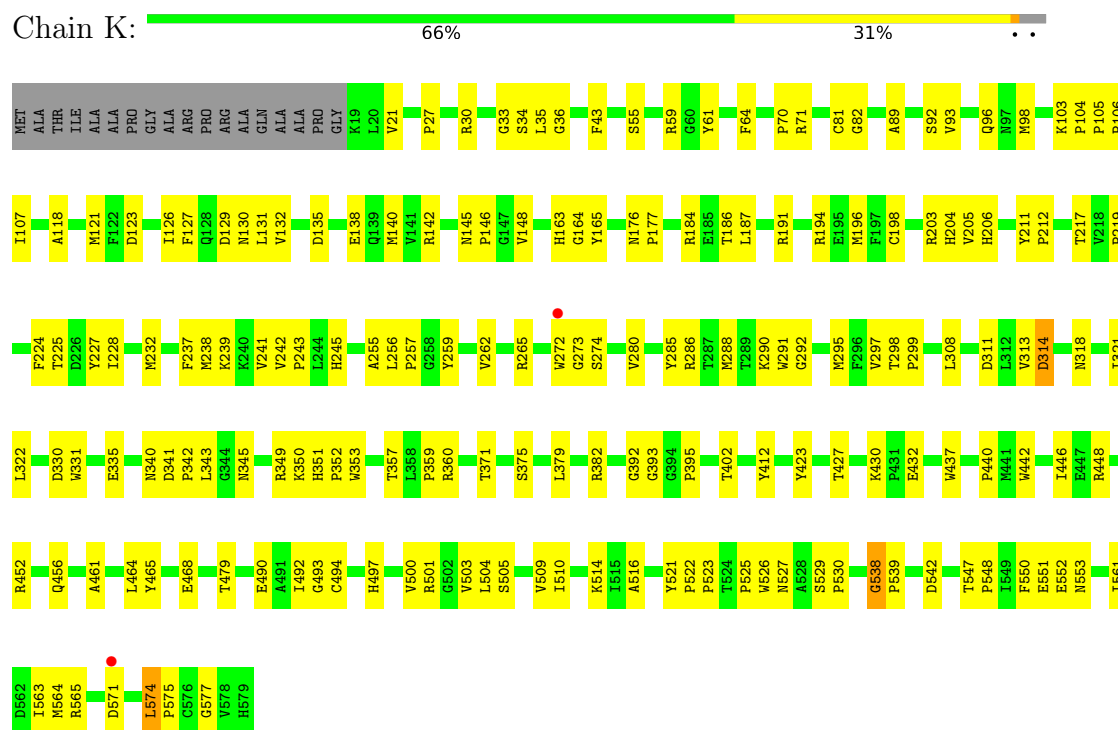


• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG





● Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG



● Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG



N527	A528	S529	P530	G535	T536	P537	G538	P539	Y540	E541	D542	A543	V544	G545	N546	T547	P548	I549	G554	F558	T563	W564	R565	F570	D571	L574	P575	C576	G577	V578	H579																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.78Å 267.97Å 144.69Å 90.00° 106.58° 90.00°	Depositor
Resolution (Å)	45.97 – 2.50 45.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.97-2.50) 97.4 (45.97-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.187 , 0.242 0.201 , 0.250	Depositor DCC
R_{free} test set	10023 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	42867	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: SF4, MLA, NI, FCO

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	0.35	0/2694	0.78	0/3683
1	B	0.37	0/2694	0.84	3/3683 (0.1%)
1	D	0.38	0/2694	0.85	5/3683 (0.1%)
1	F	0.36	0/2694	0.79	0/3683
1	H	0.37	0/2694	0.82	3/3683 (0.1%)
1	M	0.36	0/2694	0.80	2/3683 (0.1%)
2	C	0.35	0/4629	0.79	6/6296 (0.1%)
2	E	0.34	0/4612	0.80	7/6274 (0.1%)
2	G	0.37	0/4629	0.81	7/6296 (0.1%)
2	I	0.33	0/4620	0.78	6/6285 (0.1%)
2	K	0.35	0/4629	0.80	8/6296 (0.1%)
2	L	0.32	0/4620	0.76	6/6285 (0.1%)
All	All	0.35	0/43903	0.80	53/59830 (0.1%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	521	TYR	CA-C-N	8.85	129.50	120.38
2	G	521	TYR	C-N-CA	8.85	129.50	120.38
2	C	521	TYR	CA-C-N	7.39	127.99	120.38
2	C	521	TYR	C-N-CA	7.39	127.99	120.38
2	E	305	GLY	N-CA-C	-6.94	105.89	114.92

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	2616	0	2571	95	0
1	B	2616	0	2571	119	0
1	D	2616	0	2571	116	0
1	F	2616	0	2571	125	0
1	H	2616	0	2571	128	0
1	M	2616	0	2571	110	0
2	C	4495	0	4337	185	0
2	E	4478	0	4313	307	0
2	G	4495	0	4337	156	0
2	I	4486	0	4324	203	0
2	K	4495	0	4337	159	0
2	L	4486	0	4324	261	0
3	A	24	0	0	1	0
3	B	24	0	0	2	0
3	D	24	0	0	0	0
3	F	24	0	0	1	0
3	H	24	0	0	2	0
3	M	24	0	0	3	0
4	A	21	2	6	0	0
4	D	7	0	2	2	0
4	F	7	0	2	0	0
4	M	7	0	2	1	0
5	C	7	0	0	3	0
5	E	7	0	0	2	0
5	G	7	0	0	1	0
5	I	7	0	0	3	0
5	K	7	0	0	0	0
5	L	7	0	0	2	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
All	All	42865	2	41410	1811	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 21.

The worst 5 of 1811 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:C:392:GLY:HA2	2:C:396:ILE:HG22	1.31	1.11
2:L:39:THR:HG22	2:L:51:CYS:HB2	1.22	1.11
1:M:77:MET:HE1	1:M:113:MET:HG2	1.26	1.09
2:E:262:VAL:HG23	2:E:547:THR:HG23	1.30	1.08
1:A:234:ALA:HB3	1:F:234:ALA:HB3	1.35	1.06

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	343/351 (98%)	323 (94%)	19 (6%)	1 (0%)	36	55
1	B	343/351 (98%)	321 (94%)	21 (6%)	1 (0%)	36	55
1	D	343/351 (98%)	321 (94%)	20 (6%)	2 (1%)	21	38
1	F	343/351 (98%)	316 (92%)	25 (7%)	2 (1%)	21	38
1	H	343/351 (98%)	327 (95%)	14 (4%)	2 (1%)	21	38
1	M	343/351 (98%)	324 (94%)	18 (5%)	1 (0%)	36	55
2	C	559/579 (96%)	528 (94%)	30 (5%)	1 (0%)	43	63
2	E	557/579 (96%)	516 (93%)	37 (7%)	4 (1%)	18	34
2	G	559/579 (96%)	537 (96%)	21 (4%)	1 (0%)	43	63
2	I	558/579 (96%)	520 (93%)	36 (6%)	2 (0%)	30	49
2	K	559/579 (96%)	523 (94%)	36 (6%)	0	100	100
2	L	558/579 (96%)	516 (92%)	40 (7%)	2 (0%)	30	49
All	All	5408/5580 (97%)	5072 (94%)	317 (6%)	19 (0%)	30	49

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	CYS
1	B	278	CYS
1	D	278	CYS
1	F	120	HIS
1	F	278	CYS

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	277/281 (99%)	271 (98%)	6 (2%)	45	73
1	B	277/281 (99%)	271 (98%)	6 (2%)	45	73
1	D	277/281 (99%)	271 (98%)	6 (2%)	45	73
1	F	277/281 (99%)	264 (95%)	13 (5%)	23	47
1	H	277/281 (99%)	267 (96%)	10 (4%)	31	58
1	M	277/281 (99%)	275 (99%)	2 (1%)	76	89
2	C	476/485 (98%)	465 (98%)	11 (2%)	44	72
2	E	474/485 (98%)	451 (95%)	23 (5%)	22	45
2	G	476/485 (98%)	466 (98%)	10 (2%)	47	74
2	I	475/485 (98%)	460 (97%)	15 (3%)	34	62
2	K	476/485 (98%)	468 (98%)	8 (2%)	53	78
2	L	475/485 (98%)	456 (96%)	19 (4%)	28	54
All	All	4514/4596 (98%)	4385 (97%)	129 (3%)	37	65

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	241	VAL
2	L	326	SER
2	E	541	GLU
2	E	464	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	356	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	203	GLN
2	I	546	ASN
1	H	250	ASN
2	I	355	GLN
2	K	362	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 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	$\# Z > 2$
5	FCO	I	580	2	1,6,6	0.33	0	-		
5	FCO	K	580	2	1,6,6	0.23	0	-		
3	SF4	B	502	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	M	704	1	0,12,12	-	-	-		
3	SF4	B	501	1	0,12,12	-	-	-		
3	SF4	F	704	1	0,12,12	-	-	-		
3	SF4	F	703	1	0,12,12	-	-	-		
3	SF4	A	503	1	0,12,12	-	-	-		
4	MLA	D	701	-	6,6,6	1.16	0	7,7,7	0.84	0
5	FCO	C	580	2	1,6,6	1.32	0	-		
4	MLA	A	505	-	6,6,6	1.04	0	7,7,7	1.23	0
5	FCO	E	580	2	1,6,6	0.39	0	-		
3	SF4	H	503	1	0,12,12	-	-	-		
3	SF4	F	702	1	0,12,12	-	-	-		
3	SF4	D	702	1	0,12,12	-	-	-		
4	MLA	A	701	-	6,6,6	1.11	0	7,7,7	1.06	0
3	SF4	D	704	1	0,12,12	-	-	-		
3	SF4	A	502	1	0,12,12	-	-	-		
3	SF4	H	502	1	0,12,12	-	-	-		
4	MLA	F	701	-	6,6,6	1.15	0	7,7,7	0.68	0
4	MLA	M	705	-	6,6,6	1.18	0	7,7,7	0.79	0
5	FCO	G	580	2	1,6,6	0.47	0	-		
3	SF4	H	501	1	0,12,12	-	-	-		
3	SF4	M	703	1	0,12,12	-	-	-		
3	SF4	B	503	1	0,12,12	-	-	-		
3	SF4	D	703	1	0,12,12	-	-	-		
3	SF4	M	702	1	0,12,12	-	-	-		
5	FCO	L	580	2	1,6,6	1.46	0	-		
3	SF4	A	501	1	0,12,12	-	-	-		
4	MLA	A	504	-	6,6,6	1.15	0	7,7,7	0.79	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
3	SF4	B	502	1	-	-	0/6/5/5
3	SF4	M	704	1	-	-	0/6/5/5
3	SF4	B	501	1	-	-	0/6/5/5
3	SF4	F	704	1	-	-	0/6/5/5
3	SF4	F	703	1	-	-	0/6/5/5
3	SF4	A	503	1	-	-	0/6/5/5
4	MLA	D	701	-	-	2/4/4/4	-
4	MLA	A	505	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	H	503	1	-	-	0/6/5/5
3	SF4	F	702	1	-	-	0/6/5/5
4	MLA	F	701	-	-	0/4/4/4	-
4	MLA	A	701	-	-	2/4/4/4	-
4	MLA	M	705	-	-	2/4/4/4	-
3	SF4	A	502	1	-	-	0/6/5/5
3	SF4	D	702	1	-	-	0/6/5/5
3	SF4	D	704	1	-	-	0/6/5/5
3	SF4	H	502	1	-	-	0/6/5/5
3	SF4	H	501	1	-	-	0/6/5/5
3	SF4	M	703	1	-	-	0/6/5/5
3	SF4	B	503	1	-	-	0/6/5/5
3	SF4	D	703	1	-	-	0/6/5/5
3	SF4	M	702	1	-	-	0/6/5/5
3	SF4	A	501	1	-	-	0/6/5/5
4	MLA	A	504	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	705	MLA	O1A-C1-C2-C3
4	A	701	MLA	O1A-C1-C2-C3
4	M	705	MLA	O1B-C1-C2-C3
4	A	701	MLA	O1B-C1-C2-C3
4	A	504	MLA	C1-C2-C3-O3B

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	580	FCO	3	0
3	B	502	SF4	1	0
3	M	704	SF4	1	0
3	B	501	SF4	1	0
3	F	703	SF4	1	0
4	D	701	MLA	2	0
5	C	580	FCO	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	580	FCO	2	0
3	H	503	SF4	1	0
4	M	705	MLA	1	0
5	G	580	FCO	1	0
3	H	501	SF4	1	0
3	M	702	SF4	2	0
5	L	580	FCO	2	0
3	A	501	SF4	1	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 ⓘ

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	345/351 (98%)	-0.44	4 (1%) 76 73	14, 31, 67, 122	0
1	B	345/351 (98%)	-0.30	1 (0%) 90 87	16, 35, 73, 101	0
1	D	345/351 (98%)	-0.29	5 (1%) 73 70	16, 38, 77, 148	0
1	F	345/351 (98%)	-0.20	5 (1%) 73 70	19, 41, 77, 124	0
1	H	345/351 (98%)	-0.33	4 (1%) 76 73	18, 34, 77, 107	0
1	M	345/351 (98%)	-0.29	3 (0%) 81 78	19, 38, 73, 115	0
2	C	561/579 (96%)	-0.34	2 (0%) 88 86	23, 42, 63, 87	0
2	E	559/579 (96%)	0.38	34 (6%) 27 23	20, 61, 94, 141	0
2	G	561/579 (96%)	-0.53	1 (0%) 91 89	15, 32, 54, 78	0
2	I	560/579 (96%)	-0.13	2 (0%) 88 86	22, 49, 78, 112	0
2	K	561/579 (96%)	-0.28	2 (0%) 88 86	19, 43, 65, 90	0
2	L	560/579 (96%)	0.18	7 (1%) 75 71	21, 64, 92, 123	0
All	All	5432/5580 (97%)	-0.19	70 (1%) 75 71	14, 42, 80, 148	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	314	ILE	4.8
2	E	310	THR	4.0
2	C	274	SER	3.8
2	E	52	TYR	3.8
1	M	313	LEU	3.7

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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
4	MLA	A	505	7/7	0.78	0.16	53,56,66,66	0
4	MLA	A	701	7/7	0.90	0.11	44,50,56,57	0
6	NI	C	581	1/1	0.90	0.13	62,62,62,62	0
4	MLA	F	701	7/7	0.91	0.09	35,36,39,41	0
6	NI	K	581	1/1	0.91	0.13	57,57,57,57	0
4	MLA	A	504	7/7	0.92	0.08	45,47,49,50	0
4	MLA	M	705	7/7	0.92	0.08	37,38,41,42	0
6	NI	I	581	1/1	0.94	0.11	59,59,59,59	0
3	SF4	B	501	8/8	0.94	0.09	28,37,63,88	0
6	NI	G	581	1/1	0.95	0.10	32,32,32,32	0
4	MLA	D	701	7/7	0.95	0.07	32,34,36,37	0
6	NI	E	581	1/1	0.95	0.09	55,55,55,55	0
6	NI	L	581	1/1	0.97	0.08	72,72,72,72	0
3	SF4	F	703	8/8	0.98	0.05	15,20,31,33	0
5	FCO	E	580	7/7	0.98	0.09	40,44,64,65	0
5	FCO	I	580	7/7	0.98	0.09	33,36,52,53	0
5	FCO	L	580	7/7	0.98	0.11	24,47,72,72	0
3	SF4	H	502	8/8	0.98	0.04	17,19,24,28	0
3	SF4	A	503	8/8	0.98	0.04	15,19,22,30	0
3	SF4	B	502	8/8	0.98	0.05	14,20,25,25	0
3	SF4	D	702	8/8	0.98	0.05	17,21,23,26	0
3	SF4	D	703	8/8	0.98	0.04	13,17,18,31	0
3	SF4	F	702	8/8	0.98	0.04	17,22,25,28	0
3	SF4	A	501	8/8	0.99	0.03	14,21,30,35	0
5	FCO	C	580	7/7	0.99	0.08	26,33,59,60	0
3	SF4	H	503	8/8	0.99	0.04	17,21,23,24	0
5	FCO	G	580	7/7	0.99	0.09	26,40,50,51	0
3	SF4	M	702	8/8	0.99	0.04	25,28,31,34	0
5	FCO	K	580	7/7	0.99	0.09	32,40,42,48	0
3	SF4	M	703	8/8	0.99	0.06	20,24,33,42	0
3	SF4	M	704	8/8	0.99	0.06	30,33,37,40	0
3	SF4	D	704	8/8	0.99	0.04	19,21,29,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SF4	B	503	8/8	0.99	0.03	12,19,21,24	0
3	SF4	A	502	8/8	0.99	0.04	15,20,27,31	0
3	SF4	F	704	8/8	0.99	0.05	22,24,36,39	0
3	SF4	H	501	8/8	0.99	0.03	24,25,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.