



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1M1Y
Title : Chemical Crosslink of Nitrogenase MoFe Protein and Fe Protein
Authors : Schmid, B.; Einsle, O.; Chiu, H.J.; Willing, A.; Yoshida, M.; Howard, J.B.;
Rees, D.C.
Deposited on : 2002-06-20
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

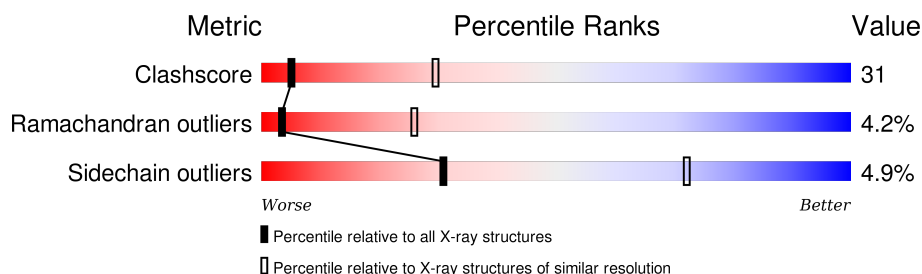
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)




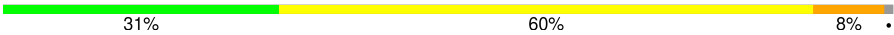

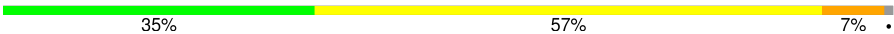
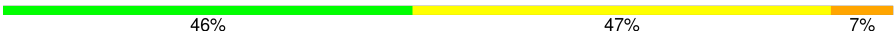
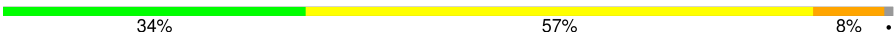
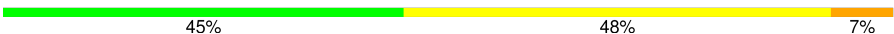
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	
1	C	491	
1	I	491	
1	K	491	
2	B	522	
2	D	522	
2	J	522	

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Mol	Chain	Length	Quality of chain
2	L	522	
3	E	289	
3	F	289	
3	G	289	
3	H	289	
3	M	289	
3	N	289	
3	O	289	
3	P	289	

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
6	CFM	A	6496	-	-	X	-
6	CFM	C	7496	-	-	X	-
7	CLF	A	6498	-	-	X	-
8	SF4	E	290	-	-	X	-
8	SF4	G	1290	-	-	X	-
8	SF4	N	2290	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 49464 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	C	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	I	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	K	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	J	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	L	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called nitrogenase IRON protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	F	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			
3	G	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	H	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			

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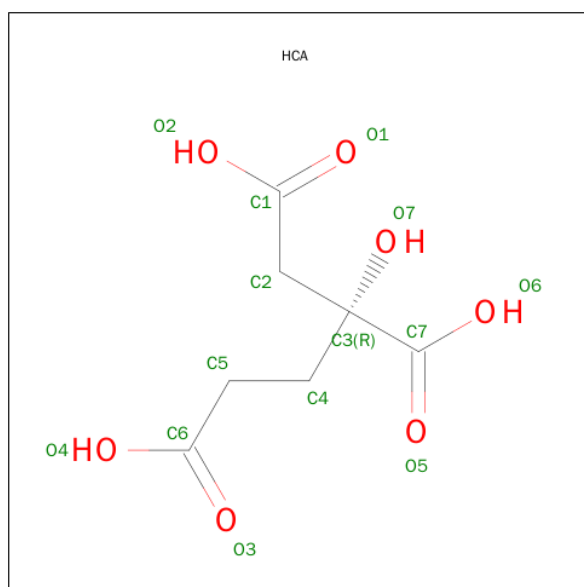
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	N	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			
3	O	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	P	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



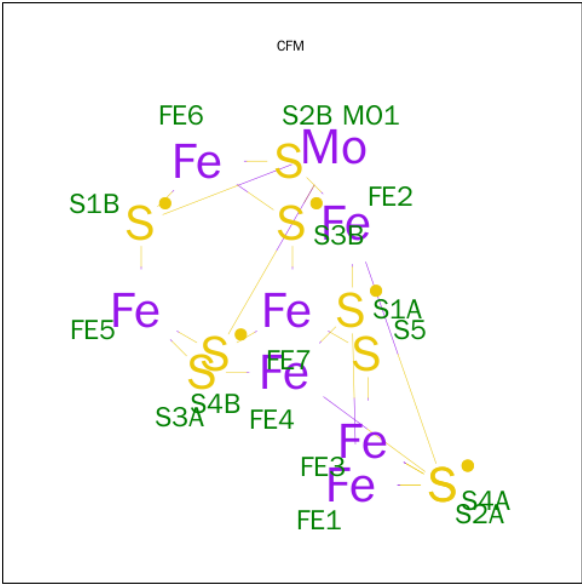
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	7	7		

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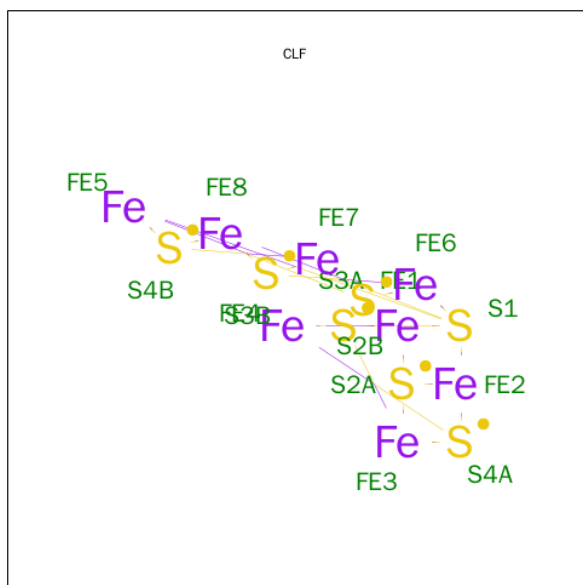
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			14	7	7		
5	I	1	Total	C	O	0	0
			14	7	7		
5	K	1	Total	C	O	0	0
			14	7	7		

- Molecule 6 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe₇MoS₉).



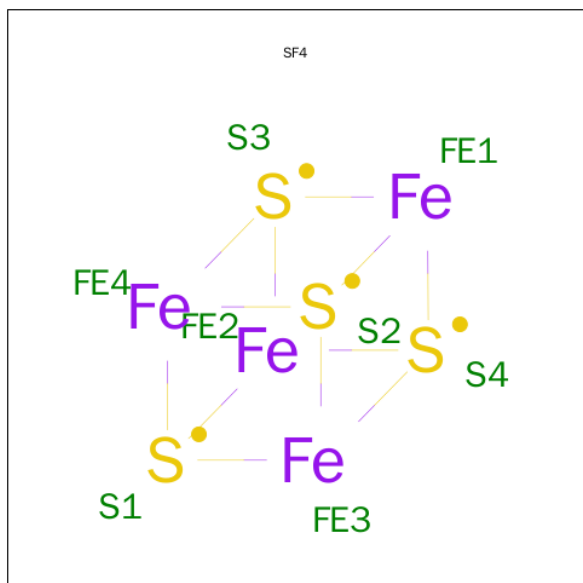
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
6	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
6	I	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
6	K	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 7 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			15	8	7		
7	D	1	Total	Fe	S	0	0
			15	8	7		
7	J	1	Total	Fe	S	0	0
			15	8	7		
7	K	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



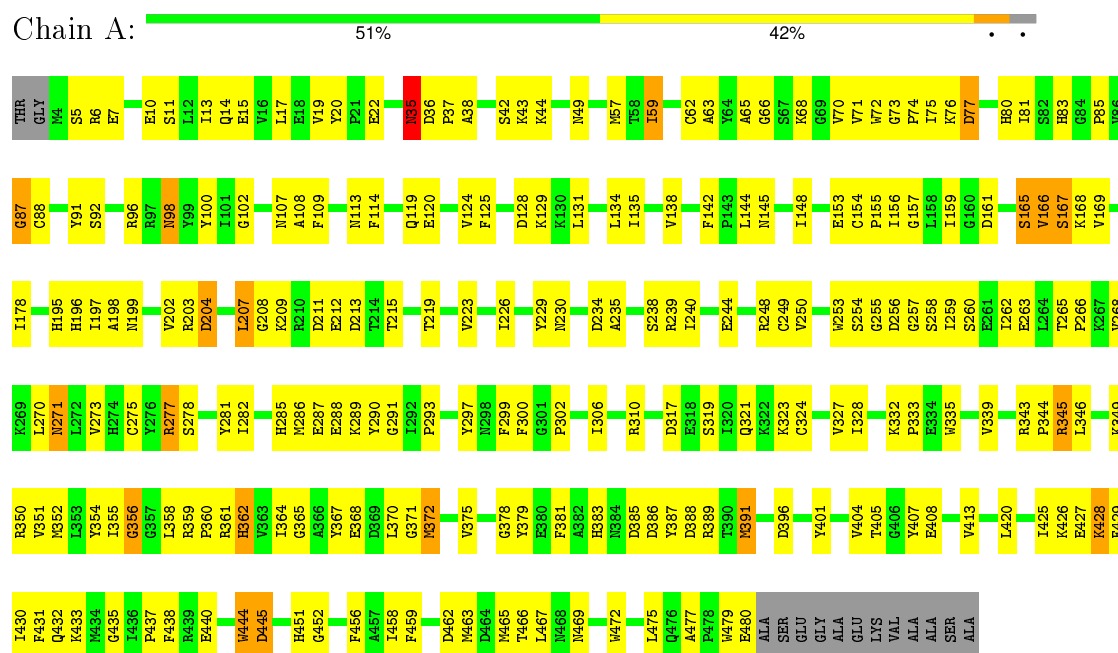
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total 8	Fe 4	S 4	0	0
8	G	1	Total 8	Fe 4	S 4	0	0
8	N	1	Total 8	Fe 4	S 4	0	0
8	P	1	Total 8	Fe 4	S 4	0	0

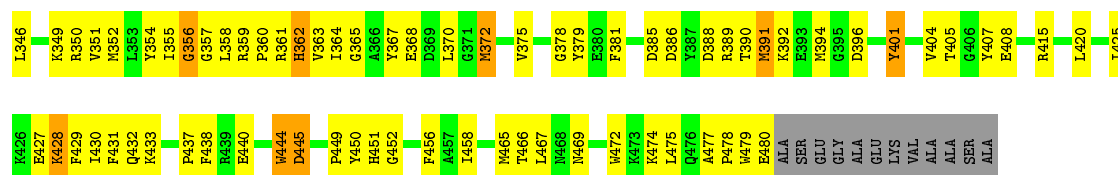
3 Residue-property plots

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

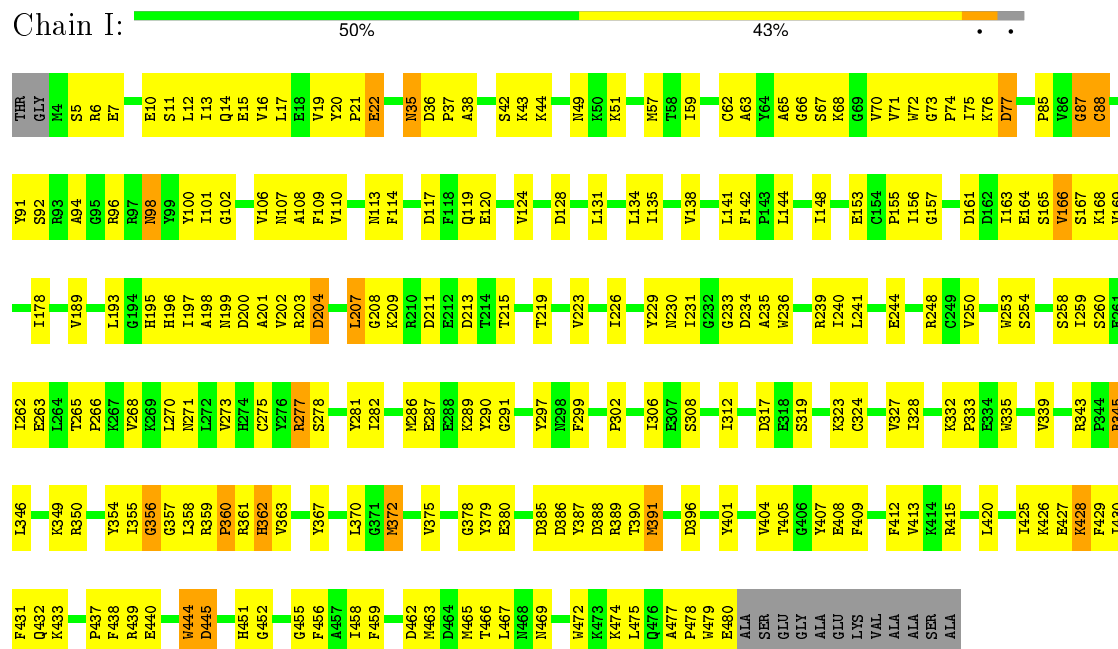
Note EDS was not executed.

- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

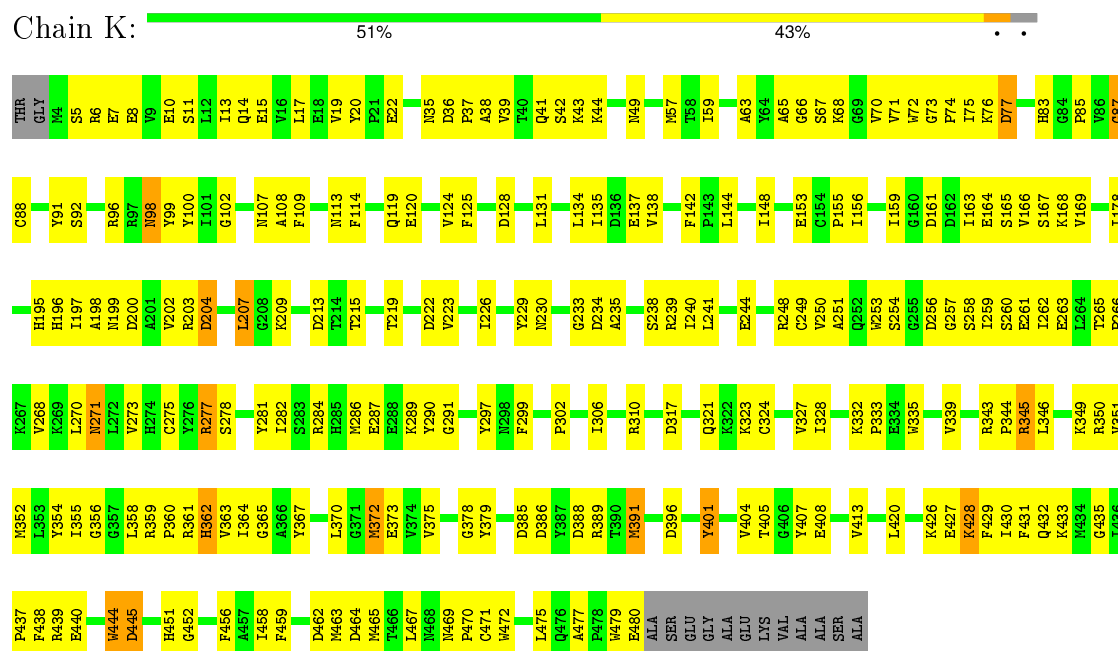




• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

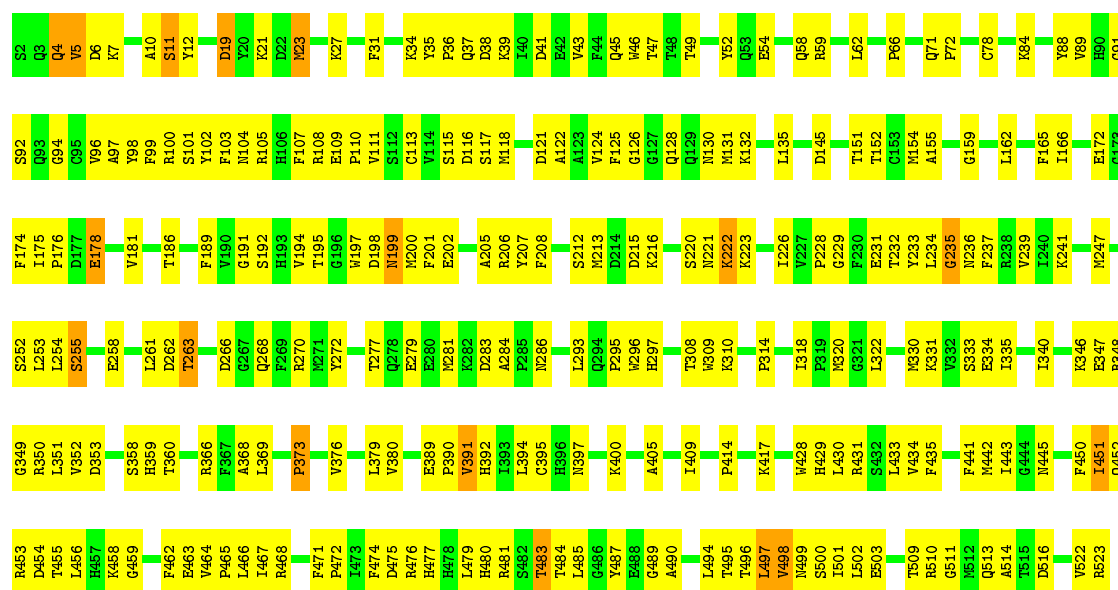


• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



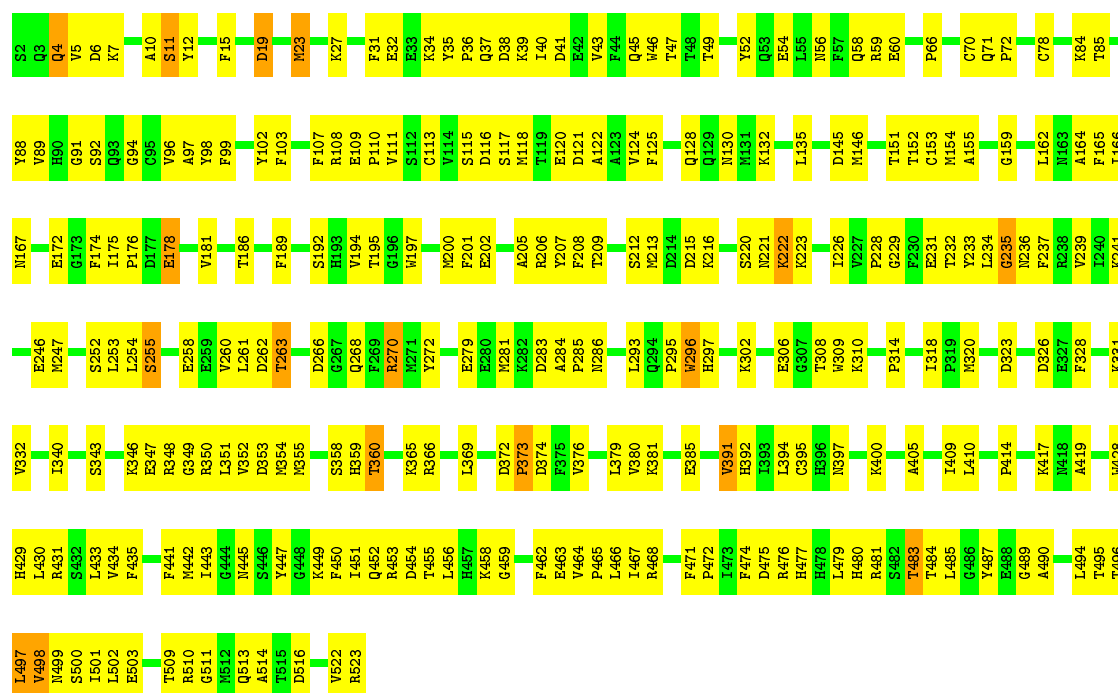
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B:  53% 44%



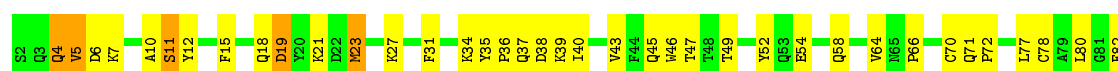
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

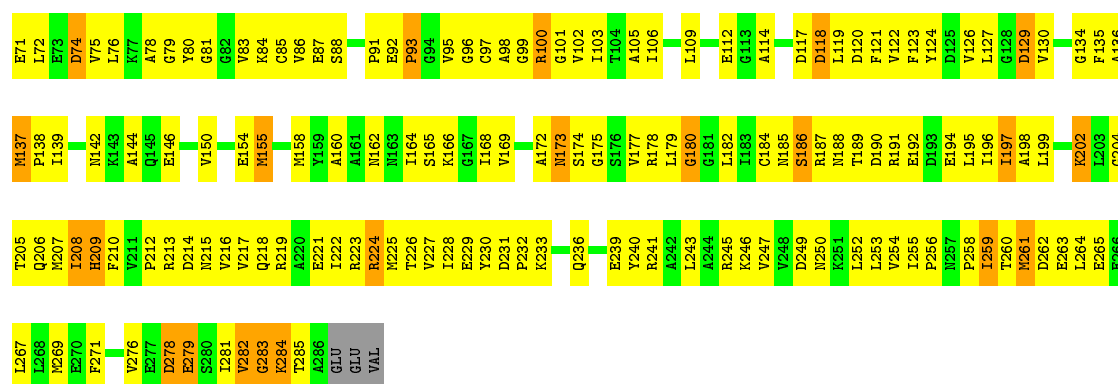
Chain D:  50% 47%



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

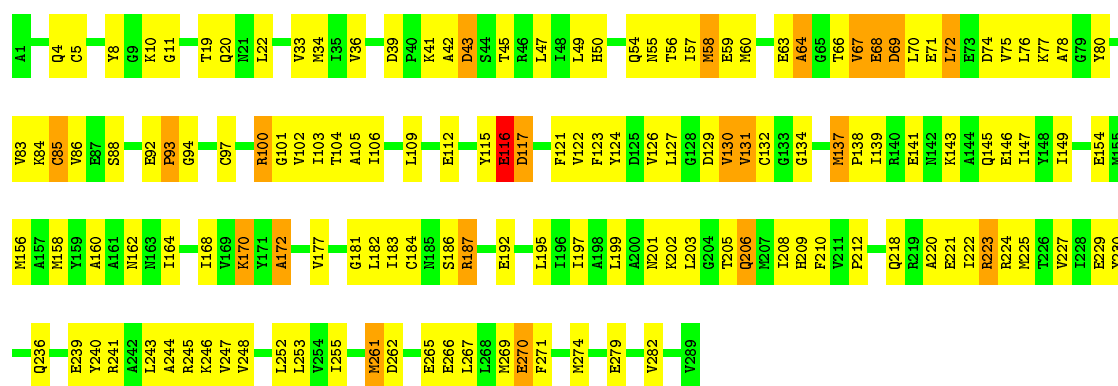
Chain J:  49% 47%





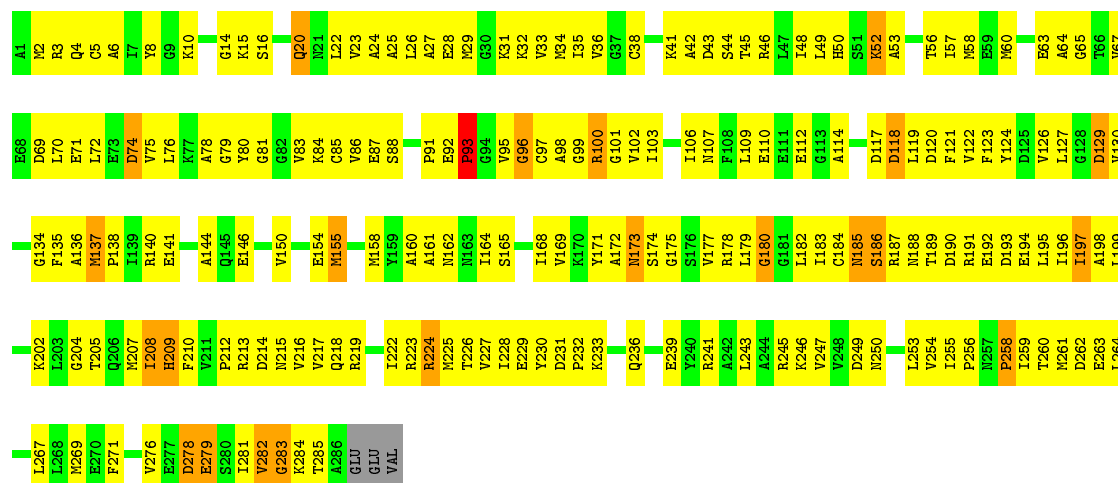
• Molecule 3: nitrogenase IRON protein 1

Chain F: 50% 43% 7%



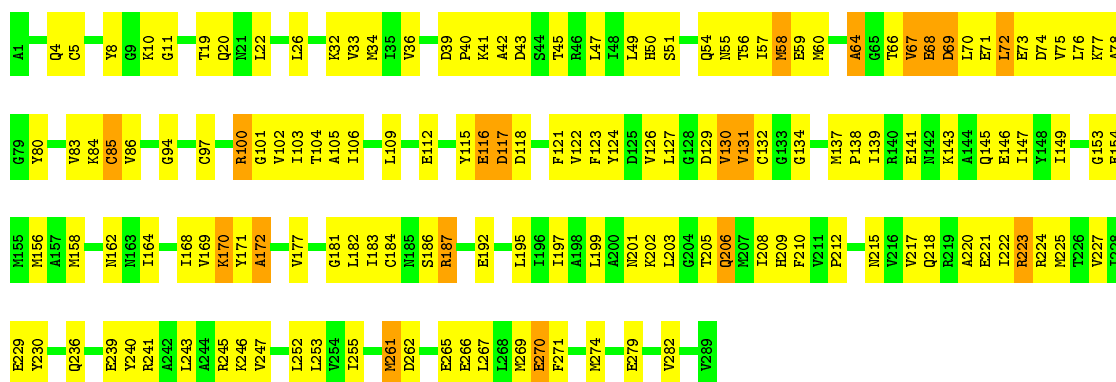
• Molecule 3: nitrogenase IRON protein 1

Chain G: 31% 60% 8%



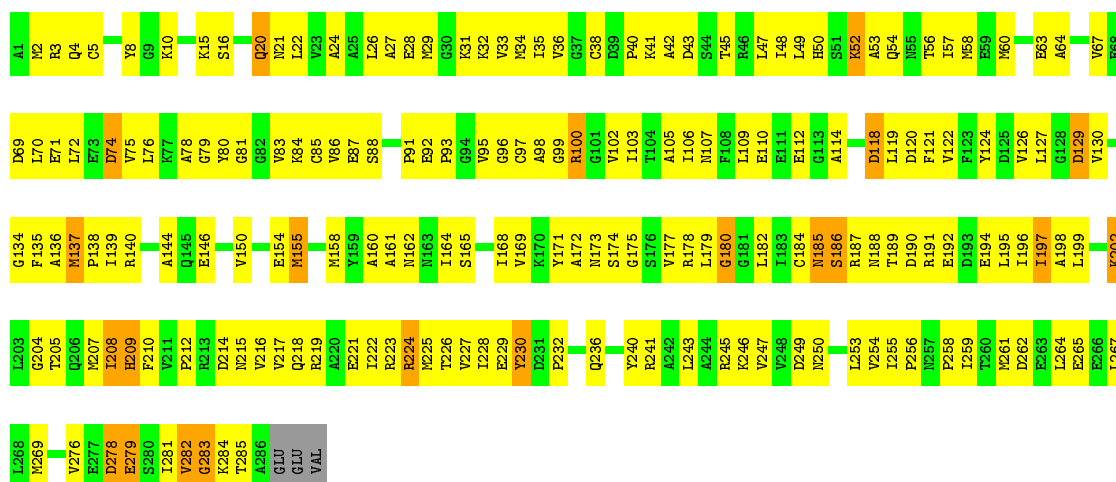
• Molecule 3: nitrogenase IRON protein 1

Chain H: 48% 45% 7%



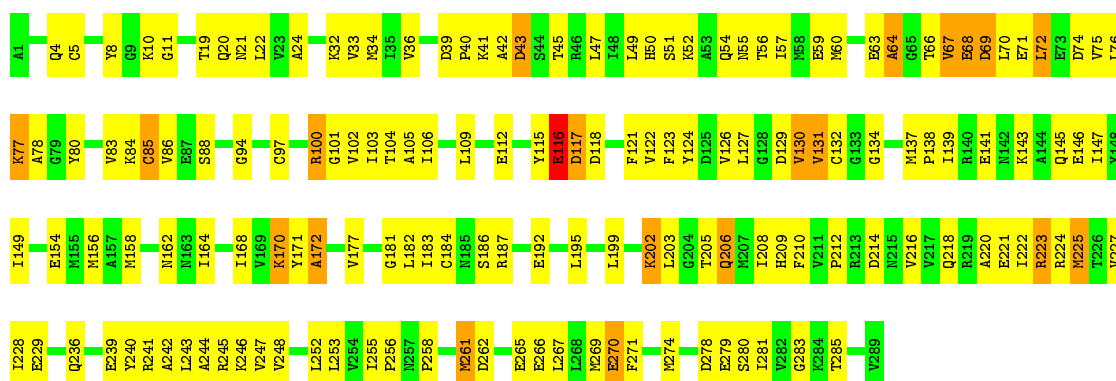
• Molecule 3: nitrogenase IRON protein 1

Chain M: 35% 57% 7% .



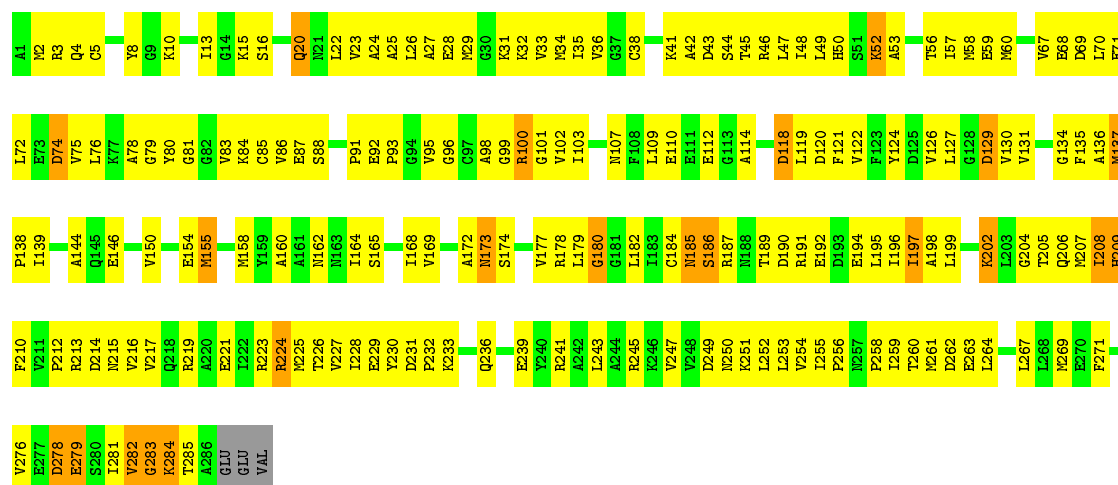
• Molecule 3: nitrogenase IRON protein 1

Chain N: 46% 47% 7%



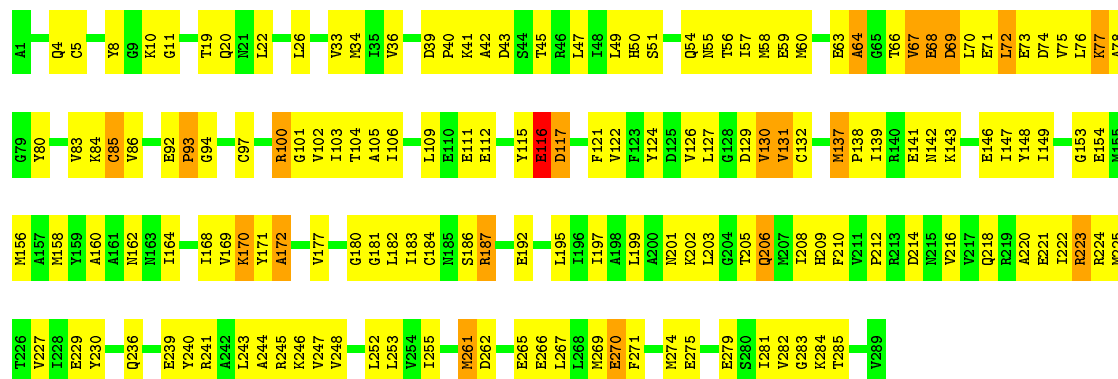
• Molecule 3: nitrogenase IRON protein 1

Chain O: 34% 57% 8% .



• Molecule 3: nitrogenase IRON protein 1

Chain P: 45% 48% 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.27Å 214.94Å 320.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	4.1 (50.00-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49464	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, HCA, CLF, CA, CFM

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	0.49	0/3878	0.68	0/5229
1	C	0.43	0/3878	0.65	0/5229
1	I	0.43	0/3878	0.66	0/5229
1	K	0.41	0/3878	0.65	0/5229
2	B	0.53	0/4280	0.68	0/5786
2	D	0.49	0/4280	0.67	0/5786
2	J	0.46	0/4280	0.67	1/5786 (0.0%)
2	L	0.49	0/4280	0.67	0/5786
3	E	0.42	0/2185	0.61	0/2943
3	F	0.45	0/2210	0.62	0/2975
3	G	0.43	0/2185	0.61	0/2943
3	H	0.42	0/2210	0.62	0/2975
3	M	0.47	0/2185	0.62	0/2943
3	N	0.46	0/2210	0.62	0/2975
3	O	0.42	0/2185	0.63	0/2943
3	P	0.44	0/2210	0.63	0/2975
All	All	0.46	0/50212	0.65	1/67732 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	368	ALA	N-CA-C	-5.13	97.16	111.00

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	3790	0	3732	214	0
1	C	3790	0	3732	217	0
1	I	3790	0	3731	216	0
1	K	3790	0	3730	194	0
2	B	4174	0	4088	238	0
2	D	4174	0	4088	243	0
2	J	4174	0	4089	245	0
2	L	4174	0	4089	246	0
3	E	2161	0	2176	195	0
3	F	2186	0	2197	153	0
3	G	2161	0	2176	194	0
3	H	2186	0	2197	155	0
3	M	2161	0	2176	198	0
3	N	2186	0	2197	171	0
3	O	2161	0	2176	195	0
3	P	2186	0	2197	174	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	14	0	6	1	0
5	C	14	0	6	1	0
5	I	14	0	6	1	0
5	K	14	0	6	1	0
6	A	17	0	0	7	0
6	C	17	0	0	5	0
6	I	17	0	0	3	0
6	K	17	0	0	3	0
7	A	15	0	0	4	0
7	D	15	0	0	3	0
7	J	15	0	0	3	0
7	K	15	0	0	3	0
8	E	8	0	0	2	0
8	G	8	0	0	2	0
8	N	8	0	0	5	0
8	P	8	0	0	0	0
All	All	49464	0	48795	3018	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 31.

The worst 5 of 3018 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:B:400:LYS:NZ	3:F:112:GLU:CD	1.81	1.34
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.32	1.11
2:B:400:LYS:HZ3	3:F:112:GLU:CD	1.43	1.09
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.35	1.08
2:L:96:VAL:HG21	2:L:115:SER:HB2	1.34	1.08

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	475/491 (97%)	364 (77%)	96 (20%)	15 (3%)	5	33
1	C	475/491 (97%)	358 (75%)	102 (22%)	15 (3%)	5	33
1	I	475/491 (97%)	357 (75%)	104 (22%)	14 (3%)	6	36
1	K	475/491 (97%)	364 (77%)	99 (21%)	12 (2%)	7	41
2	B	520/522 (100%)	423 (81%)	74 (14%)	23 (4%)	3	24
2	D	520/522 (100%)	417 (80%)	82 (16%)	21 (4%)	4	27
2	J	520/522 (100%)	421 (81%)	74 (14%)	25 (5%)	3	22
2	L	520/522 (100%)	423 (81%)	75 (14%)	22 (4%)	3	26
3	E	284/289 (98%)	219 (77%)	50 (18%)	15 (5%)	2	19
3	F	287/289 (99%)	228 (79%)	43 (15%)	16 (6%)	2	18
3	G	284/289 (98%)	221 (78%)	47 (16%)	16 (6%)	2	18
3	H	287/289 (99%)	224 (78%)	50 (17%)	13 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	284/289 (98%)	223 (78%)	47 (16%)	14 (5%)	3	22
3	N	287/289 (99%)	230 (80%)	44 (15%)	13 (4%)	3	24
3	O	284/289 (98%)	221 (78%)	48 (17%)	15 (5%)	2	19
3	P	287/289 (99%)	228 (79%)	45 (16%)	14 (5%)	3	22
All	All	6264/6364 (98%)	4921 (79%)	1080 (17%)	263 (4%)	3	26

5 of 263 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
2	B	296	TRP
1	C	22	GLU
3	E	118	ASP
3	E	208	ILE

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	407/414 (98%)	390 (96%)	17 (4%)	36	75
1	C	407/414 (98%)	390 (96%)	17 (4%)	36	75
1	I	407/414 (98%)	391 (96%)	16 (4%)	39	78
1	K	407/414 (98%)	392 (96%)	15 (4%)	41	79
2	B	454/454 (100%)	439 (97%)	15 (3%)	45	81
2	D	454/454 (100%)	438 (96%)	16 (4%)	43	80
2	J	454/454 (100%)	438 (96%)	16 (4%)	43	80
2	L	454/454 (100%)	438 (96%)	16 (4%)	43	80
3	E	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	F	233/233 (100%)	216 (93%)	17 (7%)	17	57
3	G	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	H	233/233 (100%)	216 (93%)	17 (7%)	17	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	N	233/233 (100%)	215 (92%)	18 (8%)	16	54
3	O	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	P	233/233 (100%)	216 (93%)	17 (7%)	17	57
All	All	5296/5336 (99%)	5035 (95%)	261 (5%)	31	72

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	74	ASP
1	I	445	ASP
3	O	261	MET
3	H	100	ARG
1	I	49	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	142	ASN
2	J	45	GLN
3	O	188	ASN
3	H	162	ASN
1	I	49	ASN

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

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	HCA	A	6494	6	4,13,13	2.98	2 (50%)	3,18,18	1.71	1 (33%)
6	CFM	A	6496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	A	6498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
5	HCA	C	7494	6	4,13,13	3.22	1 (25%)	3,18,18	2.05	1 (33%)
6	CFM	C	7496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	D	7498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
8	SF4	E	290	3	0,12,12	0.00	-	0,24,24	0.00	-
8	SF4	G	1290	3	0,12,12	0.00	-	0,24,24	0.00	-
5	HCA	I	8494	6	4,13,13	2.43	2 (50%)	3,18,18	1.67	1 (33%)
6	CFM	I	8496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	J	8498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
5	HCA	K	9494	6	4,13,13	3.14	2 (50%)	3,18,18	2.23	1 (33%)
6	CFM	K	9496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	K	9498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
8	SF4	N	2290	3	0,12,12	0.00	-	0,24,24	0.00	-
8	SF4	P	3290	3	0,12,12	0.00	-	0,24,24	0.00	-

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
5	HCA	A	6494	6	-	0/7/17/17	0/0/0/0
6	CFM	A	6496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	A	6498	1,2	-	0/0/132/132	0/12/10/10
5	HCA	C	7494	6	-	0/7/17/17	0/0/0/0
6	CFM	C	7496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	D	7498	1,2	-	0/0/132/132	0/12/10/10
8	SF4	E	290	3	-	0/0/48/48	0/6/5/5
8	SF4	G	1290	3	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HCA	I	8494	6	-	0/7/17/17	0/0/0/0
6	CFM	I	8496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	J	8498	1,2	-	0/0/132/132	0/12/10/10
5	HCA	K	9494	6	-	0/7/17/17	0/0/0/0
6	CFM	K	9496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	K	9498	1,2	-	0/0/132/132	0/12/10/10
8	SF4	N	2290	3	-	0/0/48/48	0/6/5/5
8	SF4	P	3290	3	-	0/0/48/48	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6494	HCA	C2-C3	-3.84	1.48	1.54
5	K	9494	HCA	C2-C3	-2.85	1.50	1.54
5	I	8494	HCA	C2-C3	-2.14	1.51	1.54
5	I	8494	HCA	O7-C3	4.33	1.50	1.43
5	A	6494	HCA	O7-C3	4.36	1.50	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	9494	HCA	C3-C2-C1	-3.75	108.96	114.96
5	C	7494	HCA	C3-C2-C1	-3.53	109.32	114.96
5	I	8494	HCA	C3-C2-C1	-2.87	110.38	114.96
5	A	6494	HCA	C3-C2-C1	-2.84	110.41	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6494	HCA	1	0
6	A	6496	CFM	7	0
7	A	6498	CLF	4	0
5	C	7494	HCA	1	0
6	C	7496	CFM	5	0
7	D	7498	CLF	3	0
8	E	290	SF4	2	0
8	G	1290	SF4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	8494	HCA	1	0
6	I	8496	CFM	3	0
7	J	8498	CLF	3	0
5	K	9494	HCA	1	0
6	K	9496	CFM	3	0
7	K	9498	CLF	3	0
8	N	2290	SF4	5	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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.