



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 06:17 PM EDT

PDB ID : 1G20 / pdb_00001g20
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
Authors : Chiu, H.-J.; Peters, J.W.; Lanzilotta, W.N.; Ryle, M.J.; Seefeldt, L.C.; Howard, J.B.; Rees, D.C.
Deposited on : 2000-10-16
Resolution : 2.20 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

<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

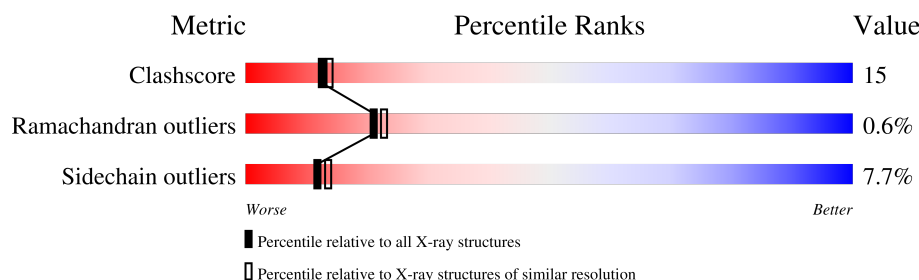
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	492	68% 23% 5% .
1	C	492	65% 28% . .
2	B	523	75% 22% .
2	D	523	72% 24% .
3	E	289	55% 29% 6% 10%
3	F	289	45% 40% . 10%
3	G	289	49% 35% 5% 11%
3	H	289	49% 36% 5% 9%

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
5	CFM	A	1496	-	-	X	-
5	CFM	C	3496	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24903 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	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			
1	C	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			

- 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			

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	259	Total	C	N	O	S	3	0	0
			1953	1227	330	376	20			
3	F	260	Total	C	N	O	S	0	0	0
			1952	1226	327	379	20			
3	G	257	Total	C	N	O	S	5	0	0
			1938	1219	327	372	20			
3	H	262	Total	C	N	O	S	3	0	0
			1984	1244	337	383	20			

There are 4 discrepancies between the modelled and reference sequences:

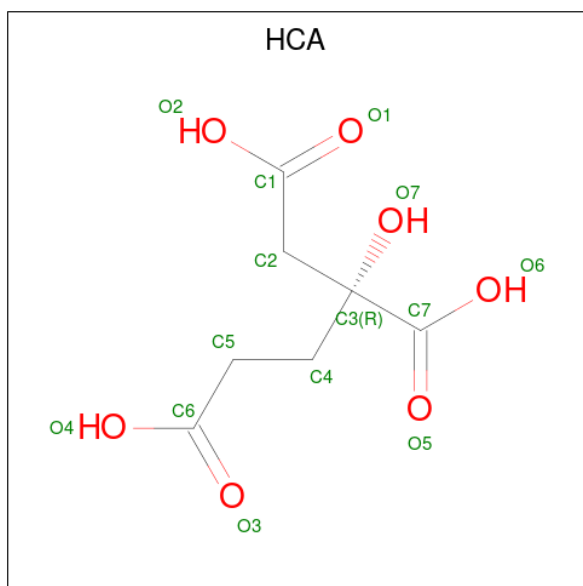
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP P00459
F	?	-	LEU	deletion	UNP P00459
G	?	-	LEU	deletion	UNP P00459

Continued on next page...

Continued from previous page...

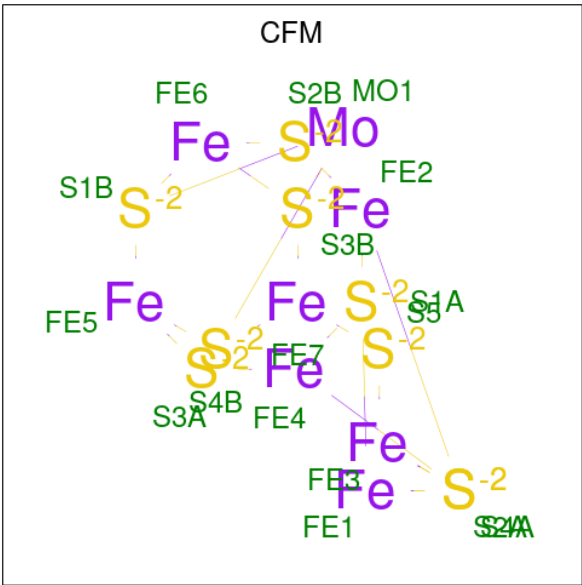
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P00459

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



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

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).

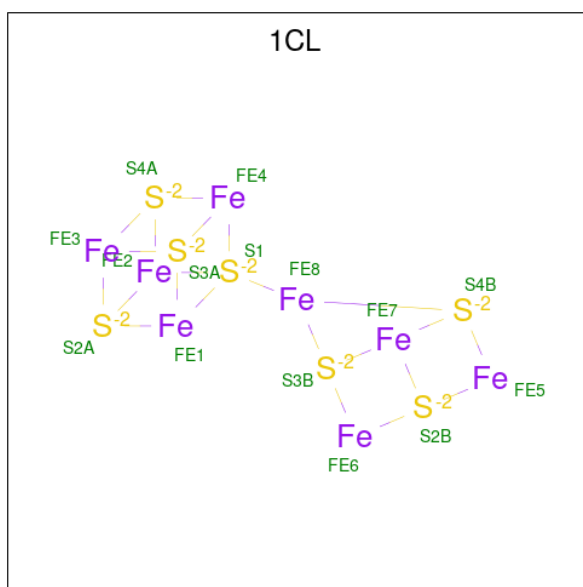


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

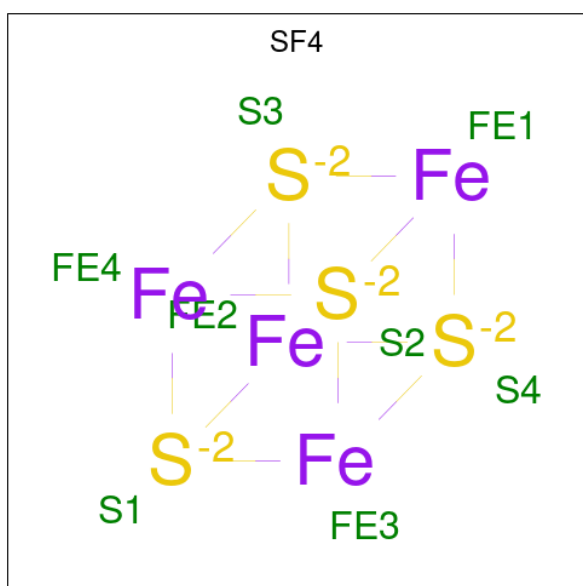
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FE(8)-S(7) CLUSTER, OXIDIZED (CCD ID: 1CL) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			15	8	7		
7	D	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	211	Total 211	O 211	0	0
9	B	309	Total 309	O 309	0	0
9	C	104	Total 104	O 104	0	0
9	D	235	Total 235	O 235	0	0
9	E	56	Total 56	O 56	0	0
9	F	62	Total 62	O 62	0	0
9	G	37	Total 37	O 37	0	0
9	H	52	Total 52	O 52	0	0

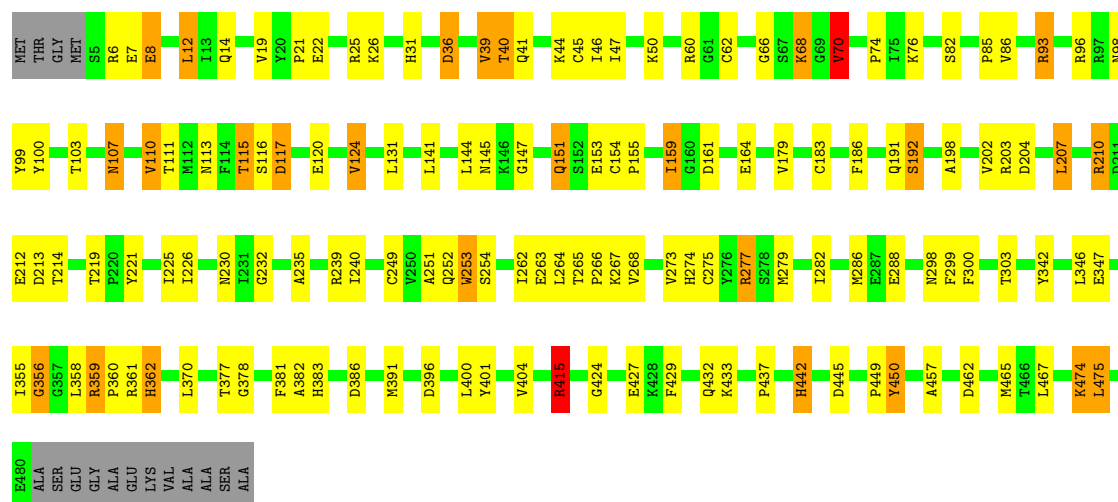
3 Residue-property plots

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. 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. 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.

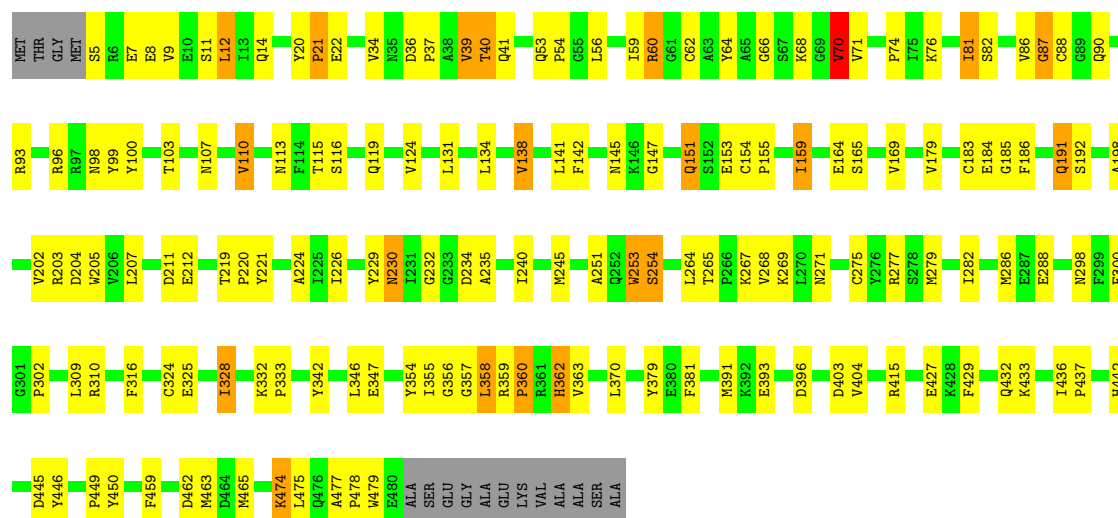
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

Chain A: 



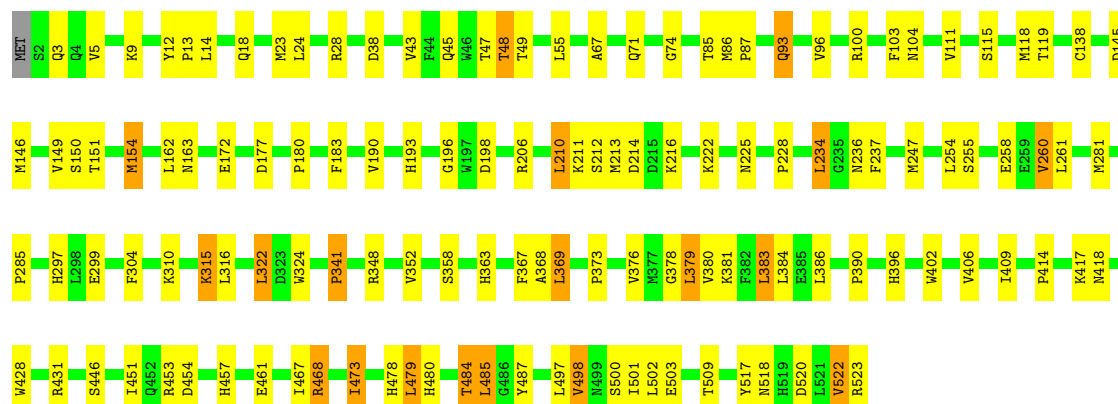
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

Chain C: 



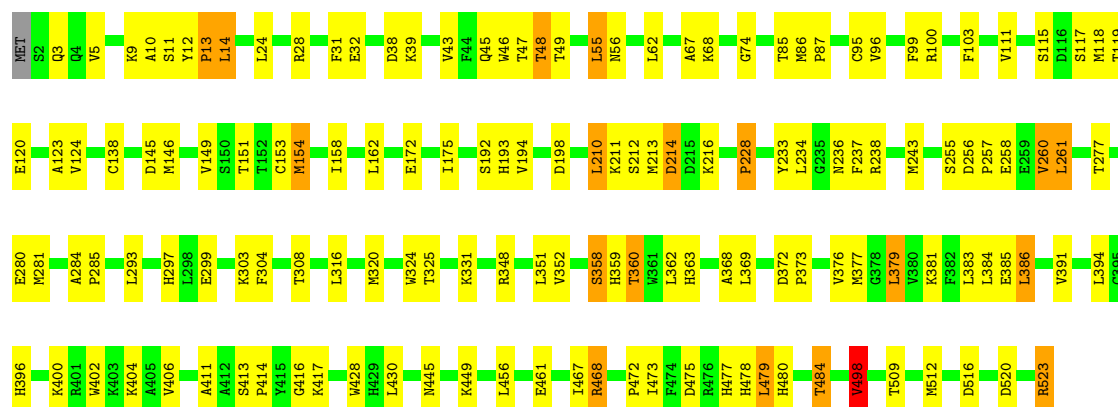
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain B:  75% 22%



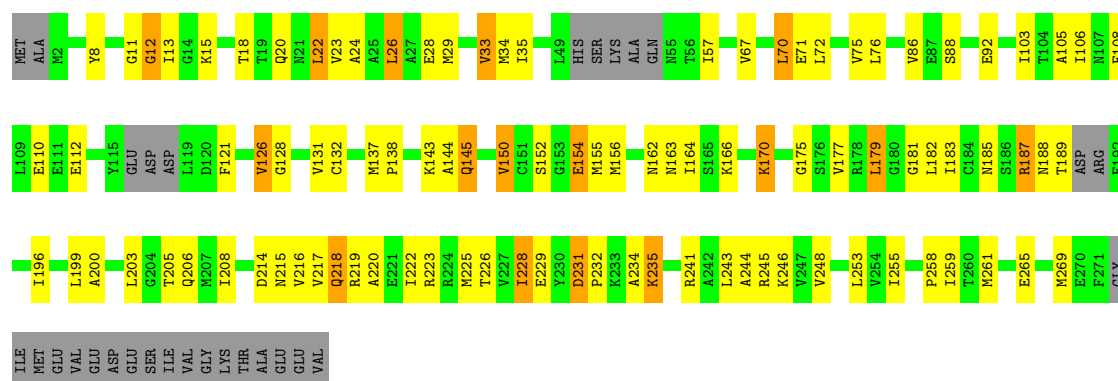
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain D:  72% 24%



• Molecule 3: NITROGENASE IRON PROTEIN

Chain E:  55% 29% 6% 10%



• Molecule 3: NITROGENASE IRON PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.24Å 111.46Å 121.59Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	89.1 (20.00-2.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24903	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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: 1CL, CA, HCA, SF4, 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	0.58	0/3864	1.25	42/5212 (0.8%)
1	C	0.58	0/3864	1.27	43/5212 (0.8%)
2	B	0.58	0/4280	1.19	35/5786 (0.6%)
2	D	0.53	0/4280	1.16	32/5786 (0.6%)
3	E	0.35	0/1973	0.99	9/2654 (0.3%)
3	F	0.34	0/1973	0.97	10/2655 (0.4%)
3	G	0.38	0/1958	0.98	5/2633 (0.2%)
3	H	0.39	0/2006	1.01	11/2699 (0.4%)
All	All	0.51	0/24198	1.15	187/32637 (0.6%)

There are no bond length outliers.

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	VAL	N-CA-C	12.33	122.42	111.81
1	C	76	LYS	N-CA-C	11.45	123.76	111.28
2	D	213	MET	N-CA-C	11.40	124.82	111.71
1	A	70	VAL	N-CA-C	11.12	120.90	111.90
1	A	76	LYS	N-CA-C	11.02	123.29	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3776	0	3708	89	0
1	C	3776	0	3708	101	0
2	B	4174	0	4087	61	0
2	D	4174	0	4087	80	0
3	E	1953	0	1971	77	0
3	F	1952	0	1958	106	0
3	G	1938	0	1958	121	0
3	H	1984	0	1993	141	0
4	A	14	0	6	3	0
4	C	14	0	6	2	0
5	A	17	0	0	5	0
5	C	17	0	0	6	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	15	0	0	1	0
7	D	15	0	0	1	0
8	E	8	0	0	0	0
8	G	8	0	0	0	0
9	A	211	0	0	6	0
9	B	309	0	0	6	0
9	C	104	0	0	1	0
9	D	235	0	0	6	0
9	E	56	0	0	2	0
9	F	62	0	0	0	0
9	G	37	0	0	0	0
9	H	52	0	0	3	0
All	All	24903	0	23482	722	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 15.

The worst 5 of 722 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)
3:G:231:ASP:OD2	3:G:234:ALA:HB2	1.31	1.25
3:G:129:ASP:CG	3:H:41:LYS:HZ3	1.48	1.21
1:C:253:TRP:CZ3	1:C:282:ILE:HD13	1.78	1.16
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.28	1.14
3:F:23:VAL:HG21	3:F:35:ILE:HD11	1.32	1.04

There are no symmetry-related clashes.

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	474/492 (96%)	443 (94%)	28 (6%)	3 (1%)	21	23
1	C	474/492 (96%)	441 (93%)	29 (6%)	4 (1%)	16	16
2	B	520/523 (99%)	502 (96%)	17 (3%)	1 (0%)	43	51
2	D	520/523 (99%)	507 (98%)	11 (2%)	2 (0%)	30	34
3	E	251/289 (87%)	234 (93%)	16 (6%)	1 (0%)	30	34
3	F	254/289 (88%)	240 (94%)	12 (5%)	2 (1%)	16	16
3	G	249/289 (86%)	231 (93%)	16 (6%)	2 (1%)	16	16
3	H	256/289 (89%)	244 (95%)	10 (4%)	2 (1%)	16	16
All	All	2998/3186 (94%)	2842 (95%)	139 (5%)	17 (1%)	21	23

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	THR
3	F	118	ASP
1	A	40	THR
1	C	396	ASP
3	G	44	SER

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	405/415 (98%)	373 (92%)	32 (8%)	11	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	405/415 (98%)	375 (93%)	30 (7%)	13	14
2	B	454/455 (100%)	419 (92%)	35 (8%)	12	13
2	D	454/455 (100%)	421 (93%)	33 (7%)	13	15
3	E	206/233 (88%)	185 (90%)	21 (10%)	7	7
3	F	205/233 (88%)	186 (91%)	19 (9%)	8	9
3	G	204/233 (88%)	191 (94%)	13 (6%)	16	19
3	H	209/233 (90%)	197 (94%)	12 (6%)	18	23
All	All	2542/2672 (95%)	2347 (92%)	195 (8%)	12	13

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	281	MET
3	E	199	LEU
2	D	383	LEU
3	E	22	LEU
3	E	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	257	ASN
3	G	21	ASN
3	H	162	ASN
1	C	113	ASN
1	C	107	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
4	HCA	A	1494	5	13,13,13	2.63	4 (30%)	15,18,18	3.60	7 (46%)
7	1CL	B	1498	1,2	0,22,22	-	-	-		
7	1CL	D	3498	1,2	0,22,22	-	-	-		
4	HCA	C	3494	5	13,13,13	2.99	5 (38%)	15,18,18	4.24	9 (60%)
8	SF4	G	7290	3	0,12,12	-	-	-		
5	CFM	A	1496	4,1	0,24,24	-	-	-		
8	SF4	E	5290	3	0,12,12	-	-	-		
5	CFM	C	3496	4,1	0,24,24	-	-	-		

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
4	HCA	A	1494	5	-	4/17/17/17	-
7	1CL	B	1498	1,2	-	-	0/10/8/8
7	1CL	D	3498	1,2	-	-	0/10/8/8
4	HCA	C	3494	5	-	5/17/17/17	-
8	SF4	G	7290	3	-	-	0/6/5/5
8	SF4	E	5290	3	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3494	HCA	O5-C7	8.80	1.49	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1494	HCA	O5-C7	7.30	1.45	1.22
4	C	3494	HCA	C3-C7	3.50	1.57	1.53
4	C	3494	HCA	O1-C1	3.37	1.33	1.22
4	A	1494	HCA	O6-C7	-3.35	1.18	1.30

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	HCA	O7-C3-C4	-10.40	92.25	108.88
4	C	3494	HCA	O7-C3-C2	-8.49	90.01	109.38
4	A	1494	HCA	O7-C3-C2	-8.19	90.70	109.38
4	A	1494	HCA	O7-C3-C4	-7.49	96.90	108.88
4	A	1494	HCA	C3-C2-C1	6.10	130.60	113.92

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3494	HCA	C1-C2-C3-C4
4	C	3494	HCA	O7-C3-C4-C5
4	A	1494	HCA	C1-C2-C3-C4
4	A	1494	HCA	C7-C3-C4-C5
4	C	3494	HCA	C7-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1494	HCA	3	0
7	B	1498	1CL	1	0
7	D	3498	1CL	1	0
4	C	3494	HCA	2	0
5	A	1496	CFM	5	0
5	C	3496	CFM	6	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.