



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 02:44 AM EDT

PDB ID : 3K1A  
Title : Insights into substrate binding at FeMo-cofactor in nitrogenase from the structure of an alpha-70Ile MoFe protein variant  
Authors : Peters, J.W.; Sarma, R.; Barney, B.M.; Keable, S.; Seefeldt, L.C.; Dean, D.R.  
Deposited on : 2009-09-26  
Resolution : 2.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

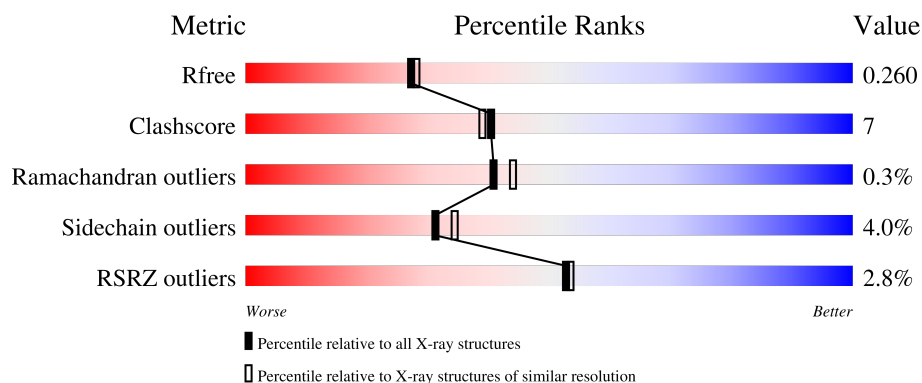
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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  $\geq 3$ , 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	491	 2% 77% 16% • 5%
1	C	491	 4% 77% 16% • 5%
2	B	522	 2% 83% 15% •
2	D	522	 2% 85% 15% •

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16704 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	467	Total	C	N	O	S	0	0	0
			3716	2365	633	694	24			
1	C	468	Total	C	N	O	S	0	0	0
			3714	2365	631	694	24			

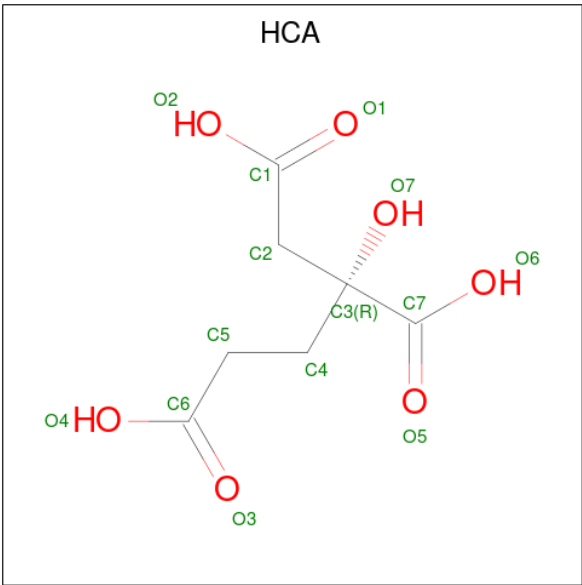
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ILE	VAL	engineered mutation	UNP P07328
C	70	ILE	VAL	engineered mutation	UNP P07328

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

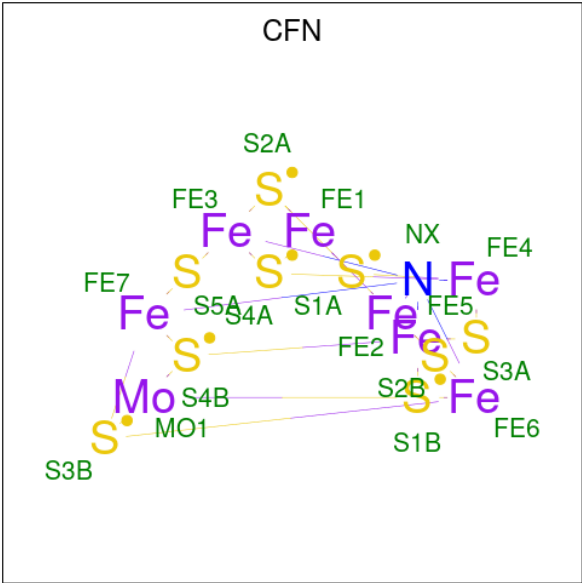
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>7</sub>).



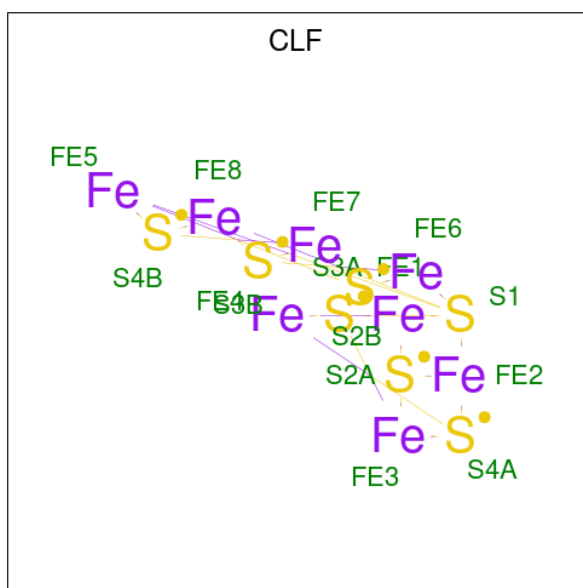
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is FE(7)-MO-S(9)-N CLUSTER (three-letter code: CFN) (formula: Fe<sub>7</sub>MoNS<sub>9</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 18	Fe 7	Mo 1	N 1	S 9	0	0
4	C	1	Total 18	Fe 7	Mo 1	N 1	S 9	0	0

- Molecule 5 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula:  $\text{Fe}_8\text{S}_7$ ).



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

- Molecule 6 is CALCIUM ION (three-letter code: 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		

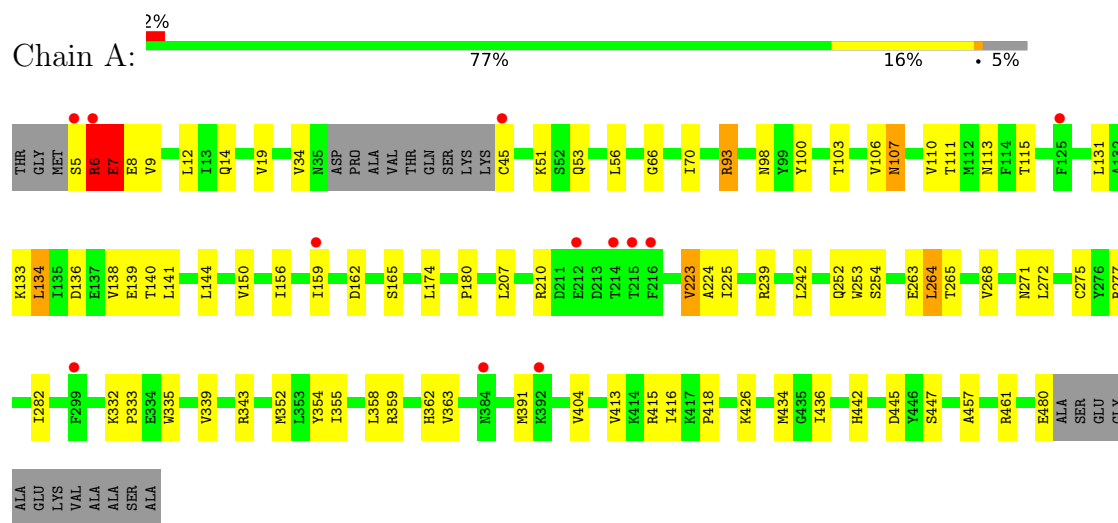
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	166	Total	O	0	0
			166	166		
7	B	255	Total	O	0	0
			255	255		
7	C	175	Total	O	0	0
			175	175		
7	D	234	Total	O	0	0
			234	234		

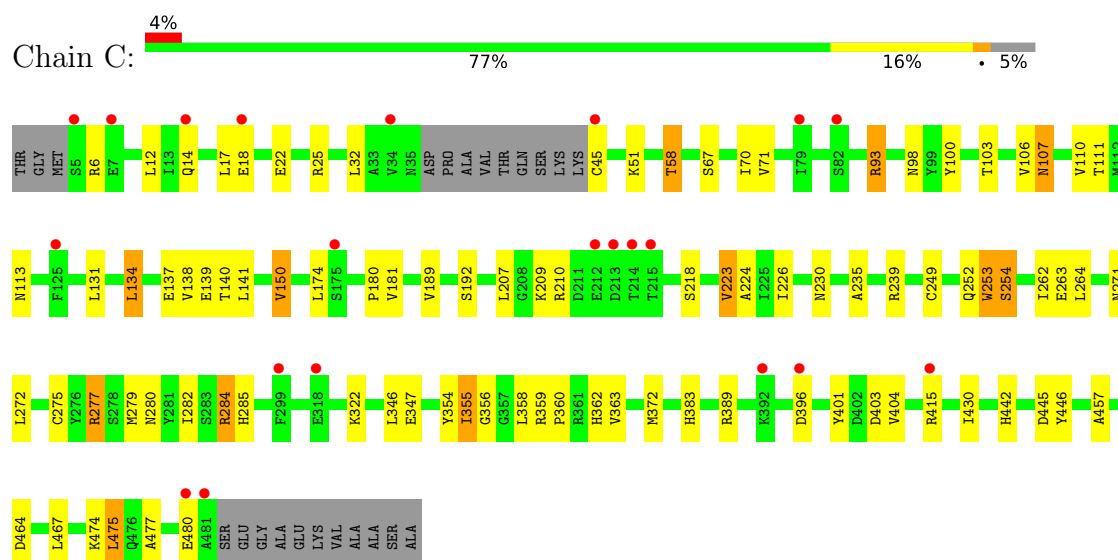
### 3 Residue-property plots [i](#)

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.

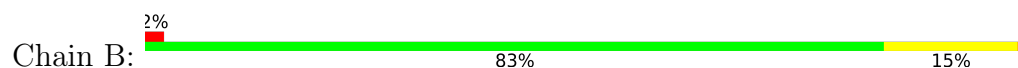
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

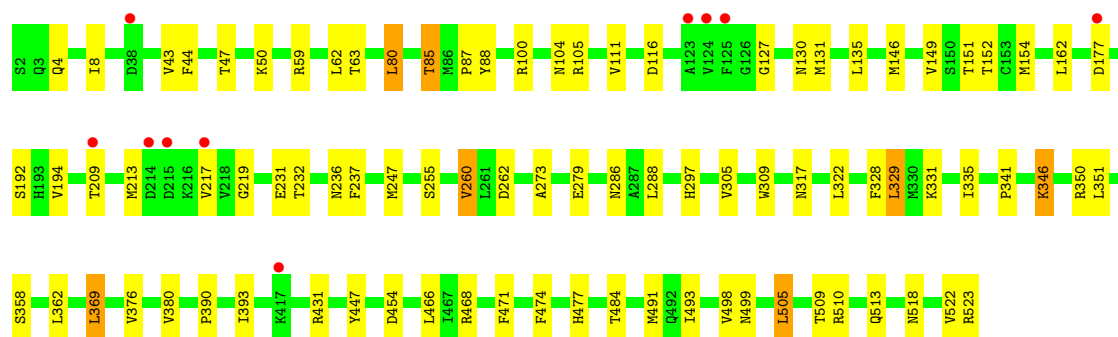


- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

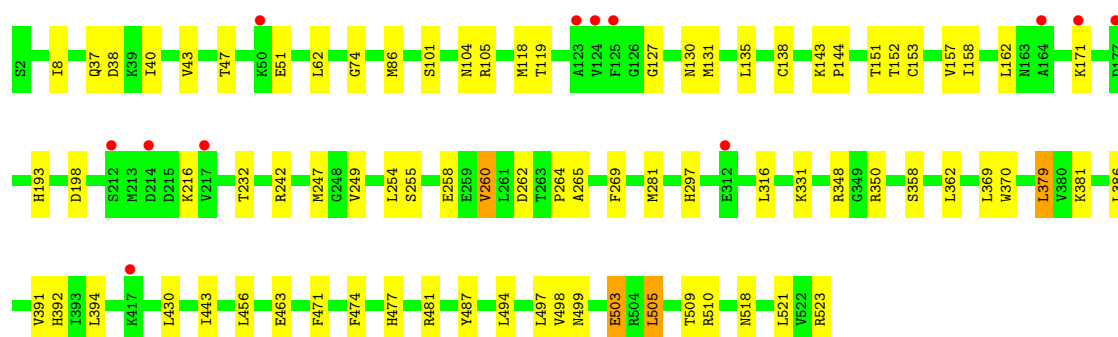
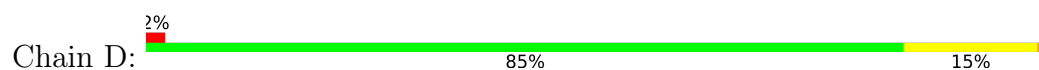


- Molecule 2: Nitrogenase molybdenum-iron protein beta chain





• Molecule 2: Nitrogenase molybdenum-iron protein beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.02Å 129.46Å 107.09Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	50.00 – 2.23 27.15 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.23) 98.5 (27.15-2.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.204 , 0.254 0.209 , 0.260	Depositor DCC
$R_{free}$ test set	4778 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HCA, CLF, CA, CFN

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	0.33	0/3802	0.55	0/5125
1	C	0.34	0/3800	0.56	0/5124
2	B	0.33	0/4280	0.53	0/5786
2	D	0.33	0/4280	0.52	0/5786
All	All	0.33	0/16162	0.54	0/21821

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	SER	Peptide
1	A	6	ARG	Peptide
1	C	253	TRP	Peptide

## 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	3716	0	3650	59	0
1	C	3714	0	3641	60	0
2	B	4174	0	4089	73	0
2	D	4174	0	4089	59	0
3	A	14	0	6	0	0
3	C	14	0	6	0	0
4	A	18	0	0	2	0
4	C	18	0	0	3	0
5	B	15	0	0	1	0
5	D	15	0	0	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	166	0	0	4	0
7	B	255	0	0	11	0
7	C	175	0	0	6	0
7	D	234	0	0	3	0
All	All	16704	0	15481	225	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 7.

All (225) 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:447:TYR:CE1	7:B:779:HOH:O	1.82	1.33
7:B:779:HOH:O	2:D:521:LEU:HD21	1.14	1.25
7:B:779:HOH:O	2:D:521:LEU:CD2	1.81	0.96
2:D:499:ASN:O	2:D:503:GLU:HG3	1.73	0.88
1:C:239:ARG:HE	1:C:252:GLN:HE21	1.19	0.86
1:A:70:ILE:HD13	4:A:6496:CFN:S2B	2.17	0.85
2:D:131:MET:HE2	2:D:135:LEU:HD11	1.58	0.85
1:C:70:ILE:HD13	4:C:7496:CFN:S2B	2.16	0.84
2:D:499:ASN:O	2:D:503:GLU:CG	2.27	0.82
1:C:457:ALA:HB1	2:D:8:ILE:HD12	1.61	0.82
2:B:513:GLN:HE22	2:D:37:GLN:HE22	1.30	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:ASN:HD21	2:D:477:HIS:H	1.29	0.79
1:C:415:ARG:HD2	7:C:692:HOH:O	1.82	0.79
2:B:131:MET:HE2	2:B:135:LEU:HD11	1.66	0.78
2:B:477:HIS:H	2:D:499:ASN:HD21	1.30	0.78
2:B:4:GLN:HG3	7:B:600:HOH:O	1.84	0.77
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.00	0.77
1:A:239:ARG:HE	1:A:252:GLN:HE21	1.31	0.76
1:A:6:ARG:HB3	1:A:7:GLU:HB2	1.67	0.75
2:B:80:LEU:HD13	2:B:87:PRO:HG3	1.67	0.75
2:B:209:THR:HG21	2:B:309:TRP:HE1	1.52	0.74
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.69	0.74
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.28	0.69
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.75	0.68
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.77	0.67
1:A:70:ILE:CD1	4:A:6496:CFN:S2B	2.82	0.67
1:C:239:ARG:HE	1:C:252:GLN:NE2	1.92	0.66
1:C:93:ARG:HG3	1:C:113:ASN:HB2	1.78	0.66
1:A:156:ILE:O	1:A:159:ILE:HG22	1.96	0.64
1:A:45:CYS:N	7:A:828:HOH:O	2.30	0.64
2:B:100:ARG:HD2	2:B:111:VAL:O	1.97	0.64
1:A:457:ALA:HB1	2:B:8:ILE:HD12	1.80	0.64
2:D:509:THR:HG21	2:D:518:ASN:HD22	1.63	0.63
1:A:352:MET:HE1	1:A:416:ILE:HB	1.79	0.62
1:C:51:LYS:HD3	1:C:189:VAL:HG12	1.81	0.62
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.34	0.62
2:B:43:VAL:O	2:B:47:THR:HG23	1.99	0.61
2:B:484:THR:HG22	2:B:493:ILE:HD11	1.83	0.61
2:D:499:ASN:O	2:D:503:GLU:HG2	2.01	0.61
2:D:379:LEU:HD11	2:D:443:ILE:HG21	1.84	0.59
2:B:509:THR:HG21	2:B:518:ASN:HD22	1.66	0.59
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.37	0.59
1:A:66:GLY:HA2	1:A:70:ILE:HD12	1.85	0.59
2:D:316:LEU:HD11	2:D:331:LYS:HG2	1.85	0.59
1:C:70:ILE:CD1	4:C:7496:CFN:S2B	2.91	0.59
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.85	0.59
1:A:103:THR:H	1:A:107:ASN:HD21	1.50	0.58
1:C:224:ALA:HB3	1:C:271:ASN:HD22	1.66	0.58
1:C:210:ARG:HD3	1:C:263:GLU:HB3	1.84	0.58
5:D:7498:CLF:S3A	5:D:7498:CLF:S4B	3.01	0.58
1:C:106:VAL:HG21	2:D:40:ILE:HG23	1.85	0.58
2:B:505:LEU:HD13	2:B:523:ARG:CZ	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD22	1:C:282:ILE:HD11	1.87	0.57
1:C:230:ASN:HD22	1:C:235:ALA:H	1.52	0.56
1:C:51:LYS:HD2	2:D:119:THR:HG21	1.89	0.55
1:A:224:ALA:HB3	1:A:271:ASN:HD22	1.71	0.55
2:D:151:THR:CG2	2:D:162:LEU:HD11	2.37	0.55
1:A:277:ARG:HD3	7:A:582:HOH:O	2.06	0.55
2:B:447:TYR:CD1	7:B:779:HOH:O	2.29	0.55
1:A:93:ARG:HD2	1:A:111:THR:O	2.06	0.55
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.88	0.55
1:C:140:THR:HG23	1:C:141:LEU:HG	1.89	0.54
1:A:150:VAL:HG13	1:A:180:PRO:HA	1.89	0.54
1:C:137:GLU:HA	1:C:140:THR:HG22	1.90	0.54
1:A:134:LEU:HD13	2:B:62:LEU:HD13	1.89	0.54
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.42	0.53
1:C:134:LEU:HD13	2:D:62:LEU:HD13	1.89	0.53
1:C:139:GLU:HG3	1:C:174:LEU:HD13	1.89	0.53
2:D:118:MET:HE1	2:D:158:ILE:HD11	1.89	0.53
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.43	0.53
1:C:359:ARG:O	1:C:363:VAL:HG22	2.08	0.53
2:D:394:LEU:HD13	2:D:430:LEU:HB2	1.91	0.53
1:C:346:LEU:HD21	1:C:464:ASP:HA	1.92	0.52
1:A:207:LEU:HD22	1:A:282:ILE:HD11	1.91	0.52
2:D:260:VAL:HG22	7:D:539:HOH:O	2.10	0.52
2:D:43:VAL:O	2:D:47:THR:HG23	2.09	0.51
1:A:6:ARG:HG2	1:A:7:GLU:H	1.75	0.51
1:C:67:SER:OG	1:C:181:VAL:HG11	2.10	0.51
1:C:106:VAL:HG23	1:C:107:ASN:N	2.25	0.51
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.45	0.51
2:B:358:SER:HB3	2:B:498:VAL:HG21	1.93	0.50
1:C:106:VAL:CG2	1:C:107:ASN:N	2.74	0.50
2:B:362:LEU:HG	2:B:498:VAL:HG22	1.93	0.50
2:B:260:VAL:HG22	7:B:532:HOH:O	2.11	0.50
2:B:351:LEU:HD13	2:B:491:MET:HG3	1.94	0.50
1:A:93:ARG:HD3	1:A:113:ASN:HB2	1.93	0.50
1:A:141:LEU:CD1	2:B:59:ARG:HD2	2.41	0.50
1:A:352:MET:HE3	1:A:418:PRO:HG3	1.93	0.50
1:C:17:LEU:HD21	1:C:32:LEU:CD1	2.42	0.50
1:C:22:GLU:CD	1:C:25:ARG:HH12	2.15	0.49
2:B:105:ARG:HB3	2:B:474:PHE:CD1	2.47	0.49
2:B:127:GLY:HA2	2:B:130:ASN:HD22	1.77	0.49
1:A:210:ARG:NH2	1:A:264:LEU:HD11	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:MET:HE1	2:B:149:VAL:HG21	1.94	0.49
2:D:362:LEU:HG	2:D:498:VAL:HG22	1.94	0.49
2:B:493:ILE:HD13	7:B:616:HOH:O	2.12	0.49
1:A:359:ARG:O	1:A:363:VAL:HG22	2.11	0.49
2:D:131:MET:HE2	2:D:135:LEU:CD1	2.38	0.48
2:D:358:SER:HB3	2:D:498:VAL:HG21	1.93	0.48
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.96	0.48
1:C:477:ALA:HB3	1:C:480:GLU:HB2	1.95	0.48
1:A:103:THR:H	1:A:107:ASN:ND2	2.10	0.48
1:C:192:SER:OG	1:C:383:HIS:HE1	1.96	0.48
2:D:105:ARG:HB3	2:D:474:PHE:CD1	2.48	0.48
1:C:93:ARG:HD3	1:C:111:THR:O	2.14	0.48
2:D:348:ARG:HG3	2:D:487:TYR:CE1	2.49	0.48
2:B:85:THR:HG21	2:B:146:MET:HE1	1.94	0.48
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.96	0.47
1:A:115:THR:HG23	2:B:63:THR:HB	1.96	0.47
1:A:223:VAL:HG22	1:A:272:LEU:HG	1.96	0.47
1:A:335:TRP:O	1:A:339:VAL:HG12	2.15	0.47
1:A:224:ALA:HB3	1:A:271:ASN:ND2	2.30	0.47
1:A:6:ARG:O	1:A:8:GLU:N	2.48	0.47
1:A:339:VAL:HG23	1:A:343:ARG:HB2	1.97	0.47
2:B:192:SER:OG	2:B:194:VAL:HG22	2.15	0.47
1:A:210:ARG:NH2	1:A:264:LEU:CD1	2.78	0.46
1:A:447:SER:HA	7:A:859:HOH:O	2.14	0.46
1:C:134:LEU:HD12	1:C:134:LEU:C	2.35	0.46
1:A:207:LEU:CD2	1:A:282:ILE:HD11	2.46	0.46
1:A:352:MET:CE	1:A:418:PRO:HD3	2.45	0.46
2:D:86:MET:HG2	2:D:138:CYS:SG	2.56	0.46
2:B:262:ASP:O	2:D:350:ARG:HD3	2.16	0.46
2:B:447:TYR:HE1	7:B:779:HOH:O	1.52	0.46
2:B:131:MET:HE2	2:B:135:LEU:CD1	2.41	0.46
1:A:150:VAL:CG1	1:A:180:PRO:HA	2.45	0.46
2:B:317:ASN:ND2	7:B:726:HOH:O	2.41	0.46
1:C:209:LYS:HE2	7:C:774:HOH:O	2.15	0.46
1:C:442:HIS:HB2	7:C:500:HOH:O	2.16	0.46
1:A:6:ARG:O	1:A:9:VAL:N	2.25	0.46
2:B:151:THR:CG2	2:B:162:LEU:HD11	2.45	0.46
1:C:150:VAL:HG13	1:C:180:PRO:HA	1.98	0.46
1:C:280:ASN:O	1:C:284:ARG:HD3	2.16	0.46
1:A:210:ARG:HG3	1:A:263:GLU:HB3	1.98	0.45
2:B:305:VAL:O	2:B:309:TRP:HB2	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:MET:CB	2:D:249:VAL:HG23	2.45	0.45
2:D:456:LEU:HD13	2:D:463:GLU:OE1	2.17	0.45
2:D:505:LEU:HD13	2:D:523:ARG:CZ	2.46	0.45
2:B:431:ARG:HD2	2:B:454:ASP:OD2	2.17	0.45
2:B:85:THR:HG21	2:B:146:MET:CE	2.46	0.45
1:C:475:LEU:HD13	2:D:265:ALA:O	2.16	0.45
2:D:523:ARG:HD3	7:D:684:HOH:O	2.16	0.45
1:A:354:TYR:CE1	1:A:404:VAL:HG12	2.51	0.45
1:C:22:GLU:CD	1:C:25:ARG:NH1	2.70	0.45
1:C:71:VAL:O	1:C:254:SER:OG	2.30	0.45
1:C:430:ILE:HG23	2:D:269:PHE:CG	2.51	0.45
1:A:134:LEU:C	1:A:134:LEU:HD12	2.36	0.45
1:A:144:LEU:CD1	2:B:43:VAL:HG21	2.45	0.45
2:B:390:PRO:HB2	2:B:393:ILE:HD11	1.97	0.45
1:C:223:VAL:HG12	1:C:249:CYS:HA	1.99	0.45
2:B:346:LYS:HZ2	2:B:346:LYS:CB	2.29	0.45
2:B:152:THR:HB	5:B:6498:CLF:S3B	2.57	0.44
1:C:17:LEU:O	1:C:25:ARG:HG3	2.18	0.44
2:D:443:ILE:HD11	2:D:497:LEU:HD21	1.99	0.44
1:C:106:VAL:CG2	2:D:40:ILE:HG23	2.47	0.44
2:D:316:LEU:HD11	2:D:331:LYS:CG	2.48	0.44
2:B:231:GLU:HB3	2:B:237:PHE:CZ	2.53	0.44
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.98	0.44
1:C:103:THR:HB	1:C:106:VAL:HG22	1.99	0.44
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.44
2:B:209:THR:HG23	2:B:213:MET:SD	2.58	0.44
2:B:491:MET:HE1	2:D:481:ARG:NH1	2.32	0.44
2:D:509:THR:HG21	2:D:518:ASN:ND2	2.32	0.44
2:D:391:VAL:HG12	2:D:392:HIS:CE1	2.53	0.43
2:B:346:LYS:HZ2	2:B:346:LYS:CA	2.31	0.43
1:A:426:LYS:HA	2:B:104:ASN:ND2	2.33	0.43
1:A:6:ARG:HG2	1:A:7:GLU:N	2.33	0.43
2:D:254:LEU:HD22	2:D:281:MET:SD	2.59	0.43
1:A:9:VAL:CG1	1:A:34:VAL:HG22	2.49	0.43
1:C:285:HIS:HE1	7:C:558:HOH:O	2.02	0.43
2:D:242:ARG:NH1	7:D:731:HOH:O	2.51	0.43
1:C:230:ASN:HD22	1:C:235:ALA:N	2.15	0.43
2:B:219:GLY:CA	2:B:288:LEU:HD23	2.49	0.43
2:B:466:LEU:HD23	2:B:468:ARG:NH1	2.33	0.42
1:A:12:LEU:HD13	1:A:415:ARG:HG2	2.00	0.42
1:A:434:MET:HB2	1:A:436:ILE:HD12	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:ASP:HB2	2:D:297:HIS:O	2.20	0.42
2:B:369:LEU:C	2:B:369:LEU:HD22	2.39	0.42
1:C:224:ALA:HB3	1:C:271:ASN:ND2	2.33	0.42
1:C:356:GLY:HA3	4:C:7496:CFN:S1B	2.60	0.42
1:C:359:ARG:N	1:C:360:PRO:CD	2.82	0.42
2:B:509:THR:HG21	2:B:518:ASN:ND2	2.34	0.42
1:C:6:ARG:CB	7:C:524:HOH:O	2.68	0.42
2:D:101:SER:HA	2:D:104:ASN:HD22	1.84	0.42
2:D:153:CYS:O	2:D:157:VAL:HG23	2.19	0.42
2:D:386:LEU:HD21	2:D:494:LEU:HD23	2.00	0.42
1:A:352:MET:HE1	1:A:413:VAL:HA	2.01	0.42
2:B:260:VAL:HG13	2:B:273:ALA:H	1.85	0.42
1:C:277:ARG:HD3	7:C:548:HOH:O	2.20	0.42
1:A:53:GLN:HB2	1:A:56:LEU:HD12	2.02	0.42
2:B:88:TYR:OH	2:B:116:ASP:HB3	2.20	0.42
1:C:58:THR:CG2	1:C:403:ASP:OD1	2.68	0.42
2:D:370:TRP:CE3	2:D:430:LEU:HD21	2.55	0.42
1:A:134:LEU:O	1:A:138:VAL:HG23	2.19	0.41
2:B:219:GLY:HA2	2:B:288:LEU:HD23	2.01	0.41
2:B:328:PHE:HD2	2:B:329:LEU:HD13	1.85	0.41
1:A:253:TRP:HA	1:A:254:SER:HA	1.84	0.41
2:B:331:LYS:O	2:B:335:ILE:HG12	2.20	0.41
2:B:376:VAL:O	2:B:380:VAL:HG23	2.21	0.41
2:B:177:ASP:HB3	7:B:564:HOH:O	2.19	0.41
2:B:350:ARG:HD3	2:D:262:ASP:O	2.20	0.41
2:B:510:ARG:HG2	2:D:456:LEU:HD23	2.03	0.41
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.56	0.41
1:A:136:ASP:O	1:A:140:THR:HG23	2.20	0.41
2:B:369:LEU:CD2	2:B:376:VAL:HG13	2.51	0.41
1:A:332:LYS:N	1:A:333:PRO:HD2	2.36	0.41
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.24	0.41
2:B:522:VAL:HG12	1:C:446:TYR:CE1	2.56	0.41
7:B:552:HOH:O	2:D:510:ARG:HD3	2.20	0.41
1:C:134:LEU:O	1:C:138:VAL:HG23	2.21	0.41
1:C:226:ILE:HG22	1:C:279:MET:HB3	2.02	0.41
1:A:265:THR:O	1:A:268:VAL:HG22	2.20	0.41
1:C:138:VAL:HG23	2:D:62:LEU:HD22	2.03	0.41
2:B:217:VAL:H	2:B:286:ASN:ND2	2.19	0.40
2:B:346:LYS:HE3	2:D:264:PRO:HG3	2.02	0.40
2:B:369:LEU:HD22	2:B:369:LEU:O	2.21	0.40
2:B:513:GLN:NE2	2:D:37:GLN:HE22	2.07	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:HIS:HB2	7:A:516:HOH:O	2.22	0.40
1:C:223:VAL:HG22	1:C:272:LEU:HG	2.02	0.40
2:D:127:GLY:HA2	2:D:130:ASN:HD22	1.86	0.40
2:D:143:LYS:N	2:D:144:PRO:HD3	2.35	0.40
2:D:152:THR:HB	5:D:7498:CLF:S3B	2.60	0.40
1:A:225:ILE:HD11	1:A:242:LEU:HD12	2.03	0.40
1:C:346:LEU:HD13	1:C:372:MET:CE	2.51	0.40
2:D:74:GLY:HA3	2:D:193:HIS:O	2.21	0.40
1:A:106:VAL:HG21	2:B:44:PHE:HB2	2.03	0.40

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	463/491 (94%)	441 (95%)	20 (4%)	2 (0%)	34	35
1	C	464/491 (94%)	440 (95%)	23 (5%)	1 (0%)	47	53
2	B	520/522 (100%)	509 (98%)	10 (2%)	1 (0%)	47	53
2	D	520/522 (100%)	508 (98%)	11 (2%)	1 (0%)	47	53
All	All	1967/2026 (97%)	1898 (96%)	64 (3%)	5 (0%)	41	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	GLU
2	B	255	SER
2	D	255	SER
1	C	355	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	398/414 (96%)	378 (95%)	20 (5%)	24	24
1	C	396/414 (96%)	369 (93%)	27 (7%)	16	13
2	B	454/454 (100%)	444 (98%)	10 (2%)	52	59
2	D	454/454 (100%)	443 (98%)	11 (2%)	49	55
All	All	1702/1736 (98%)	1634 (96%)	68 (4%)	31	34

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	14	GLN
1	A	19	VAL
1	A	51	LYS
1	A	93	ARG
1	A	98	ASN
1	A	107	ASN
1	A	131	LEU
1	A	133	LYS
1	A	134	LEU
1	A	162	ASP
1	A	165	SER
1	A	223	VAL
1	A	264	LEU
1	A	355	ILE
1	A	362	HIS
1	A	391	MET
1	A	445	ASP
1	A	461	ARG
1	A	480	GLU
2	B	50	LYS
2	B	80	LEU
2	B	85	THR
2	B	154	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	260	VAL
2	B	279	GLU
2	B	329	LEU
2	B	346	LYS
2	B	369	LEU
2	B	505	LEU
1	C	12	LEU
1	C	14	GLN
1	C	18	GLU
1	C	45	CYS
1	C	58	THR
1	C	93	ARG
1	C	98	ASN
1	C	107	ASN
1	C	131	LEU
1	C	134	LEU
1	C	150	VAL
1	C	218	SER
1	C	223	VAL
1	C	254	SER
1	C	264	LEU
1	C	277	ARG
1	C	284	ARG
1	C	322	LYS
1	C	347	GLU
1	C	355	ILE
1	C	362	HIS
1	C	389	ARG
1	C	396	ASP
1	C	401	TYR
1	C	445	ASP
1	C	467	LEU
1	C	475	LEU
2	D	38	ASP
2	D	51	GLU
2	D	171	LYS
2	D	216	LYS
2	D	258	GLU
2	D	260	VAL
2	D	369	LEU
2	D	379	LEU
2	D	381	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	503	GLU
2	D	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	49	ASN
1	A	53	GLN
1	A	107	ASN
1	A	196	HIS
1	A	252	GLN
1	A	271	ASN
1	A	285	HIS
1	A	362	HIS
1	A	383	HIS
2	B	37	GLN
2	B	104	ASN
2	B	128	GLN
2	B	130	ASN
2	B	168	ASN
2	B	268	GLN
2	B	286	ASN
2	B	317	ASN
2	B	457	HIS
2	B	499	ASN
2	B	518	ASN
2	B	519	HIS
1	C	107	ASN
1	C	230	ASN
1	C	252	GLN
1	C	271	ASN
1	C	285	HIS
1	C	362	HIS
1	C	383	HIS
2	D	37	GLN
2	D	58	GLN
2	D	104	ASN
2	D	128	GLN
2	D	129	GLN
2	D	130	ASN
2	D	167	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	168	ASN
2	D	268	GLN
2	D	286	ASN
2	D	499	ASN
2	D	513	GLN
2	D	518	ASN
2	D	519	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	CFN	A	6496	1	18,30,30	8.44	12 (66%)	-		
5	CLF	B	6498	2,1	0,24,24	-	-	-		
3	HCA	A	494	-	4,13,13	0.90	0	4,18,18	1.32	1 (25%)
4	CFN	C	7496	1	18,30,30	8.38	12 (66%)	-		
3	HCA	C	494	-	4,13,13	1.02	0	4,18,18	1.64	1 (25%)
5	CLF	D	7498	2,1	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
3	HCA	A	494	-	-	4/7/17/17	-
5	CLF	D	7498	2,1	-	-	0/12/10/10
3	HCA	C	494	-	-	4/7/17/17	-
5	CLF	B	6498	2,1	-	-	0/12/10/10

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6496	CFN	S1A-FE2	-11.45	2.07	2.29
4	C	7496	CFN	S1A-FE2	-11.39	2.07	2.29
4	A	6496	CFN	S1B-FE6	-11.36	2.07	2.29
4	C	7496	CFN	S3B-FE6	-10.90	2.08	2.29
4	C	7496	CFN	S1B-FE5	-10.89	2.08	2.29
4	C	7496	CFN	S1B-FE6	-10.76	2.08	2.29
4	C	7496	CFN	S4A-FE4	-10.74	2.08	2.29
4	A	6496	CFN	S4A-FE4	-10.70	2.08	2.29
4	A	6496	CFN	S4A-FE3	-10.57	2.08	2.29
4	A	6496	CFN	S3B-FE6	-10.56	2.08	2.29
4	C	7496	CFN	S4A-FE3	-10.51	2.09	2.29
4	C	7496	CFN	S4B-FE5	-10.44	2.09	2.29
4	A	6496	CFN	S1A-FE4	-10.41	2.09	2.29
4	A	6496	CFN	S1B-FE5	-10.34	2.09	2.29
4	A	6496	CFN	S4B-FE5	-10.18	2.09	2.29
4	C	7496	CFN	S2A-FE2	-10.03	2.09	2.29
4	A	6496	CFN	S2A-FE3	-9.78	2.10	2.29
4	A	6496	CFN	S2A-FE2	-9.75	2.10	2.29
4	C	7496	CFN	S2A-FE3	-9.54	2.10	2.29
4	A	6496	CFN	S3B-FE7	-9.47	2.11	2.29
4	C	7496	CFN	S4B-FE7	-9.41	2.11	2.29
4	C	7496	CFN	S1A-FE4	-9.35	2.11	2.29
4	A	6496	CFN	S4B-FE7	-9.15	2.11	2.29
4	C	7496	CFN	S3B-FE7	-8.90	2.12	2.29

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	494	HCA	C4-C5-C6	2.54	115.24	111.39
3	A	494	HCA	C4-C5-C6	2.49	115.16	111.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

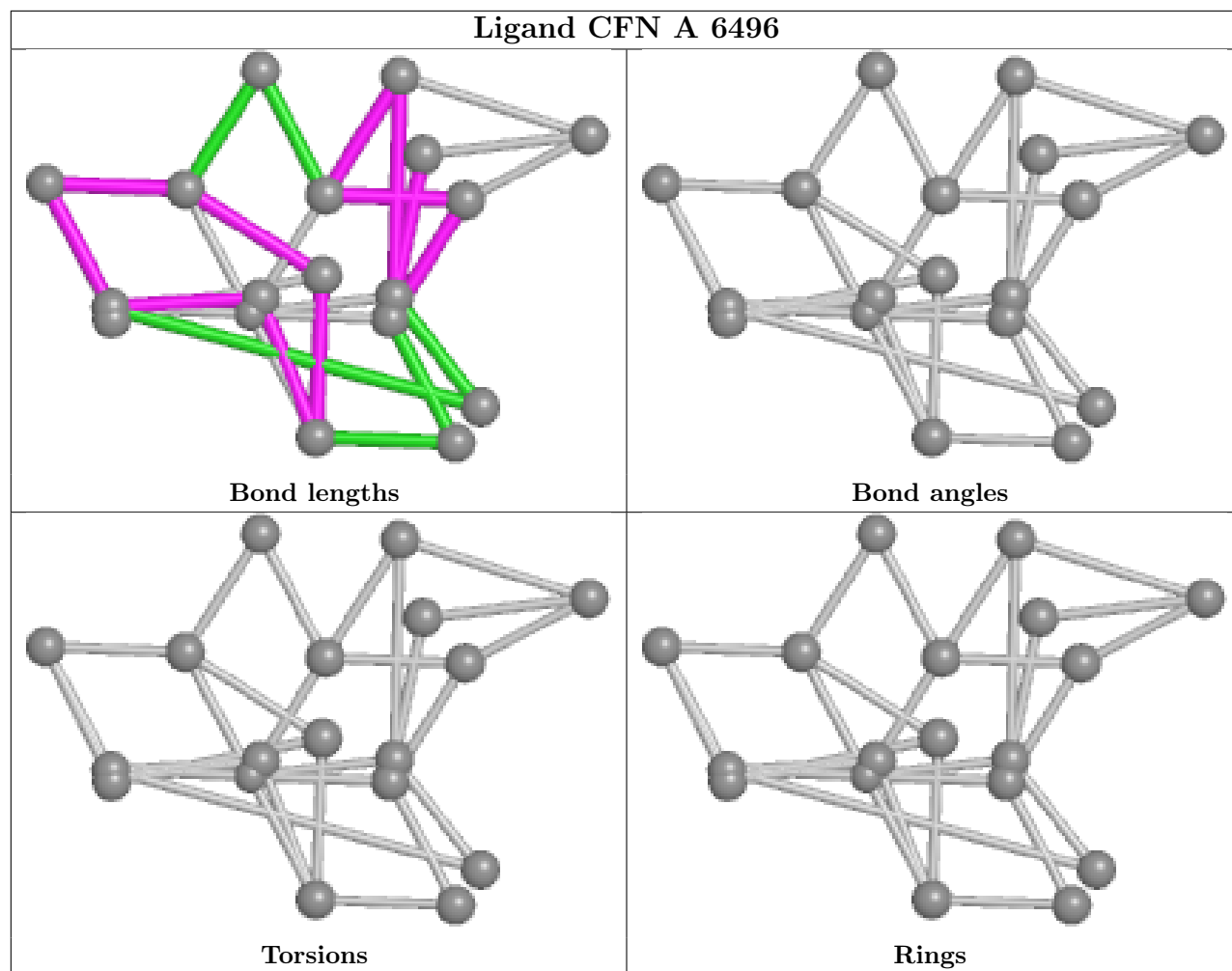
Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C2-C3-C4-C5
3	A	494	HCA	C7-C3-C4-C5
3	A	494	HCA	O7-C3-C4-C5
3	C	494	HCA	C2-C3-C4-C5
3	C	494	HCA	C7-C3-C4-C5
3	C	494	HCA	O7-C3-C4-C5
3	A	494	HCA	C3-C4-C5-C6
3	C	494	HCA	C3-C4-C5-C6

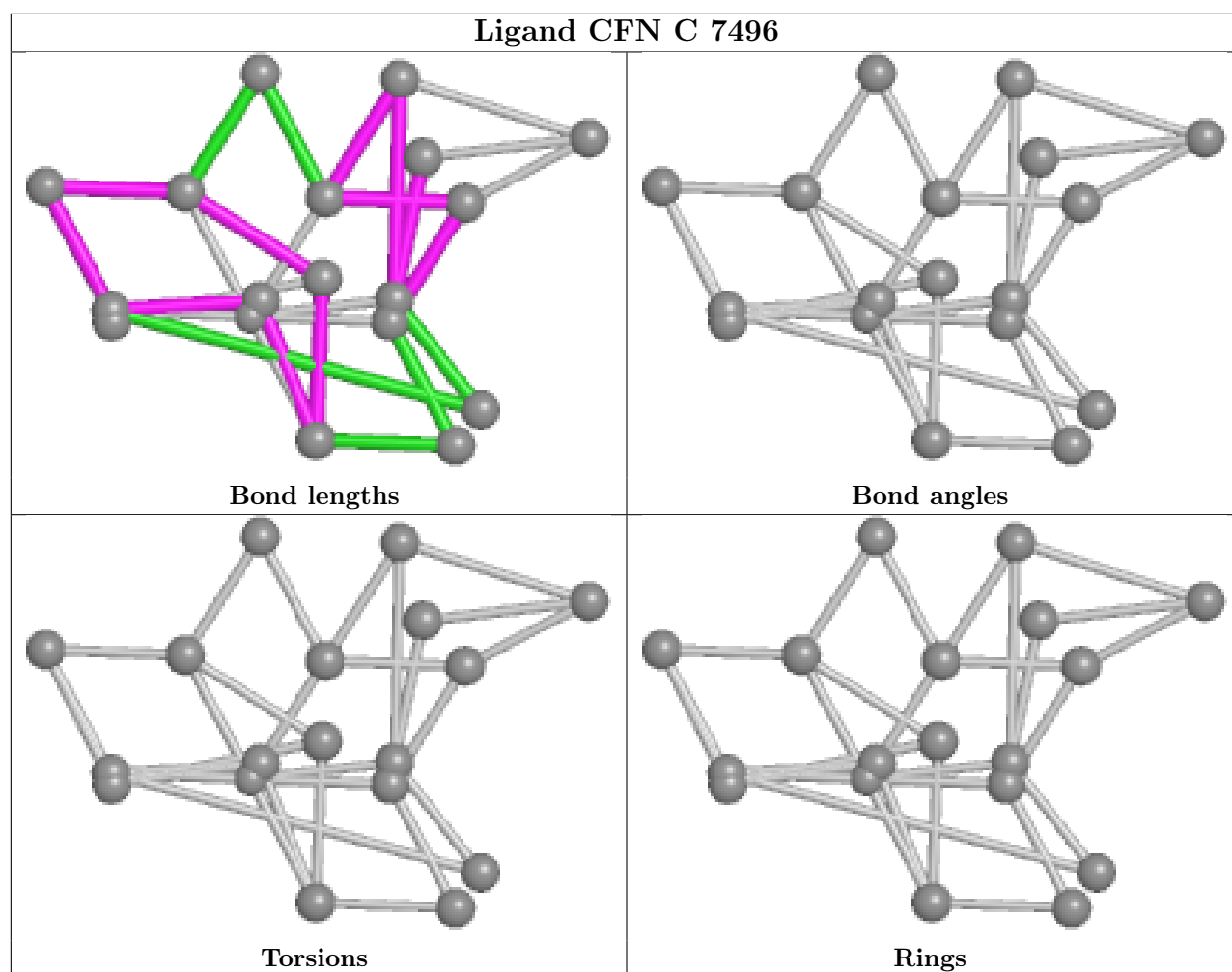
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6496	CFN	2	0
5	B	6498	CLF	1	0
4	C	7496	CFN	3	0
5	D	7498	CLF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	467/491 (95%)	0.21	12 (2%) 56 57	25, 37, 53, 73	0
1	C	468/491 (95%)	0.31	21 (4%) 33 33	27, 37, 55, 73	0
2	B	522/522 (100%)	-0.01	10 (1%) 66 68	27, 35, 49, 63	0
2	D	522/522 (100%)	0.06	12 (2%) 60 61	27, 37, 50, 67	0
All	All	1979/2026 (97%)	0.14	55 (2%) 53 53	25, 36, 52, 73	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	125	PHE	5.3
1	A	212	GLU	4.9
2	B	214	ASP	4.8
1	C	212	GLU	4.6
1	C	481	ALA	4.4
2	D	123	ALA	4.1
1	A	6	ARG	4.1
1	C	215	THR	3.8
1	C	396	ASP	3.6
1	A	125	PHE	3.6
1	C	415	ARG	3.5
1	C	392	LYS	3.4
2	B	38	ASP	3.2
1	A	216	PHE	3.2
2	B	123	ALA	3.1
2	D	217	VAL	3.1
1	A	159	ILE	3.1
2	D	214	ASP	3.0
1	A	215	THR	3.0
2	D	124	VAL	3.0
1	C	14	GLN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	480	GLU	2.9
1	C	5	SER	2.9
2	B	177	ASP	2.9
1	A	45	CYS	2.9
2	B	125	PHE	2.8
1	A	384	ASN	2.8
2	B	124	VAL	2.8
1	C	79	ILE	2.8
1	A	392	LYS	2.8
2	B	215	ASP	2.7
1	C	213	ASP	2.7
1	A	299	PHE	2.6
1	C	7	GLU	2.6
2	D	212	SER	2.5
1	C	214	THR	2.5
1	C	175	SER	2.5
2	D	177	ASP	2.5
1	C	18	GLU	2.4
1	C	125	PHE	2.4
1	A	214	THR	2.4
2	D	50	LYS	2.3
1	C	299	PHE	2.3
2	B	417	LYS	2.3
1	C	45	CYS	2.2
1	C	318	GLU	2.2
2	B	209	THR	2.2
1	C	34	VAL	2.2
1	C	82	SER	2.1
2	B	217	VAL	2.1
2	D	171	LYS	2.1
1	A	5	SER	2.1
2	D	164	ALA	2.1
2	D	417	LYS	2.0
2	D	312	GLU	2.0

## 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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

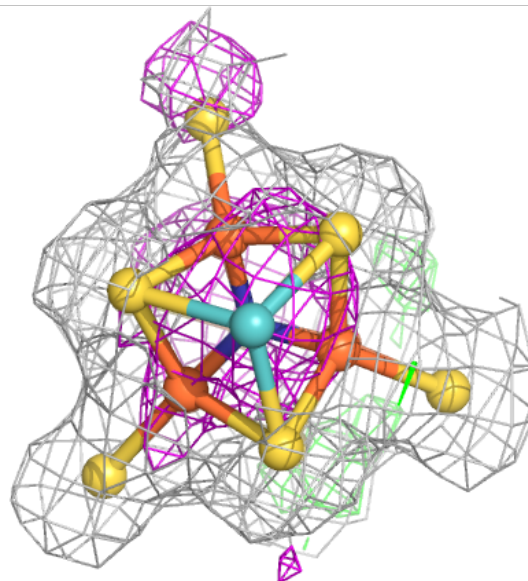
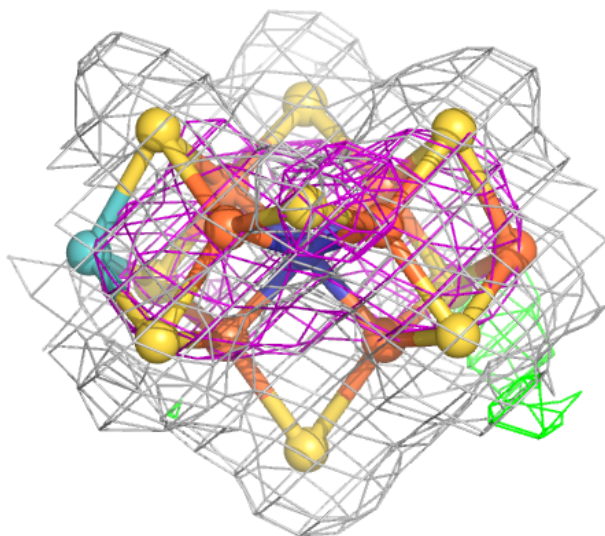
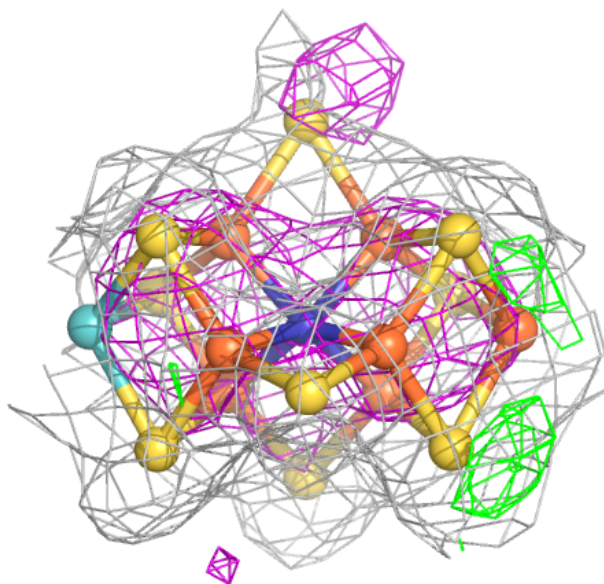
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CLF	B	6498	15/15	0.62	0.23	21,31,40,46	2
5	CLF	D	7498	15/15	0.64	0.22	20,28,44,54	0
6	CA	B	524	1/1	0.85	0.07	57,57,57,57	0
6	CA	D	524	1/1	0.87	0.08	61,61,61,61	0
4	CFN	A	6496	18/18	0.94	0.09	22,27,33,42	0
4	CFN	C	7496	18/18	0.94	0.09	18,25,32,38	0
3	HCA	A	494	14/14	0.96	0.13	27,30,34,37	0
3	HCA	C	494	14/14	0.97	0.12	30,33,36,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

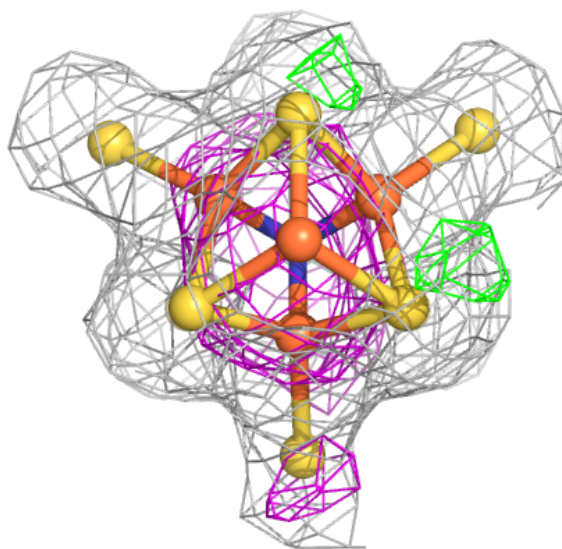
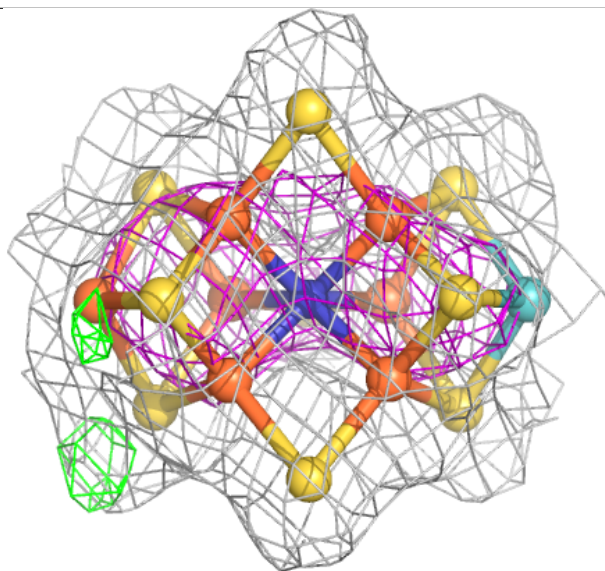
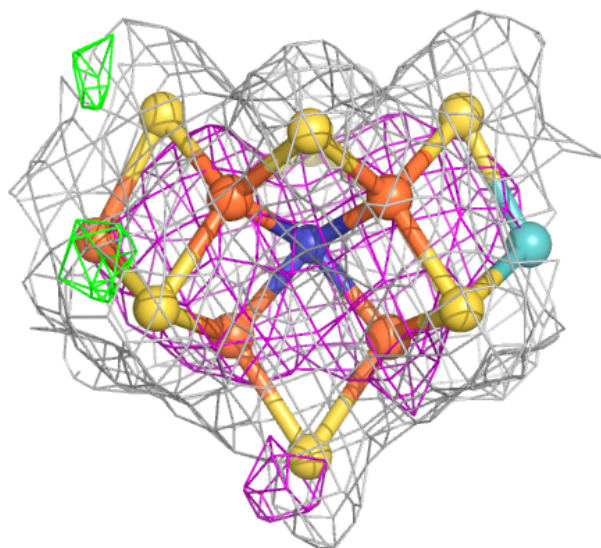
**Electron density around CFN A 6496:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CFN C 7496:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.