



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:41 AM UTC

PDB ID : 6BBL / pdb\_00006bbl  
Title : Crystal structure of the a-96Gln MoFe protein variant in the presence of the substrate acetylene  
Authors : Zadvornyy, O.A.; Keable, S.M.; Vertemara, J.; Eilers, B.J.; Karamatullah, D.; Rasmussen, A.J.; De Gioia, L.; Zampella, G.; Seefeldt, L.C.; Peters, J.W.  
Deposited on : 2017-10-18  
Resolution : 1.68 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 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) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

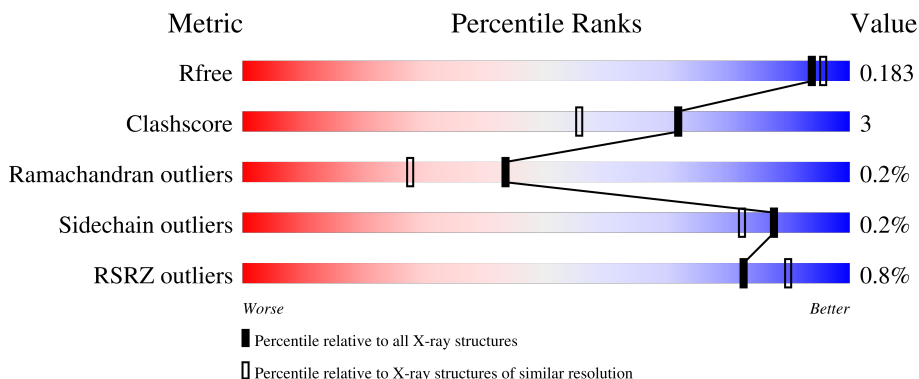
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


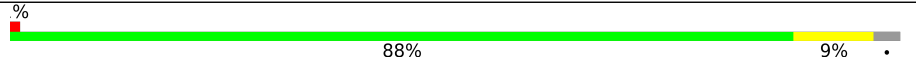
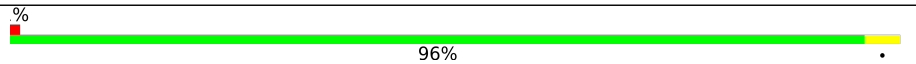
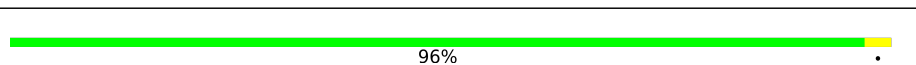
The reported resolution of this entry is 1.68 Å.

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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	492	 88% 8% .
1	C	492	 88% 9% .
2	B	523	 96% .
2	D	523	 96% .

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	C2H	C	501	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33891 atoms, of which 15669 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
			Total	C	H	N	O	S			
1	A	477	7525	2412	3731	645	711	26	0	2	0
1	C	477	7525	2412	3731	645	711	26	0	2	0

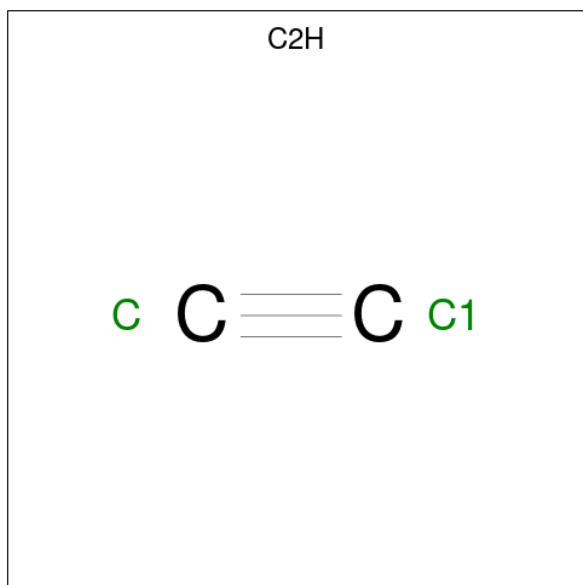
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLN	ARG	variant	UNP P07328
C	96	GLN	ARG	variant	UNP P07328

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

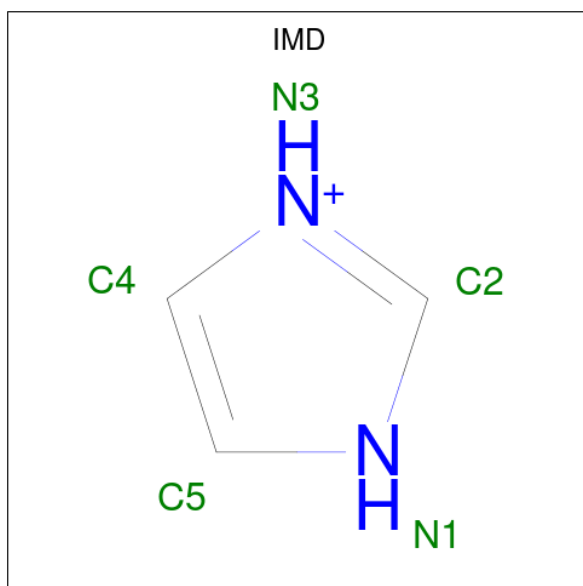
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	522	8262	2666	4088	705	775	28	0	0	0
2	D	522	8262	2666	4088	705	775	28	0	0	0

- Molecule 3 is acetylene (CCD ID: C2H) (formula: C<sub>2</sub>H<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	H	0	0
			4	2	2		
3	C	1	Total	C	H	0	0
			4	2	2		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



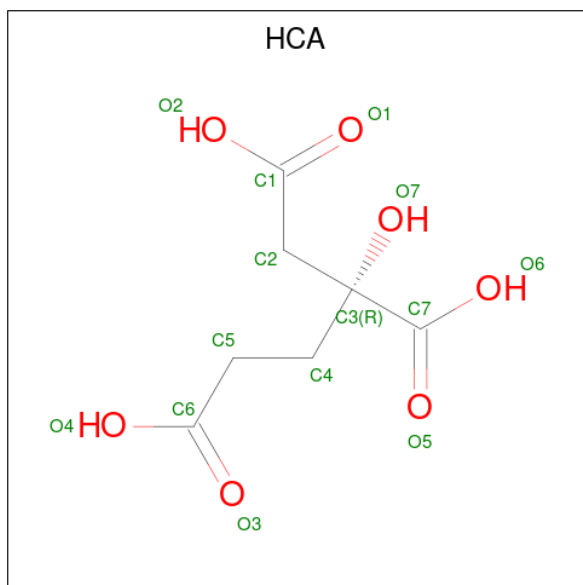
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	0	0
			10	3	5	2		
4	C	1	Total	C	H	N	0	0
			10	3	5	2		

*Continued on next page...*

Continued from previous page...

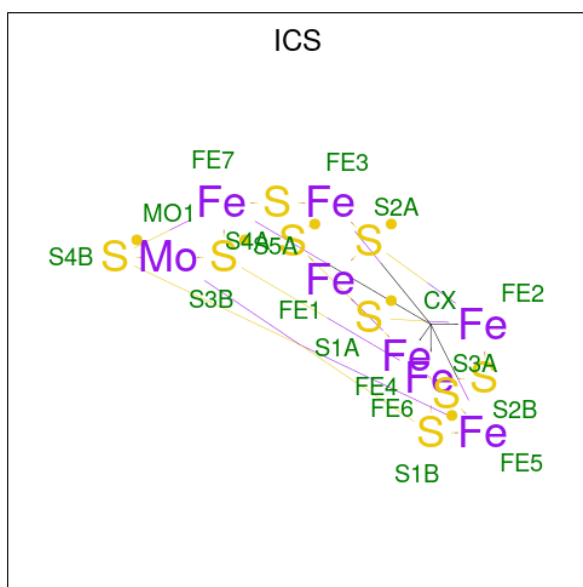
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
4	D	1	10	3	5	2	0	0

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula:  $C_7H_{10}O_7$ ).



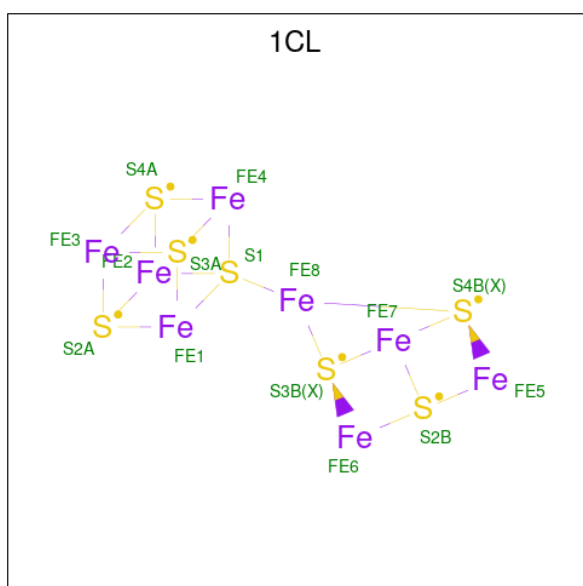
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	20	7	6	7	0	0
5	C	1	20	7	6	7	0	0

- Molecule 6 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula:  $CFe_7MoS_9$ ).



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

- Molecule 7 is FE(8)-S(7) CLUSTER, OXIDIZED (CCD ID: 1CL) (formula:  $\text{Fe}_8\text{S}_7$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	A	1	Total	Fe	S	0	0
			15	8	7		
7	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Fe	0	0
			2	2		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

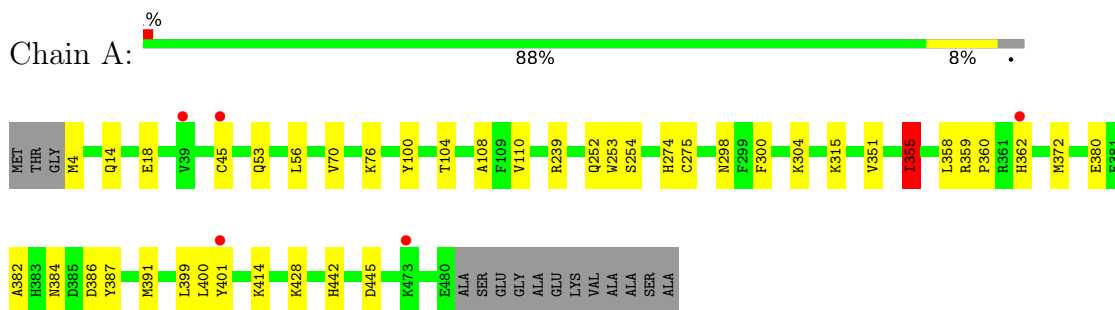
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	455	Total	O	0	0
			455	455		
10	B	620	Total	O	0	0
			620	620		
10	C	483	Total	O	0	0
			483	483		
10	D	612	Total	O	0	0
			612	612		

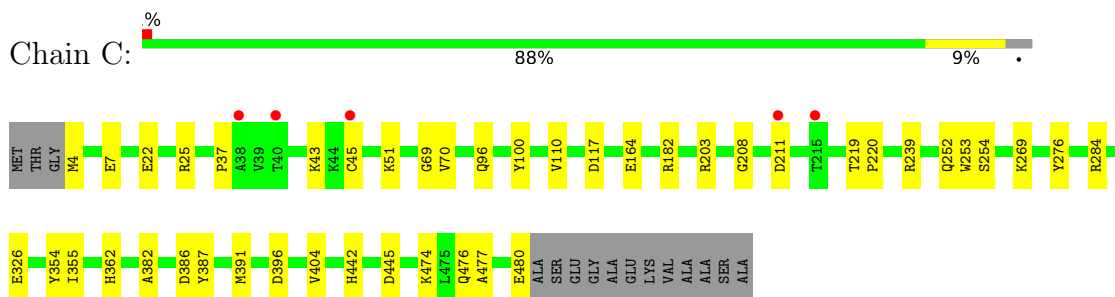
### 3 Residue-property plots [i](#)

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.

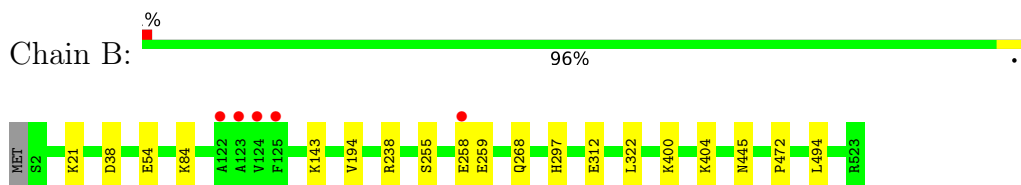
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



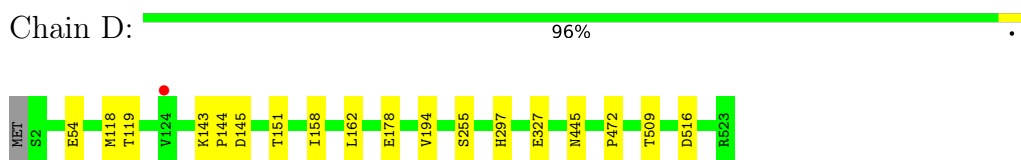
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.78Å 128.25Å 107.27Å 90.00° 109.11° 90.00°	Depositor
Resolution (Å)	39.76 – 1.68 39.76 – 1.68	Depositor EDS
% Data completeness (in resolution range)	91.9 (39.76-1.68) 91.8 (39.76-1.68)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.68Å)	Xtrriage
Refinement program	PHENIX (DEV_2880: ???)	Depositor
R, $R_{free}$	0.151 , 0.185 0.151 , 0.183	Depositor DCC
$R_{free}$ test set	10163 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtrriage
Anisotropy	0.378	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: MG, ICS, FE, HCA, IMD, C2H, 1CL

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	0.43	3/3889 (0.1%)	0.58	0/5245
1	C	0.38	0/3889	0.57	0/5245
2	B	0.39	0/4280	0.56	0/5786
2	D	0.40	0/4280	0.56	0/5786
All	All	0.40	3/16338 (0.0%)	0.57	0/22062

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	LEU	C-O	-6.20	1.17	1.24
1	A	399	LEU	C-O	-6.04	1.16	1.23
1	A	401	TYR	C-O	-5.33	1.18	1.24

There are no bond angle outliers.

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	3794	3731	3720	36	0
1	C	3794	3731	3720	37	0
2	B	4174	4088	4088	19	0
2	D	4174	4088	4088	12	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	2	0	1	0
3	C	2	2	0	2	0
4	A	5	5	5	0	0
4	C	5	5	5	2	0
4	D	5	5	5	0	0
5	A	14	6	6	2	0
5	C	14	6	6	4	0
6	A	18	0	0	0	0
6	C	18	0	0	0	0
7	A	15	0	0	0	0
7	C	15	0	0	0	0
8	B	2	0	0	0	0
9	B	1	0	0	0	0
10	A	455	0	0	12	0
10	B	620	0	0	10	1
10	C	483	0	0	20	4
10	D	612	0	0	5	2
All	All	18222	15669	15643	106	4

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 3.

All (106) 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:238:ARG:HG3	2:B:258:GLU:OE1	1.45	1.16
2:B:238:ARG:CG	2:B:258:GLU:OE1	1.96	1.12
2:B:312:GLU:OE2	10:B:701:HOH:O	1.81	0.99
1:C:326:GLU:OE1	10:C:601:HOH:O	1.80	0.97
2:B:21:LYS:NZ	10:B:703:HOH:O	2.01	0.93
1:C:22:GLU:OE1	1:C:25:ARG:NH1	2.06	0.88
4:C:504:IMD:N1	10:C:603:HOH:O	2.05	0.87
1:A:384:ASN:OD1	10:A:601:HOH:O	1.91	0.86
2:B:238:ARG:HG2	2:B:258:GLU:OE1	1.74	0.84
2:B:38:ASP:OD1	10:B:702:HOH:O	1.98	0.81
1:C:117:ASP:O	10:C:602:HOH:O	2.00	0.79
2:D:327:GLU:OE2	10:D:701:HOH:O	2.01	0.79
2:D:145:ASP:OD2	10:D:702:HOH:O	2.02	0.78
1:C:480:GLU:HB2	10:C:604:HOH:O	1.87	0.74
2:B:84:LYS:NZ	10:B:706:HOH:O	2.21	0.73
1:C:4:MET:N	10:C:608:HOH:O	2.21	0.72

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ARG:HD3	10:C:640:HOH:O	1.91	0.71
2:B:54:GLU:OE2	10:B:704:HOH:O	2.10	0.69
2:D:178:GLU:OE1	10:D:703:HOH:O	2.11	0.68
2:B:238:ARG:HE	2:B:258:GLU:CD	2.03	0.66
1:A:18:GLU:OE1	10:A:602:HOH:O	2.14	0.65
1:C:269:LYS:NZ	10:C:613:HOH:O	2.31	0.62
1:C:477:ALA:O	10:C:604:HOH:O	2.16	0.60
1:C:7:GLU:OE2	10:C:605:HOH:O	2.16	0.60
1:C:45:CYS:SG	1:C:391:MET:HE1	2.41	0.60
1:A:298:ASN:CG	1:A:362:HIS:CD2	2.80	0.60
1:A:380:GLU:HG3	10:A:610:HOH:O	2.03	0.59
1:A:414:LYS:NZ	10:A:608:HOH:O	2.35	0.59
1:A:428:LYS:HE3	10:A:880:HOH:O	2.03	0.58
1:C:164:GLU:OE1	10:C:606:HOH:O	2.17	0.58
1:C:203:ARG:NH2	10:C:617:HOH:O	2.37	0.58
1:A:4:MET:N	10:A:609:HOH:O	2.35	0.57
1:C:477:ALA:N	10:C:604:HOH:O	2.37	0.57
1:A:274:HIS:CE1	1:A:362:HIS:CE1	2.93	0.56
1:A:298:ASN:HA	1:A:362:HIS:HE2	1.71	0.56
1:C:208:GLY:HA2	1:C:211:ASP:OD1	2.06	0.56
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.42	0.55
1:A:45:CYS:SG	1:A:391:MET:HE1	2.47	0.54
2:D:54:GLU:OE1	10:D:704:HOH:O	2.18	0.54
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.44	0.53
1:A:358:LEU:HD21	1:A:362:HIS:ND1	2.24	0.53
1:C:51:LYS:NZ	2:D:119:THR:OG1	2.42	0.53
2:B:259:GLU:OE2	10:B:705:HOH:O	2.19	0.53
4:C:504:IMD:C2	10:C:603:HOH:O	2.49	0.52
2:B:268:GLN:HG3	10:B:1010:HOH:O	2.08	0.52
1:A:304:LYS:NZ	10:A:615:HOH:O	2.41	0.52
1:C:387:TYR:O	1:C:391:MET:HG3	2.10	0.52
1:C:476:GLN:HG3	10:C:604:HOH:O	2.10	0.52
2:D:54:GLU:OE2	10:D:705:HOH:O	2.19	0.50
1:C:476:GLN:CG	10:C:604:HOH:O	2.60	0.49
1:A:14:GLN:HG2	10:A:617:HOH:O	2.12	0.49
1:A:442:HIS:HB3	5:A:503:HCA:O6	2.13	0.48
1:A:387:TYR:O	1:A:391:MET:HG3	2.14	0.48
1:C:37:PRO:HD3	1:C:396:ASP:OD1	2.14	0.48
2:B:238:ARG:HE	2:B:258:GLU:CG	2.27	0.47
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.50	0.47
1:A:4:MET:C	10:A:609:HOH:O	2.56	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.97	0.47
2:B:143:LYS:HE3	10:B:871:HOH:O	2.14	0.47
1:A:359:ARG:HA	1:A:362:HIS:HB3	1.96	0.47
2:D:194:VAL:HB	2:D:297:HIS:CG	2.50	0.47
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.97	0.47
1:C:70:VAL:HG13	3:C:501:C2H:C1	2.45	0.47
1:C:182:ARG:CZ	10:C:640:HOH:O	2.63	0.46
1:A:4:MET:N	10:A:625:HOH:O	2.48	0.46
1:C:442:HIS:HB3	5:C:502:HCA:O5	2.16	0.46
5:A:503:HCA:O2	5:A:503:HCA:O7	2.34	0.46
1:A:300:PHE:HD2	1:A:362:HIS:CD2	2.34	0.45
1:A:298:ASN:CG	1:A:362:HIS:HD2	2.20	0.45
1:C:43:LYS:NZ	10:C:636:HOH:O	2.49	0.45
2:B:494:LEU:C	2:B:494:LEU:HD23	2.41	0.45
1:C:253:TRP:HA	1:C:254:SER:HA	1.80	0.45
1:A:239:ARG:HD2	1:A:252:GLN:OE1	2.16	0.45
1:C:43:LYS:CE	10:C:636:HOH:O	2.64	0.45
1:C:480:GLU:OE2	10:C:607:HOH:O	2.20	0.45
2:B:194:VAL:HB	2:B:297:HIS:CG	2.52	0.44
1:C:182:ARG:NH1	10:C:640:HOH:O	2.50	0.44
1:C:69:GLY:HA3	3:C:501:C2H:C	2.48	0.44
1:C:239:ARG:HD2	1:C:252:GLN:OE1	2.17	0.44
1:A:355:ILE:C	10:A:610:HOH:O	2.60	0.44
1:A:298:ASN:ND2	1:A:362:HIS:HD2	2.16	0.43
5:C:502:HCA:O1	5:C:502:HCA:O7	2.35	0.43
1:C:219:THR:HB	1:C:220:PRO:HD2	1.99	0.43
2:D:509:THR:O	2:D:516:ASP:HA	2.18	0.42
1:A:359:ARG:N	1:A:360:PRO:CD	2.82	0.42
2:D:118:MET:HE1	2:D:158:ILE:HD11	2.01	0.42
1:A:70:VAL:HG13	3:A:501:C2H:C1	2.49	0.42
1:A:382:ALA:HB1	1:A:386:ASP:HB2	2.00	0.42
1:A:76:LYS:O	1:A:108:ALA:HA	2.20	0.42
1:A:274:HIS:NE2	1:A:362:HIS:CE1	2.88	0.42
1:C:96:GLN:HG2	5:C:502:HCA:O6	2.20	0.42
1:A:358:LEU:HD21	1:A:362:HIS:CE1	2.55	0.42
2:B:322:LEU:HD21	1:C:474:LYS:HB3	2.02	0.42
1:C:276:TYR:OH	1:C:284:ARG:NH2	2.52	0.42
1:C:442:HIS:CG	5:C:502:HCA:H52	2.55	0.42
1:A:104:THR:HA	1:A:108:ALA:O	2.20	0.41
1:A:275:CYS:HA	1:A:358:LEU:HD22	2.01	0.41
2:D:445:ASN:HB2	2:D:472:PRO:O	2.19	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:CG2	1:A:372:MET:HE2	2.50	0.41
2:D:143:LYS:N	2:D:144:PRO:CD	2.83	0.41
1:A:315:LYS:HD3	10:A:943:HOH:O	2.20	0.41
2:D:151:THR:HG23	2:D:162:LEU:HD11	2.01	0.41
2:B:400:LYS:HG3	10:B:869:HOH:O	2.21	0.41
2:B:445:ASN:HB2	2:B:472:PRO:O	2.19	0.41
1:A:253:TRP:HA	1:A:254:SER:HA	1.85	0.41
2:B:404:LYS:NZ	10:B:719:HOH:O	2.40	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1013:HOH:O	10:C:1045:HOH:O[2_555]	1.88	0.32
10:B:1260:HOH:O	10:C:867:HOH:O[2_545]	1.99	0.21
10:C:967:HOH:O	10:D:872:HOH:O[1_655]	2.00	0.20
10:C:958:HOH:O	10:D:866:HOH:O[2_545]	2.18	0.02

## 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	477/492 (97%)	458 (96%)	18 (4%)	1 (0%)	43 27
1	C	477/492 (97%)	459 (96%)	17 (4%)	1 (0%)	43 27
2	B	520/523 (99%)	510 (98%)	9 (2%)	1 (0%)	43 27
2	D	520/523 (99%)	507 (98%)	12 (2%)	1 (0%)	43 27
All	All	1994/2030 (98%)	1934 (97%)	56 (3%)	4 (0%)	43 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	255	SER
2	B	255	SER
1	A	355	ILE
1	C	355	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/415 (99%)	407 (100%)	2 (0%)	81	72
1	C	409/415 (99%)	407 (100%)	2 (0%)	81	72
2	B	454/455 (100%)	454 (100%)	0	100	100
2	D	454/455 (100%)	454 (100%)	0	100	100
All	All	1726/1740 (99%)	1722 (100%)	4 (0%)	87	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ILE
1	A	445	ASP
1	C	362	HIS
1	C	445	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	362	HIS
1	A	432	GLN
2	B	418	ASN
1	C	14	GLN
1	C	29	ASN
1	C	119	GLN
1	C	476	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	163	ASN

### 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 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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
7	1CL	A	505	1,2	0,22,22	-	-	-		
5	HCA	C	502	-	13,13,13	1.11	2 (15%)	15,18,18	1.21	2 (13%)
3	C2H	C	501	-	1,1,1	1.07	0	-		
4	IMD	C	504	-	5,5,5	0.75	0	5,5,5	0.74	0
7	1CL	C	505	1,2	0,22,22	-	-	-		
6	ICS	C	503	1	6,30,30	1.01	0	-		
4	IMD	D	601	-	5,5,5	0.65	0	5,5,5	0.44	0
4	IMD	A	502	-	5,5,5	0.75	0	5,5,5	0.44	0
6	ICS	A	504	1	6,30,30	0.89	0	-		
5	HCA	A	503	-	13,13,13	1.67	4 (30%)	15,18,18	2.14	5 (33%)
3	C2H	A	501	-	1,1,1	1.07	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
7	1CL	A	505	1,2	-	-	0/10/8/8
5	HCA	C	502	-	-	4/17/17/17	-
4	IMD	C	504	-	-	-	0/1/1/1
7	1CL	C	505	1,2	-	-	0/10/8/8
4	IMD	D	601	-	-	-	0/1/1/1
4	IMD	A	502	-	-	-	0/1/1/1
5	HCA	A	503	-	-	5/17/17/17	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	HCA	O6-C7	-3.21	1.18	1.30
5	A	503	HCA	O5-C7	2.98	1.31	1.22
5	A	503	HCA	O1-C1	2.89	1.31	1.22
5	A	503	HCA	O2-C1	-2.85	1.21	1.30
5	C	502	HCA	O3-C6	2.80	1.31	1.22
5	C	502	HCA	O4-C6	-2.59	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	HCA	O6-C7-C3	5.02	122.77	113.14
5	A	503	HCA	O5-C7-C3	-4.26	113.83	122.09
5	C	502	HCA	C4-C5-C6	3.26	120.33	112.77
5	A	503	HCA	O1-C1-C2	-2.86	114.84	122.95
5	A	503	HCA	C4-C5-C6	2.57	118.73	112.77
5	A	503	HCA	O2-C1-C2	2.28	121.56	114.35
5	C	502	HCA	O3-C6-C5	-2.27	115.88	123.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	HCA	C2-C3-C4-C5
5	A	503	HCA	O7-C3-C4-C5
5	C	502	HCA	C2-C3-C4-C5
5	C	502	HCA	O7-C3-C4-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	503	HCA	C7-C3-C4-C5
5	C	502	HCA	C7-C3-C4-C5
5	A	503	HCA	O1-C1-C2-C3
5	C	502	HCA	C1-C2-C3-C7
5	A	503	HCA	O2-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	HCA	4	0
3	C	501	C2H	2	0
4	C	504	IMD	2	0
5	A	503	HCA	2	0
3	A	501	C2H	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	477/492 (96%)	-0.14	5 (1%) 79 86	11, 23, 41, 61	9 (1%)
1	C	477/492 (96%)	-0.19	5 (1%) 79 86	11, 23, 41, 55	2 (0%)
2	B	522/523 (99%)	-0.35	5 (0%) 79 86	16, 22, 32, 54	3 (0%)
2	D	522/523 (99%)	-0.37	1 (0%) 91 95	15, 21, 32, 48	3 (0%)
All	All	1998/2030 (98%)	-0.27	16 (0%) 82 90	11, 22, 38, 61	17 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	123	ALA	5.2
2	B	124	VAL	5.1
1	A	39	VAL	4.0
1	A	362	HIS	3.2
1	A	401	TYR	3.1
2	B	125	PHE	2.8
2	B	122	ALA	2.8
1	C	38	ALA	2.4
1	A	473	LYS	2.4
1	C	215	THR	2.2
1	C	211	ASP	2.2
2	B	258	GLU	2.2
1	C	40	THR	2.2
2	D	124	VAL	2.1
1	A	45	CYS	2.1
1	C	45	CYS	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
4	IMD	A	502	5/5	0.75	0.14	42,50,60,61	0
4	IMD	D	601	5/5	0.87	0.12	39,44,52,53	0
4	IMD	C	504	5/5	0.88	0.24	16,30,46,47	0
3	C2H	C	501	2/2	0.88	0.27	24,26,29,31	0
3	C2H	A	501	2/2	0.93	0.17	22,27,30,36	0
5	HCA	C	502	14/14	0.94	0.08	16,20,23,23	0
9	MG	B	602	1/1	0.94	0.10	42,42,42,42	0
7	1CL	A	505	15/15	0.96	0.06	14,16,26,28	0
7	1CL	C	505	15/15	0.97	0.05	14,16,26,28	0
5	HCA	A	503	14/14	0.97	0.06	18,22,27,27	0
6	ICS	C	503	18/18	0.99	0.04	11,17,18,18	1
8	FE	B	601	1/1	0.99	0.03	18,18,18,18	0
6	ICS	A	504	18/18	0.99	0.04	10,17,19,19	3
8	FE	B	603	1/1	1.00	0.05	21,21,21,21	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.