Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 12:54 AM EDT

PDB ID	:	4WZA
Title	:	Asymmetric Nucleotide Binding in the Nitrogenase Complex
Authors	:	Tezcan, F.A.; Kaiser, J.T.; Howard, J.B.; Rees, D.C.
Deposited on	:	2014-11-19
Resolution	:	1.90 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*
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:

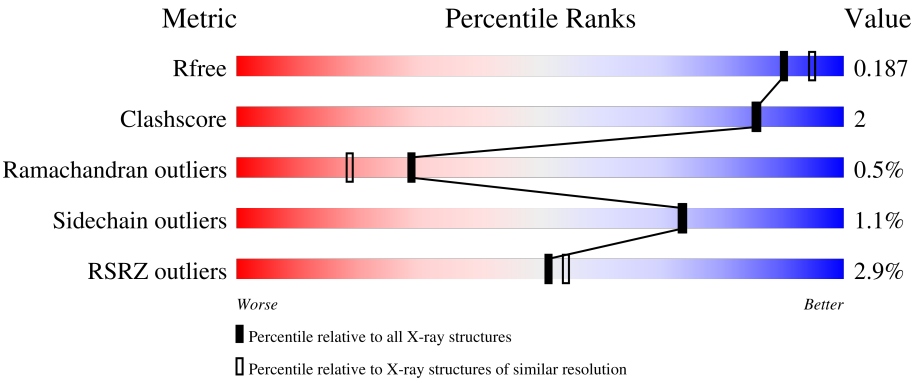
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	477	3% 92% 8%
1	C	477	% 93% 7%
2	B	522	95% 5%
2	D	522	95% 5%
3	E	276	7% 92% 8%

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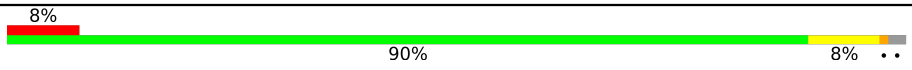
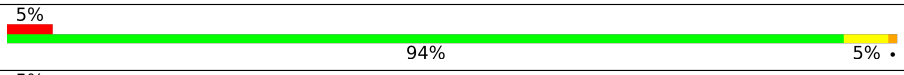
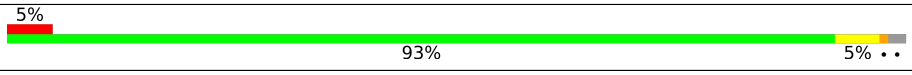
Mol	Chain	Length	Quality of chain
3	F	276	
3	G	276	
3	H	276	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 26654 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	4	0	0
			3791	2410	647	709	25			
1	C	477	Total	C	N	O	S	0	0	0
			3791	2410	647	709	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLN	GLU	variant	UNP P07328
C	440	GLN	GLU	variant	UNP P07328

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

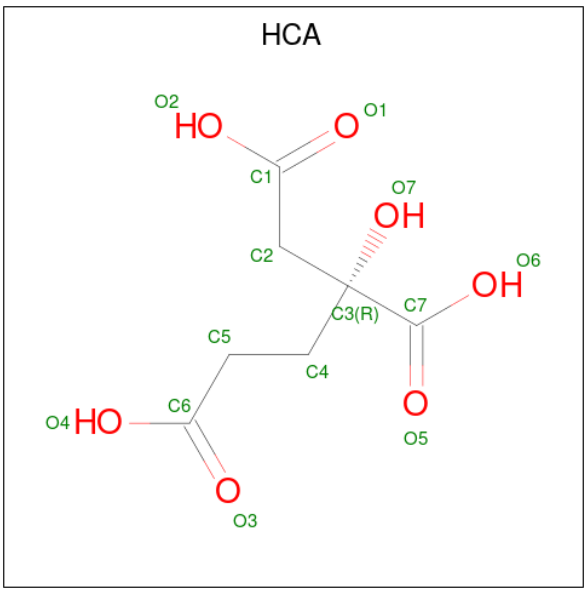
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	1	0
			4183	2671	706	778	28			

- Molecule 3 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	276	Total	C	N	O	S	100	0	0
			2090	1306	355	408	21			
3	F	271	Total	C	N	O	S	52	0	0
			2053	1283	350	400	20			
3	G	276	Total	C	N	O	S	29	0	0
			2089	1306	355	407	21			
3	H	271	Total	C	N	O	S	53	0	0
			2053	1283	350	400	20			

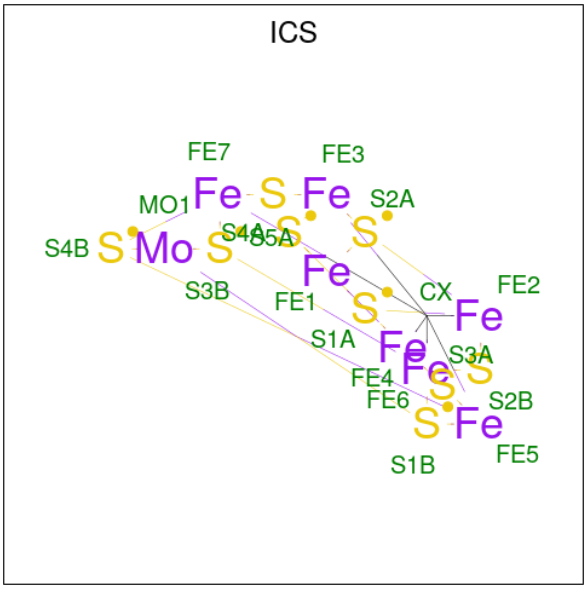
- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (for-

mula: $C_7H_{10}O_7$).



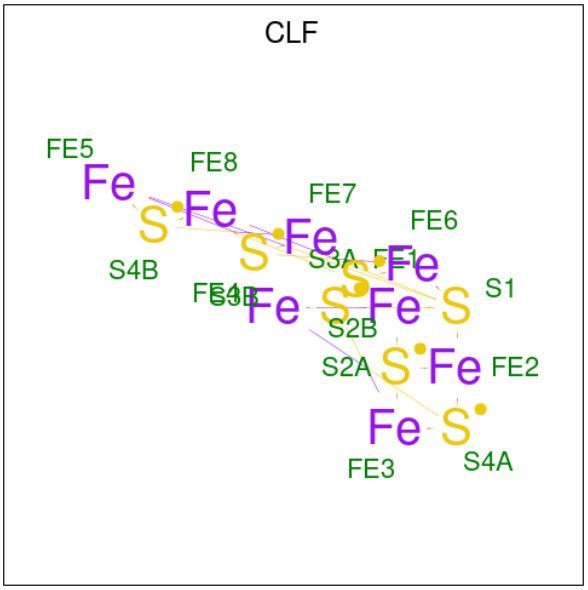
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 7 7	0	0
4	C	1	Total C O 14 7 7	0	0

- Molecule 5 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe_7MoS_9).



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

- Molecule 6 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).

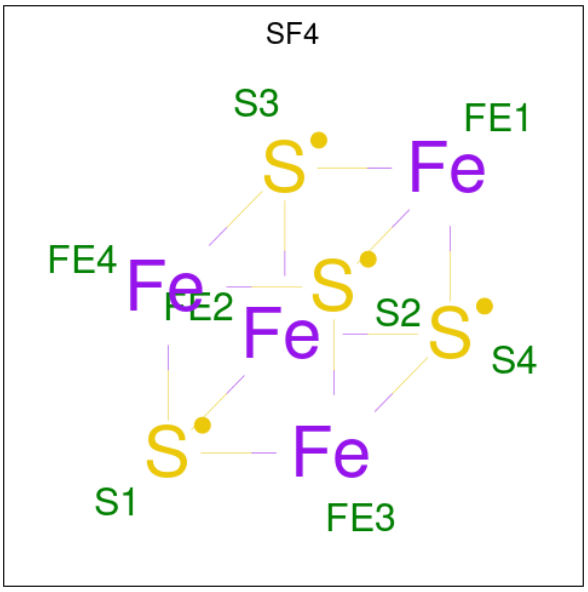


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 15 8 7	0	0
6	C	1	Total Fe S 15 8 7	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

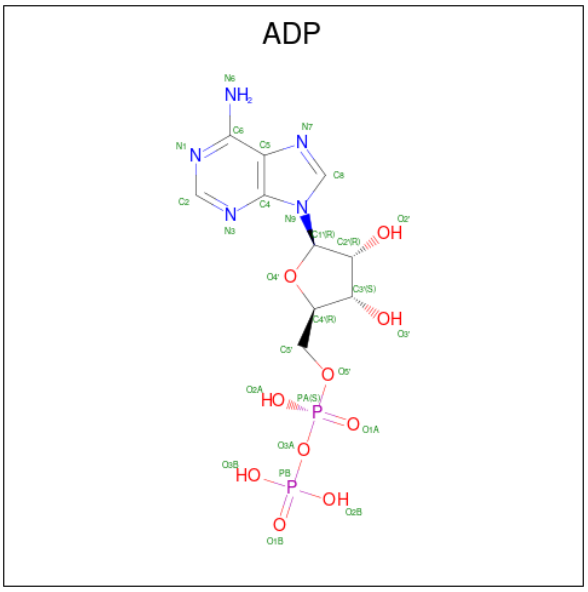


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Fe S 8 4 4	0	0
8	G	1	Total Fe S 8 4 4	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

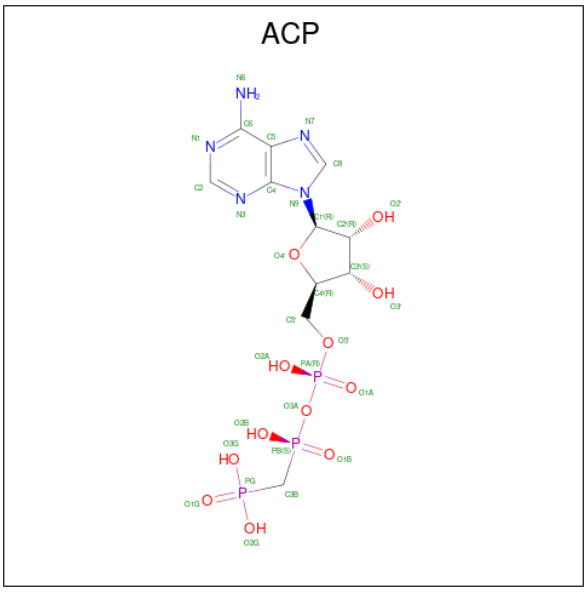
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total Mg 1 1	0	0
9	F	1	Total Mg 1 1	0	0
9	G	1	Total Mg 1 1	0	0
9	H	1	Total Mg 1 1	0	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	H	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

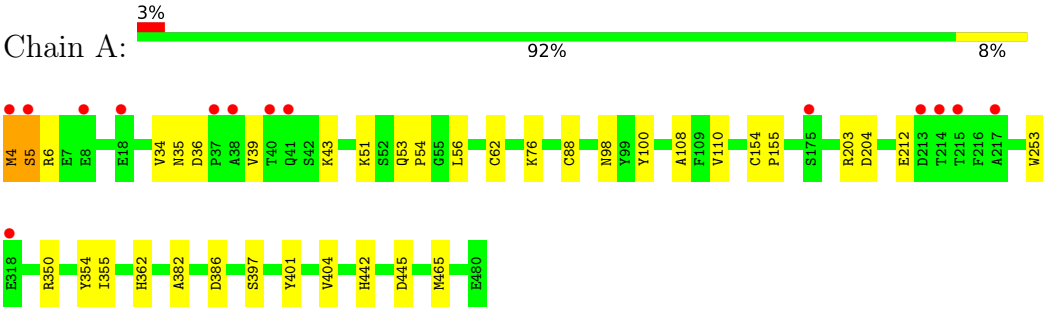
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	297	Total	O	0	0
			297	297		
12	B	525	Total	O	0	0
			525	525		
12	C	424	Total	O	0	0
			424	424		
12	D	510	Total	O	0	0
			510	510		
12	E	79	Total	O	0	0
			79	79		
12	F	95	Total	O	0	0
			95	95		
12	G	130	Total	O	0	0
			130	130		
12	H	138	Total	O	0	0
			138	138		

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.

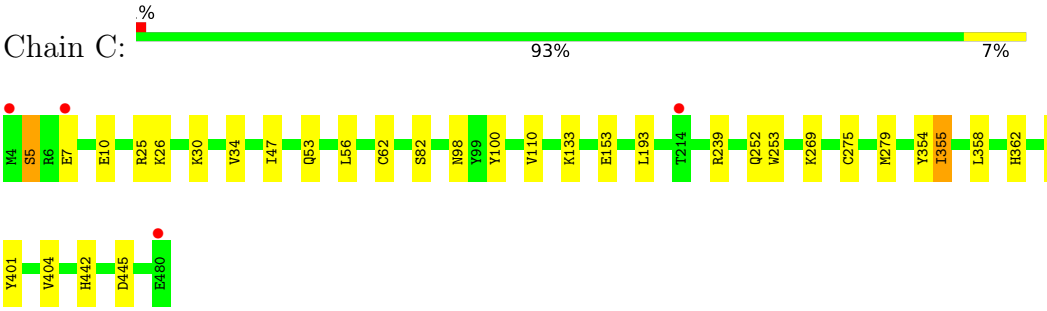
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain A:



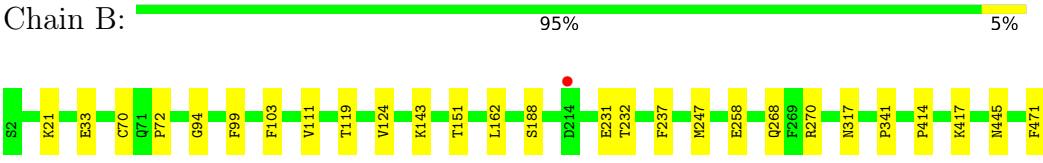
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain C:



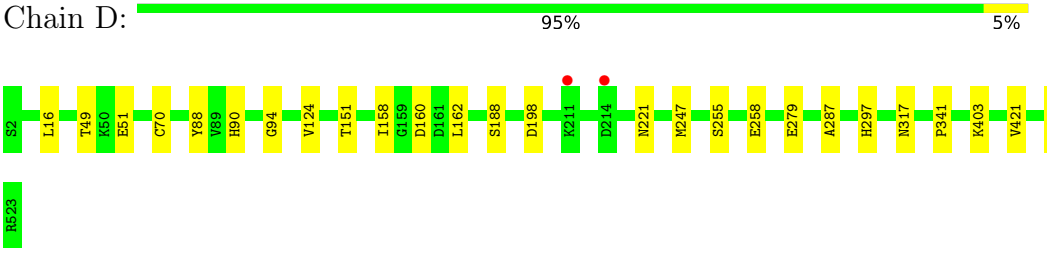
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B:



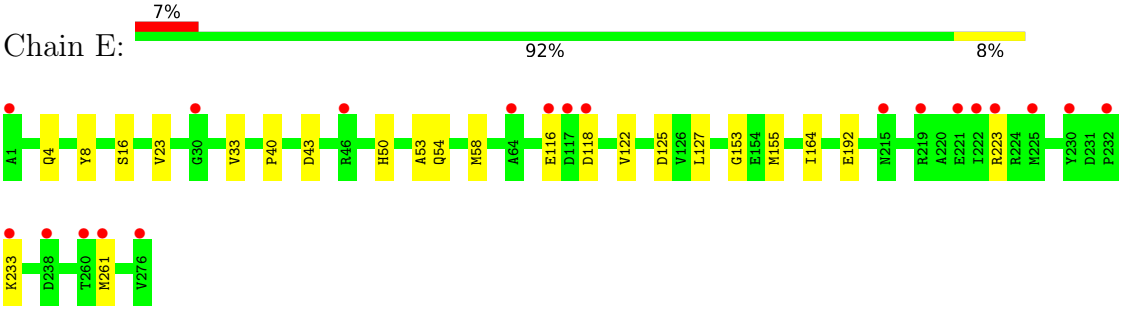
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:



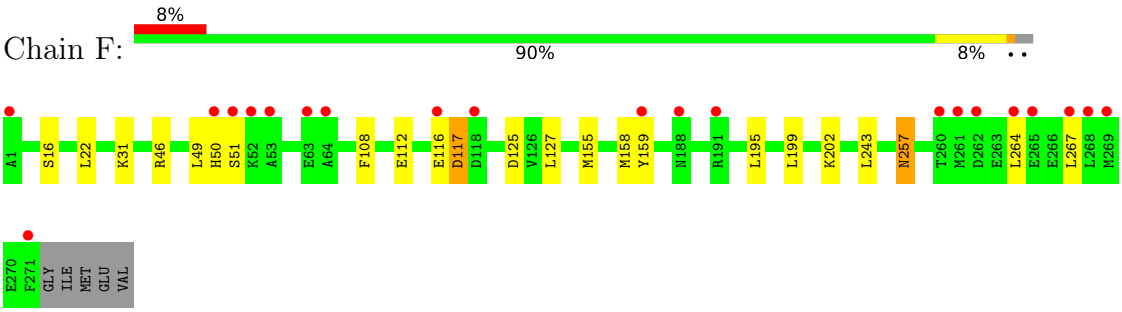
• Molecule 3: Nitrogenase iron protein 1

Chain E:



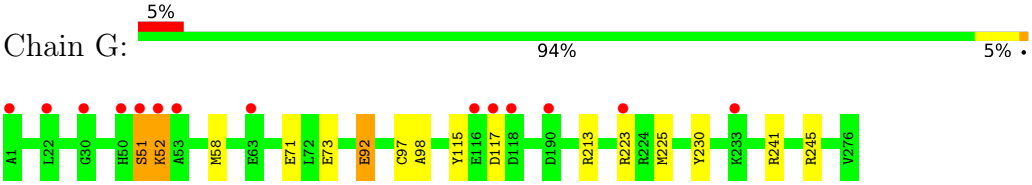
• Molecule 3: Nitrogenase iron protein 1

Chain F:



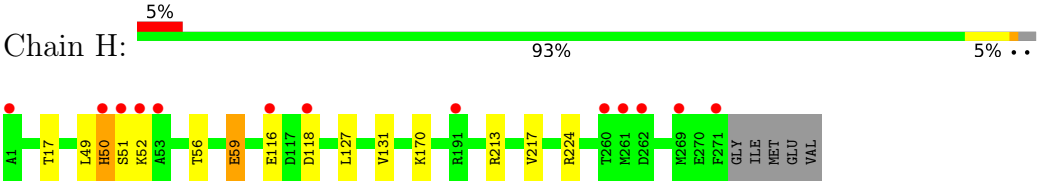
• Molecule 3: Nitrogenase iron protein 1

Chain G:



• Molecule 3: Nitrogenase iron protein 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.20Å 120.41Å 264.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 1.90 19.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.84-1.90) 97.7 (19.84-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.145 , 0.187 0.146 , 0.187	Depositor DCC
R_{free} test set	13601 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26654	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, CLF, ICS, HCA, FE, SF4, ACP

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	0.46	0/3879	0.58	0/5229
1	C	0.51	0/3879	0.60	0/5229
2	B	0.51	0/4280	0.59	0/5786
2	D	0.53	0/4289	0.60	0/5798
3	E	0.36	0/2114	0.52	0/2846
3	F	0.38	0/2077	0.55	0/2798
3	G	0.43	0/2113	0.57	0/2846
3	H	0.41	0/2077	0.55	0/2798
All	All	0.47	0/24708	0.58	0/33330

There are no bond length outliers.

There are no bond angle outliers.

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	3791	0	3731	22	0
1	C	3791	0	3731	18	0
2	B	4174	0	4088	19	0
2	D	4183	0	4093	14	0
3	E	2090	0	2107	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2053	0	2069	14	0
3	G	2089	0	2107	11	0
3	H	2053	0	2069	8	0
4	A	14	0	6	3	0
4	C	14	0	6	2	0
5	A	18	0	0	0	0
5	C	18	0	0	0	0
6	A	15	0	0	0	0
6	C	15	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	E	8	0	0	0	0
8	G	8	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
10	E	27	0	12	0	0
10	G	27	0	12	0	0
11	F	31	0	14	0	0
11	H	31	0	14	0	0
12	A	297	0	0	5	0
12	B	525	0	0	5	0
12	C	424	0	0	2	0
12	D	510	0	0	2	0
12	E	79	0	0	1	0
12	F	95	0	0	2	0
12	G	130	0	0	1	0
12	H	138	0	0	0	0
All	All	26654	0	24059	107	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 2.

All (107) 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:F:257:ASN:ND2	12:F:1371:HOH:O	2.25	0.70
2:B:317:ASN:ND2	12:B:2007:HOH:O	2.23	0.70
3:H:49:LEU:O	3:H:51:SER:N	2.29	0.66
3:F:202:LYS:HE3	3:F:267:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:116:GLU:HG3	3:E:118:ASP:H	1.65	0.62
3:G:213:ARG:NH2	12:G:1394:HOH:O	2.33	0.62
3:G:51:SER:O	3:G:52:LYS:HB2	1.99	0.62
2:B:258:GLU:OE2	12:B:1744:HOH:O	2.16	0.61
2:B:33:GLU:OE1	12:B:1906:HOH:O	2.16	0.61
3:H:50:HIS:HB3	3:H:224:ARG:O	2.00	0.61
2:D:317:ASN:ND2	12:D:1891:HOH:O	2.10	0.58
3:E:16:SER:OG	3:E:125:ASP:OD2	2.18	0.57
1:A:212:GLU:HG2	12:A:1651:HOH:O	2.05	0.57
3:F:49:LEU:O	3:F:51:SER:N	2.29	0.55
1:A:442:HIS:CG	4:A:1494:HCA:H52	2.42	0.55
1:A:315:LYS:NZ	12:A:1771:HOH:O	2.40	0.54
1:C:253:TRP:HB3	1:C:279:MET:HE1	1.88	0.54
2:B:231:GLU:HB3	2:B:237:PHE:CZ	2.43	0.54
1:C:269:LYS:NZ	12:C:1863:HOH:O	2.40	0.53
3:F:158:MET:SD	3:F:195:LEU:HD21	2.49	0.52
1:A:43:LYS:NZ	12:A:1786:HOH:O	2.41	0.52
2:B:70:CYS:HB2	2:B:188:SER:HB2	1.92	0.52
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.91	0.52
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.46	0.51
3:G:115:TYR:C	3:G:117:ASP:H	2.14	0.51
3:F:257:ASN:N	3:F:257:ASN:OD1	2.42	0.50
3:F:158:MET:HG2	3:F:199:LEU:HD22	1.92	0.50
2:D:124:VAL:HG11	3:G:58:MET:HG3	1.92	0.50
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.94	0.50
1:A:203:ARG:HD2	1:A:204:ASP:OD1	2.11	0.50
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.94	0.49
2:B:124:VAL:HG11	3:E:58:MET:HG3	1.93	0.49
3:G:92:GLU:CD	3:H:170:LYS:HZ1	2.16	0.49
2:D:49:THR:OG1	2:D:51[A]:GLU:HG2	2.13	0.49
1:A:442:HIS:ND1	4:A:1494:HCA:H52	2.28	0.49
2:B:21:LYS:HG2	12:B:1979:HOH:O	2.12	0.48
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.94	0.48
1:A:4:MET:O	1:A:5:SER:HB3	2.14	0.48
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.94	0.48
1:C:442:HIS:CG	4:C:1494:HCA:H52	2.48	0.48
2:D:445:ASN:HB2	2:D:472:PRO:O	2.13	0.48
3:E:153:GLY:HA3	3:E:192:GLU:HG3	1.96	0.48
2:D:70:CYS:HB2	2:D:188:SER:HB2	1.95	0.48
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.49	0.47
1:A:36:ASP:HB3	1:A:39:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:116:GLU:O	3:H:118:ASP:N	2.48	0.47
1:C:239:ARG:HD2	1:C:252:GLN:OE1	2.15	0.47
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.97	0.47
2:D:279:GLU:HG2	12:D:1775:HOH:O	2.14	0.46
3:E:40:PRO:HD2	3:E:127:LEU:HD13	1.98	0.46
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.98	0.45
1:C:5:SER:OG	1:C:7:GLU:HG2	2.15	0.45
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.51	0.45
3:F:16:SER:OG	3:F:125:ASP:OD2	2.30	0.45
1:C:62:CYS:HB3	2:D:94:GLY:HA3	1.99	0.45
2:B:103:PHE:HB3	2:B:111:VAL:HG21	1.99	0.45
2:B:268:GLN:HE21	2:B:270:ARG:NH2	2.14	0.44
2:B:414:PRO:HA	2:B:417:LYS:HE3	1.99	0.44
1:C:10:GLU:HG3	1:C:34:VAL:HG21	1.99	0.44
3:H:17:THR:HG21	3:H:217:VAL:CG1	2.48	0.44
1:A:442:HIS:HB3	4:A:1494:HCA:O5	2.18	0.44
2:D:198:ASP:HB2	2:D:297:HIS:O	2.17	0.44
1:C:25:ARG:NH2	1:C:26:LYS:HG3	2.33	0.44
3:G:225:MET:HG3	3:G:230:TYR:HB2	2.00	0.44
2:B:151:THR:HG23	2:B:162:LEU:HD11	2.00	0.43
1:C:30:LYS:HD2	1:C:47:ILE:HD13	1.99	0.43
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.53	0.43
1:A:51:LYS:HB3	1:A:51:LYS:HE2	1.63	0.43
3:F:22:LEU:HD13	3:F:243:LEU:HG	2.01	0.43
2:B:445:ASN:HB2	2:B:472:PRO:O	2.19	0.43
3:F:31:LYS:NZ	12:F:1357:HOH:O	2.50	0.43
1:A:253:TRP:HA	1:A:254:SER:HA	1.76	0.43
3:E:23:VAL:HG13	3:E:33:VAL:HG11	2.01	0.43
2:B:247:MET:HG2	2:B:341:PRO:CD	2.48	0.43
2:D:403:LYS:HE2	2:D:421:VAL:O	2.19	0.42
3:E:261:MET:HG2	3:F:46:ARG:HH21	1.83	0.42
3:F:108:PHE:CE1	3:F:112:GLU:HG3	2.54	0.42
2:D:247:MET:HG2	2:D:341:PRO:HD3	2.01	0.42
3:F:159:TYR:CD1	3:F:264:LEU:HD13	2.54	0.42
3:G:92:GLU:OE1	3:H:170:LYS:NZ	2.53	0.42
1:C:53:GLN:HB2	1:C:56:LEU:HD12	2.00	0.42
3:G:241:ARG:O	3:G:245:ARG:HG3	2.19	0.42
2:B:143:LYS:NZ	12:B:1992:HOH:O	2.53	0.42
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.88	0.42
3:E:43:ASP:OD1	12:E:1317:HOH:O	2.22	0.42
3:G:223:ARG:HD2	3:G:230:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:HB2	1:A:56:LEU:HD12	2.01	0.42
3:F:49:LEU:C	3:F:51:SER:H	2.19	0.42
3:H:56:THR:OG1	3:H:59:GLU:HB3	2.19	0.42
1:A:154:CYS:HB2	1:A:155:PRO:HD3	2.02	0.41
3:E:4:GLN:HG2	3:E:122:VAL:HB	2.02	0.41
1:C:82:SER:HB3	1:C:153:GLU:OE2	2.20	0.41
2:D:158:ILE:HG22	3:G:97:CYS:HB2	2.02	0.41
1:A:6:ARG:NH2	1:A:35:ASN:O	2.53	0.41
12:A:1589:HOH:O	2:B:119:THR:HB	2.21	0.41
1:A:34:VAL:HG12	1:A:397:SER:HA	2.03	0.41
1:A:76:LYS:O	1:A:108:ALA:HA	2.20	0.41
1:A:350:ARG:HD3	12:A:1690:HOH:O	2.20	0.41
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.56	0.41
2:D:90:HIS:NE2	2:D:160:ASP:OD2	2.54	0.41
2:B:72:PRO:HG2	2:B:99:PHE:CZ	2.56	0.41
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.91	0.40
3:F:155:MET:HB3	3:F:159:TYR:HE2	1.86	0.40
1:C:133:LYS:HE3	12:C:1896:HOH:O	2.21	0.40
1:C:442:HIS:HB3	4:C:1494:HCA:O5	2.22	0.40
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.21	0.40
3:G:98:ALA:HB3	3:H:131:VAL:HB	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	475/477 (100%)	459 (97%)	14 (3%)	2 (0%)	34 24
1	C	475/477 (100%)	457 (96%)	16 (3%)	2 (0%)	34 24
2	B	520/522 (100%)	511 (98%)	9 (2%)	0	100 100
2	D	521/522 (100%)	511 (98%)	9 (2%)	1 (0%)	47 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	274/276 (99%)	261 (95%)	10 (4%)	3 (1%)	14 5
3	F	269/276 (98%)	257 (96%)	10 (4%)	2 (1%)	22 12
3	G	274/276 (99%)	263 (96%)	9 (3%)	2 (1%)	22 12
3	H	269/276 (98%)	256 (95%)	11 (4%)	2 (1%)	22 12
All	All	3077/3102 (99%)	2975 (97%)	88 (3%)	14 (0%)	29 18

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	50	HIS
3	F	50	HIS
3	G	52	LYS
3	H	50	HIS
3	E	54	GLN
3	E	53	ALA
1	A	5	SER
1	C	5	SER
2	D	255	SER
3	F	117	ASP
3	G	51	SER
3	H	52	LYS
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	407/407 (100%)	400 (98%)	7 (2%)	60 57
1	C	407/407 (100%)	402 (99%)	5 (1%)	71 70
2	B	454/454 (100%)	454 (100%)	0	100 100
2	D	455/454 (100%)	452 (99%)	3 (1%)	84 84
3	E	222/222 (100%)	219 (99%)	3 (1%)	67 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	218/222 (98%)	214 (98%)	4 (2%)	59 55
3	G	222/222 (100%)	219 (99%)	3 (1%)	67 65
3	H	218/222 (98%)	215 (99%)	3 (1%)	67 65
All	All	2603/2610 (100%)	2575 (99%)	28 (1%)	73 73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	88	CYS
1	A	98	ASN
1	A	362	HIS
1	A	401	TYR
1	A	445	ASP
1	A	465	MET
1	C	98	ASN
1	C	355	ILE
1	C	362	HIS
1	C	401	TYR
1	C	445	ASP
2	D	16	LEU
2	D	88	TYR
2	D	258	GLU
3	E	155	MET
3	E	223	ARG
3	E	233	LYS
3	F	116	GLU
3	F	117	ASP
3	F	127	LEU
3	F	257	ASN
3	G	71	GLU
3	G	73	GLU
3	G	92	GLU
3	H	59	GLU
3	H	127	LEU
3	H	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	-	13,13,13	1.00	0	14,18,18	1.73	4 (28%)
10	ADP	E	1292	9	24,29,29	1.00	2 (8%)	29,45,45	1.42	4 (13%)
5	ICS	C	1496	1	18,30,30	2.53	11 (61%)	-		
10	ADP	G	1292	9	24,29,29	1.01	1 (4%)	29,45,45	1.32	4 (13%)
11	ACP	F	1292	9	27,33,33	1.71	4 (14%)	32,52,52	1.52	7 (21%)
6	CLF	A	1498	2,1	0,24,24	-	-	-		
5	ICS	A	1496	1	18,30,30	2.35	9 (50%)	-		
4	HCA	C	1494	-	13,13,13	1.27	2 (15%)	14,18,18	1.62	4 (28%)
11	ACP	H	1292	9	27,33,33	1.68	5 (18%)	32,52,52	1.45	4 (12%)
8	SF4	G	1290	3	0,12,12	-	-	-		
8	SF4	E	1290	3	0,12,12	-	-	-		
6	CLF	C	1498	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
4	HCA	A	1494	-	-	5/17/17/17	-
10	ADP	E	1292	9	-	1/12/32/32	0/3/3/3
10	ADP	G	1292	9	-	2/12/32/32	0/3/3/3
11	ACP	F	1292	9	-	0/15/38/38	0/3/3/3
6	CLF	A	1498	2,1	-	-	0/12/10/10
4	HCA	C	1494	-	-	4/17/17/17	-
11	ACP	H	1292	9	-	0/15/38/38	0/3/3/3
8	SF4	G	1290	3	-	-	0/6/5/5
8	SF4	E	1290	3	-	-	0/6/5/5
6	CLF	C	1498	2,1	-	-	0/12/10/10

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1292	ACP	PG-O1G	5.22	1.61	1.50
11	F	1292	ACP	PG-O1G	5.15	1.61	1.50
11	F	1292	ACP	PB-O3A	4.51	1.63	1.58
5	C	1496	ICS	S4B-FE7	-4.39	2.21	2.32
5	C	1496	ICS	S1B-FE6	-4.38	2.21	2.32
5	A	1496	ICS	S1B-FE6	-3.86	2.22	2.32
5	C	1496	ICS	S3B-FE6	-3.69	2.23	2.32
11	H	1292	ACP	PB-O3A	3.39	1.62	1.58
5	A	1496	ICS	S4B-FE7	-3.28	2.24	2.32
5	A	1496	ICS	S3B-FE6	-3.21	2.24	2.32
5	A	1496	ICS	S2A-FE2	-3.13	2.24	2.32
5	A	1496	ICS	S2A-FE3	-3.04	2.24	2.32
5	A	1496	ICS	S4B-FE5	-2.97	2.25	2.32
5	C	1496	ICS	S4B-FE5	-2.90	2.25	2.32
5	A	1496	ICS	S2B-FE6	-2.79	2.18	2.24
5	C	1496	ICS	S2B-FE6	-2.78	2.18	2.24
5	C	1496	ICS	S2A-FE2	-2.74	2.25	2.32
11	H	1292	ACP	PG-O2G	-2.69	1.48	1.54
5	C	1496	ICS	S5A-FE7	-2.62	2.18	2.24
11	F	1292	ACP	PG-O2G	-2.56	1.49	1.54
5	C	1496	ICS	S1B-FE5	-2.55	2.26	2.32
10	E	1292	ADP	C5-C4	2.52	1.47	1.40
11	F	1292	ACP	C5-C4	2.49	1.47	1.40
5	C	1496	ICS	S3B-FE7	-2.45	2.26	2.32
4	C	1494	HCA	O5-C7	2.42	1.29	1.22
11	H	1292	ACP	C5-C4	2.38	1.47	1.40
11	H	1292	ACP	PB-O1B	-2.35	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	1292	ADP	C5-C4	2.31	1.47	1.40
4	C	1494	HCA	C3-C7	-2.31	1.51	1.53
10	E	1292	ADP	O4'-C1'	2.25	1.44	1.41
5	A	1496	ICS	S4A-FE3	-2.19	2.27	2.32
5	C	1496	ICS	S2A-FE3	-2.14	2.27	2.32
5	C	1496	ICS	S1A-FE2	-2.04	2.27	2.32
5	A	1496	ICS	S3A-FE5	2.04	2.29	2.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	1292	ADP	N3-C2-N1	-3.52	123.17	128.68
11	H	1292	ACP	O3G-PG-C3B	3.42	114.70	106.40
11	F	1292	ACP	N3-C2-N1	-3.33	123.48	128.68
11	F	1292	ACP	O3G-PG-C3B	3.24	114.25	106.40
11	H	1292	ACP	N3-C2-N1	-3.05	123.91	128.68
10	G	1292	ADP	N3-C2-N1	-3.04	123.92	128.68
4	A	1494	HCA	O5-C7-C3	-2.86	118.20	122.25
11	H	1292	ACP	O1B-PB-C3B	2.69	116.17	109.07
4	C	1494	HCA	O4-C6-C5	2.64	122.52	114.03
11	F	1292	ACP	PB-O3A-PA	-2.63	124.23	132.56
11	F	1292	ACP	O1B-PB-C3B	2.55	115.81	109.07
4	A	1494	HCA	O6-C7-C3	2.50	117.39	113.05
10	E	1292	ADP	PA-O3A-PB	-2.45	124.41	132.83
4	A	1494	HCA	O2-C1-C2	2.38	121.99	114.35
11	F	1292	ACP	C4-C5-N7	-2.31	106.99	109.40
10	G	1292	ADP	O3B-PB-O2B	2.30	116.42	107.64
4	C	1494	HCA	O5-C7-C3	-2.24	119.09	122.25
11	H	1292	ACP	PB-O3A-PA	-2.23	125.49	132.56
4	A	1494	HCA	O4-C6-C5	2.20	121.11	114.03
10	G	1292	ADP	PA-O3A-PB	-2.20	125.29	132.83
10	G	1292	ADP	C4-C5-N7	-2.12	107.19	109.40
4	C	1494	HCA	O4-C6-O3	-2.11	118.03	123.30
10	E	1292	ADP	C3'-C2'-C1'	2.11	104.15	100.98
4	C	1494	HCA	O2-C1-C2	2.09	121.07	114.35
11	F	1292	ACP	O2B-PB-C3B	2.07	115.06	106.58
10	E	1292	ADP	C2-N1-C6	2.05	122.26	118.75
11	F	1292	ACP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1494	HCA	C2-C3-C4-C5
4	C	1494	HCA	C2-C3-C4-C5
10	G	1292	ADP	PA-O3A-PB-O2B
4	A	1494	HCA	C7-C3-C4-C5
4	C	1494	HCA	C7-C3-C4-C5
10	G	1292	ADP	PA-O3A-PB-O1B
4	A	1494	HCA	O7-C3-C4-C5
4	C	1494	HCA	O1-C1-C2-C3
10	E	1292	ADP	PA-O3A-PB-O3B
4	C	1494	HCA	O2-C1-C2-C3
4	A	1494	HCA	O1-C1-C2-C3
4	A	1494	HCA	O2-C1-C2-C3

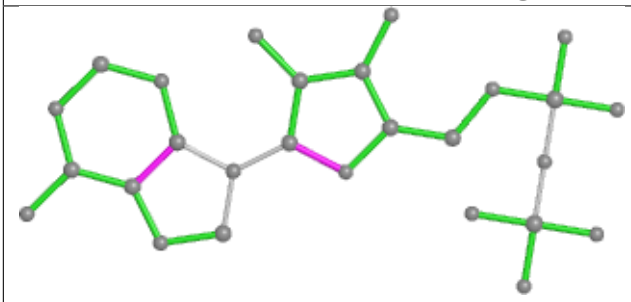
There are no ring outliers.

2 monomers are involved in 5 short contacts:

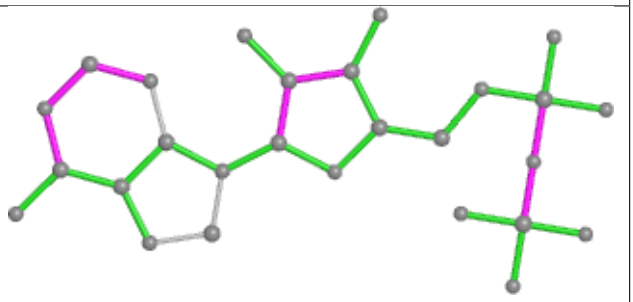
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1494	HCA	3	0
4	C	1494	HCA	2	0

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 then 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.

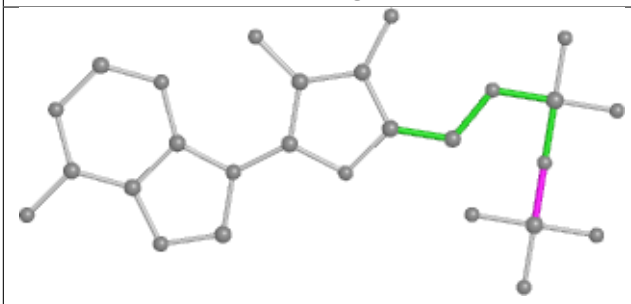
Ligand ADP E 1292



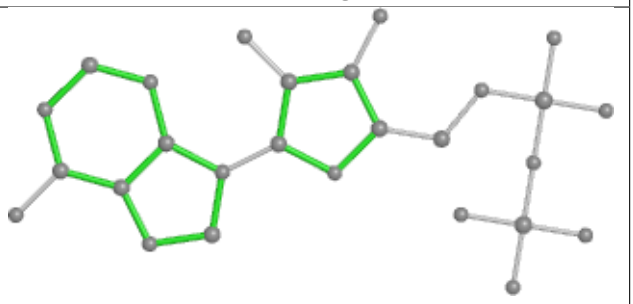
Bond lengths



Bond angles

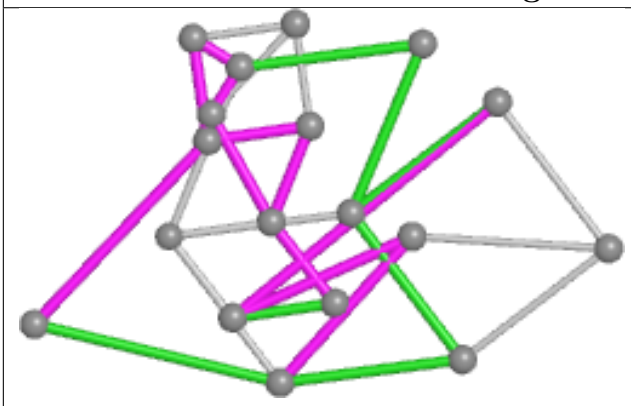


Torsions

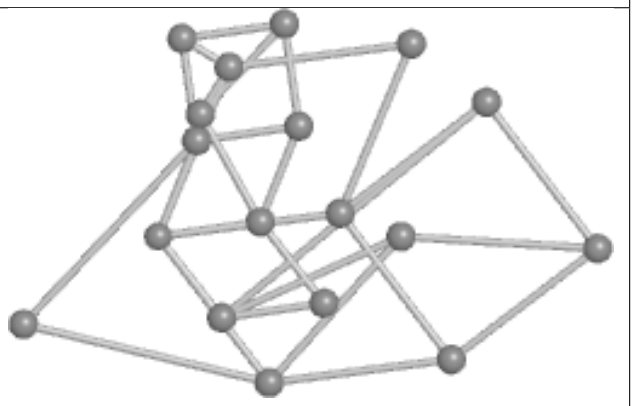


Rings

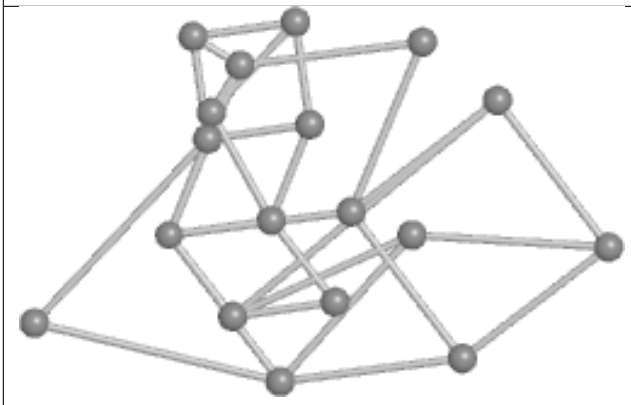
Ligand ICS C 1496



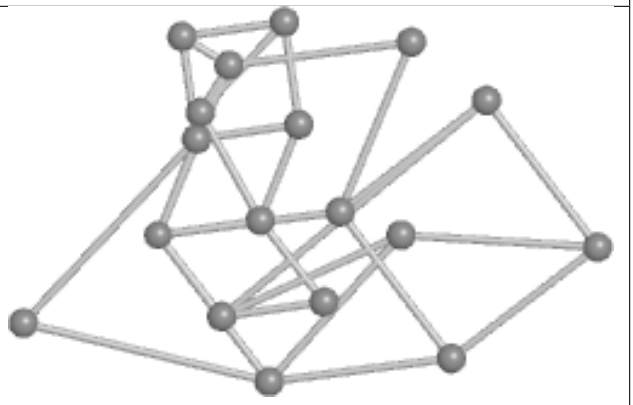
Bond lengths



Bond angles

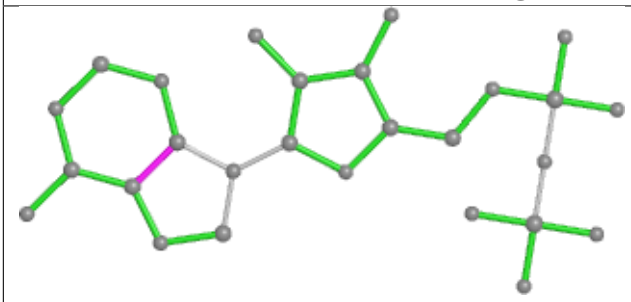


Torsions

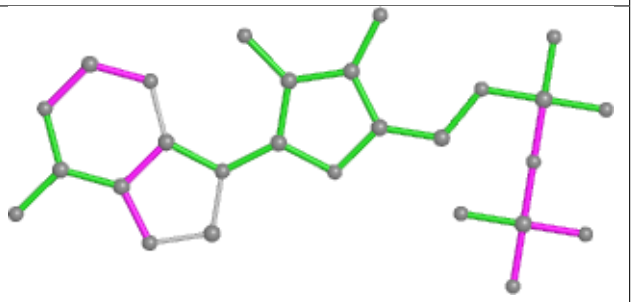


Rings

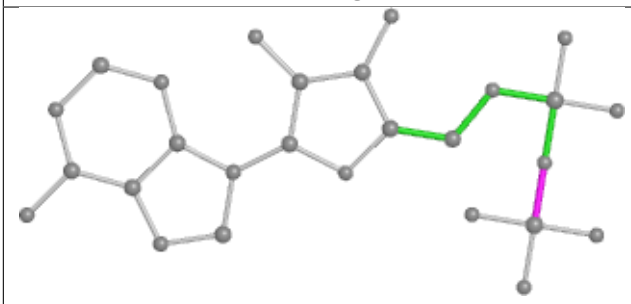
Ligand ADP G 1292



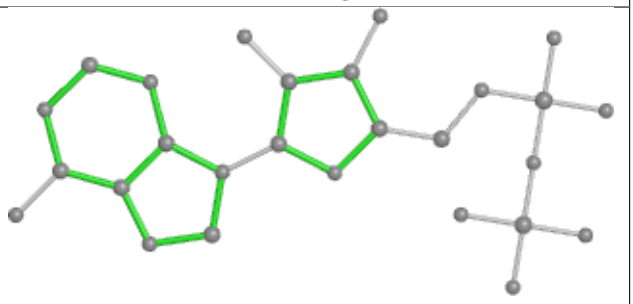
Bond lengths



Bond angles

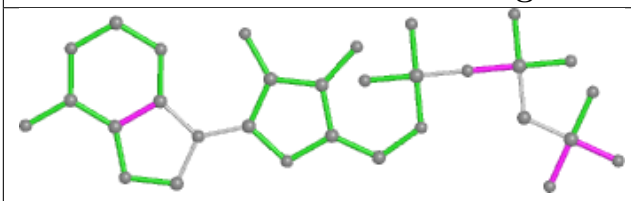


Torsions

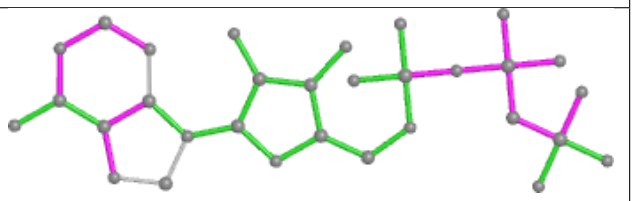


Rings

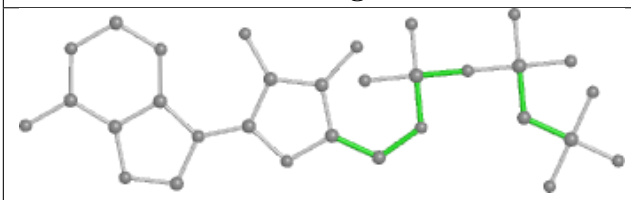
Ligand ACP F 1292



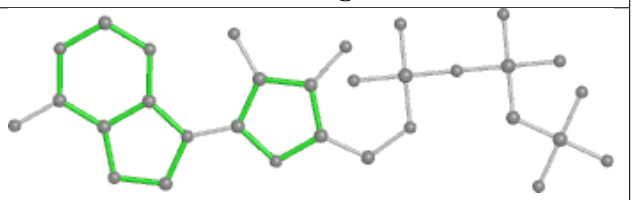
Bond lengths



Bond angles

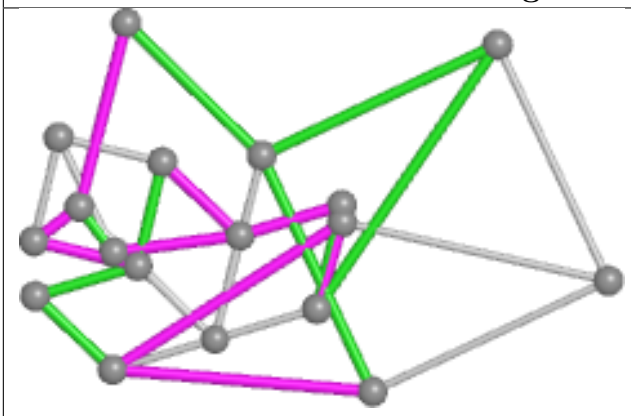


Torsions

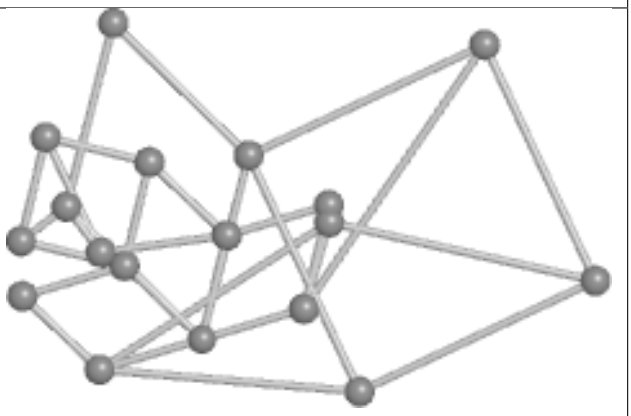


Rings

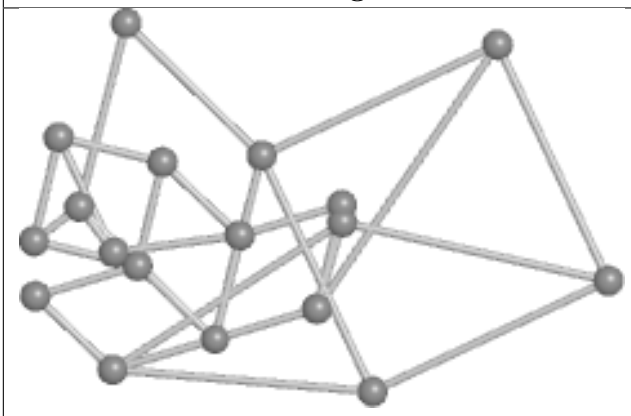
Ligand ICS A 1496



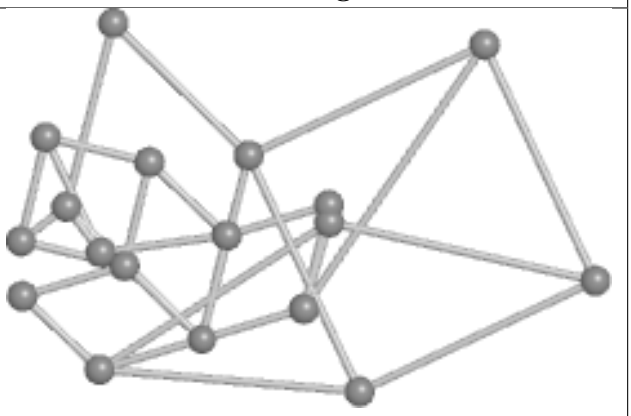
Bond lengths



Bond angles

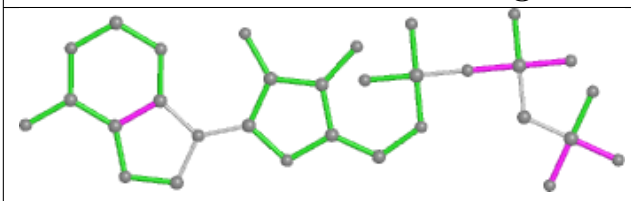


Torsions

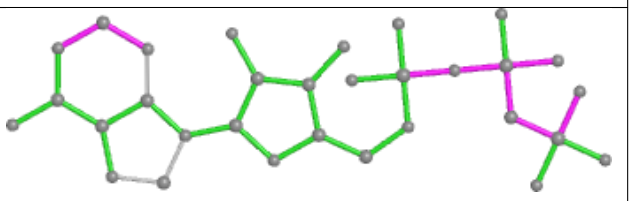


Rings

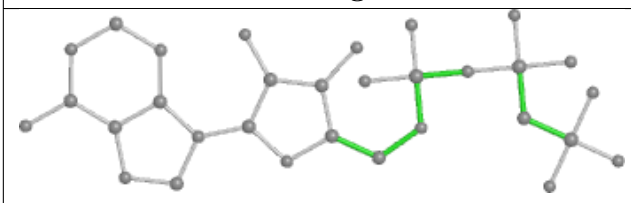
Ligand ACP H 1292



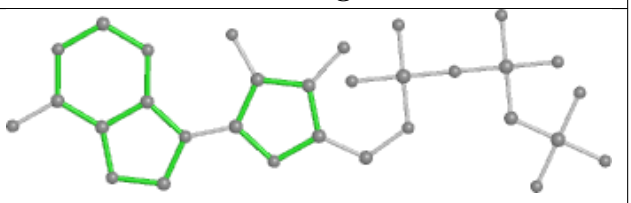
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	477/477 (100%)	-0.33	14 (2%)	51	54	13, 25, 46, 72	1 (0%)
1	C	477/477 (100%)	-0.51	4 (0%)	86	87	12, 20, 40, 85	0
2	B	522/522 (100%)	-0.58	1 (0%)	95	95	12, 19, 36, 51	0
2	D	522/522 (100%)	-0.62	2 (0%)	92	93	11, 19, 32, 48	0
3	E	271/276 (98%)	0.32	20 (7%)	14	16	20, 42, 65, 107	17 (6%)
3	F	270/276 (97%)	0.33	21 (7%)	13	14	19, 39, 80, 101	13 (4%)
3	G	276/276 (100%)	-0.18	14 (5%)	28	31	14, 30, 53, 76	10 (3%)
3	H	271/276 (98%)	-0.05	13 (4%)	30	33	14, 30, 70, 84	18 (6%)
All	All	3086/3102 (99%)	-0.30	89 (2%)	51	54	11, 24, 53, 107	59 (1%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	53	ALA	7.1
3	E	117	ASP	6.6
3	H	53	ALA	6.4
3	F	261	MET	6.3
3	F	159	TYR	6.3
3	F	269	MET	6.2
3	F	1	ALA	5.9
3	G	1	ALA	5.7
3	H	51	SER	5.4
3	E	118	ASP	5.3
1	A	38	ALA	5.1
3	G	53	ALA	4.8
1	A	40	THR	4.7
3	F	260	THR	4.7
3	F	262	ASP	4.7
1	A	214	THR	4.6

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Mol	Chain	Res	Type	RSRZ
3	H	261	MET	4.5
3	E	222	ILE	4.5
3	H	52	LYS	4.5
3	F	265	GLU	4.0
3	G	118	ASP	3.9
3	H	1	ALA	3.8
3	F	52	LYS	3.8
3	E	276	VAL	3.8
3	F	264	LEU	3.8
1	C	4	MET	3.7
3	H	262	ASP	3.7
3	F	51	SER	3.6
3	F	116	GLU	3.5
3	G	117	ASP	3.4
3	E	1	ALA	3.4
3	G	51	SER	3.4
3	F	267	LEU	3.4
3	G	52	LYS	3.4
3	H	118	ASP	3.4
3	H	271	PHE	3.3
1	C	214	THR	3.2
3	G	116	GLU	3.2
3	E	46	ARG	3.2
3	F	191	ARG	3.2
1	A	215	THR	3.0
3	E	225	MET	3.0
3	H	260	THR	3.0
3	G	190	ASP	3.0
3	H	116	GLU	2.9
3	F	118	ASP	2.9
3	H	191	ARG	2.9
3	F	271	PHE	2.8
3	E	233	LYS	2.8
1	A	41	GLN	2.8
3	E	219	ARG	2.8
3	F	63	GLU	2.7
3	G	223	ARG	2.6
3	E	261	MET	2.6
1	A	175	SER	2.6
3	E	64	ALA	2.6
3	E	230	TYR	2.6
1	A	217	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	50	HIS	2.5
1	A	4	MET	2.5
3	G	63	GLU	2.5
3	H	50	HIS	2.5
3	H	269	MET	2.5
3	E	260	THR	2.5
3	G	233	LYS	2.4
3	F	64	ALA	2.4
1	A	213	ASP	2.4
3	E	238	ASP	2.4
3	E	232	PRO	2.4
3	E	223	ARG	2.4
3	F	188	ASN	2.3
1	C	7	GLU	2.3
3	E	215	ASN	2.3
3	G	50	HIS	2.3
1	A	37	PRO	2.3
2	B	214	ASP	2.3
3	E	221	GLU	2.2
1	A	5	SER	2.2
3	G	22	LEU	2.2
3	G	30	GLY	2.2
2	D	211	LYS	2.2
1	C	480	GLU	2.2
1	A	8	GLU	2.1
1	A	318	GLU	2.1
3	E	30	GLY	2.1
3	E	116	GLU	2.1
2	D	214	ASP	2.0
3	F	268	LEU	2.0
1	A	18	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

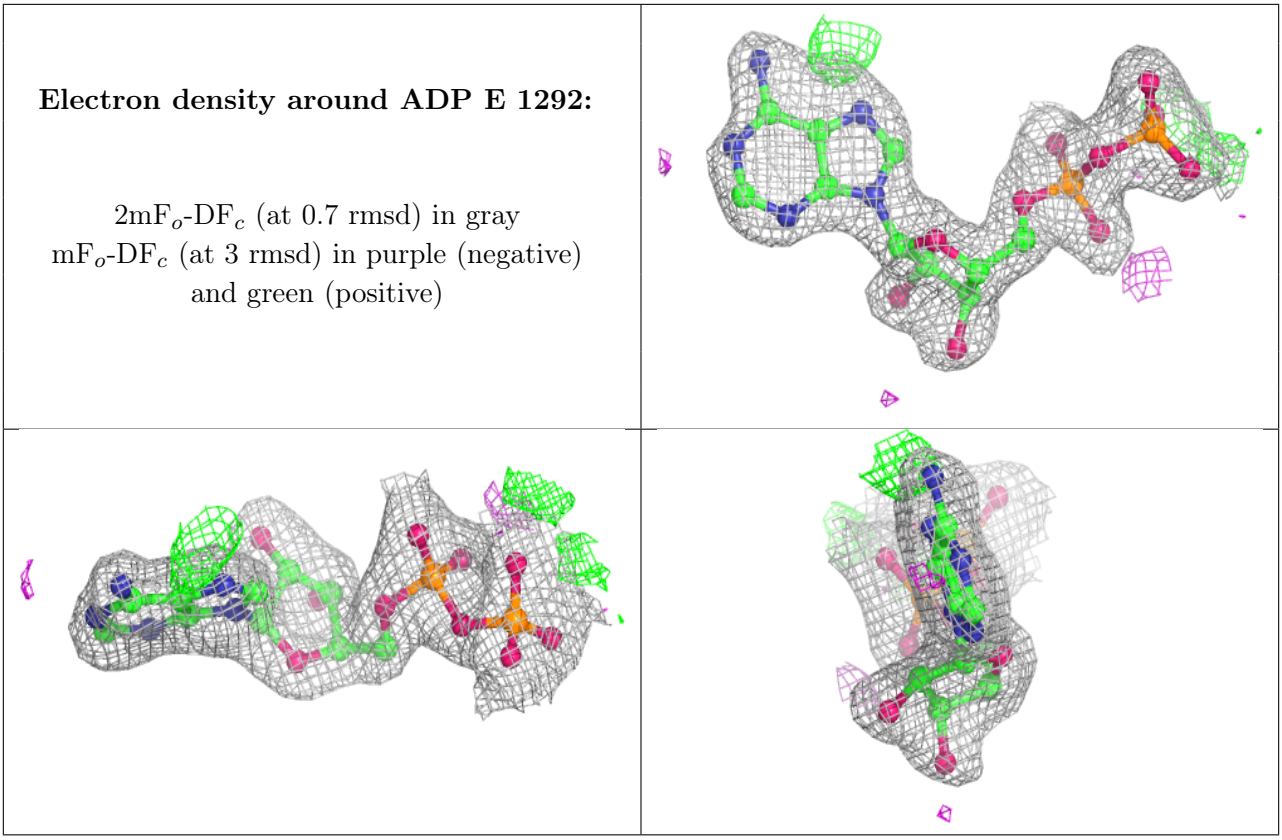
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	E	1291	1/1	0.80	0.11	39,39,39,39	0
9	MG	G	1291	1/1	0.86	0.07	32,32,32,32	0
9	MG	F	1291	1/1	0.92	0.06	27,27,27,27	0
4	HCA	A	1494	14/14	0.96	0.08	15,17,23,24	0
10	ADP	E	1292	27/27	0.96	0.09	27,39,43,47	0
11	ACP	F	1292	31/31	0.97	0.07	20,32,39,49	0
10	ADP	G	1292	27/27	0.98	0.07	19,27,35,40	0
4	HCA	C	1494	14/14	0.98	0.07	11,15,19,20	0
11	ACP	H	1292	31/31	0.98	0.07	16,23,30,41	0
6	CLF	A	1498	15/15	0.99	0.05	13,15,16,17	0
7	FE	B	1492	1/1	0.99	0.03	25,25,25,25	1
9	MG	H	1291	1/1	0.99	0.08	23,23,23,23	0
7	FE	D	1492	1/1	0.99	0.02	21,21,21,21	1
8	SF4	E	1290	8/8	0.99	0.04	16,18,19,22	0
8	SF4	G	1290	8/8	0.99	0.04	12,14,15,16	0
5	ICS	A	1496	18/18	0.99	0.05	15,18,20,20	0
5	ICS	C	1496	18/18	1.00	0.04	12,14,16,16	0
6	CLF	C	1498	15/15	1.00	0.04	11,13,13,14	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.

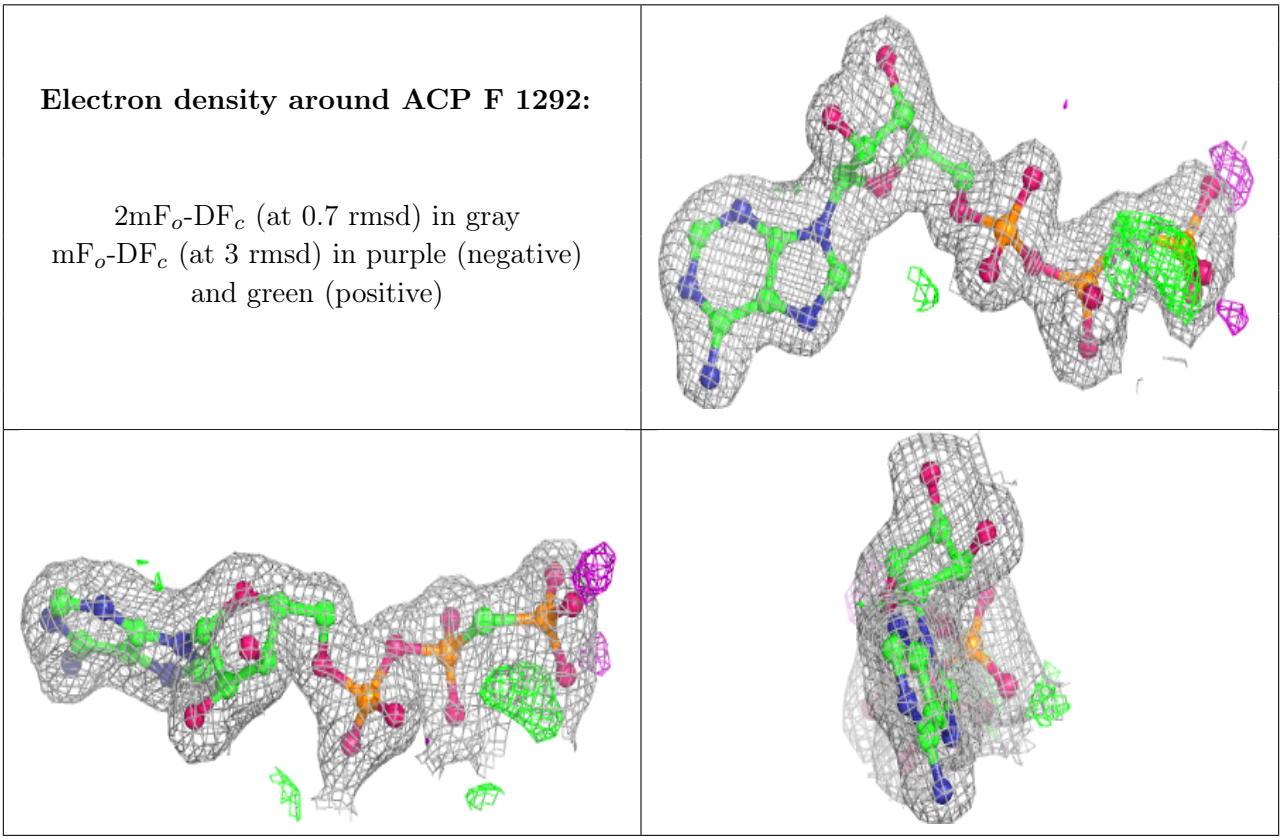
Electron density around ADP E 1292:

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



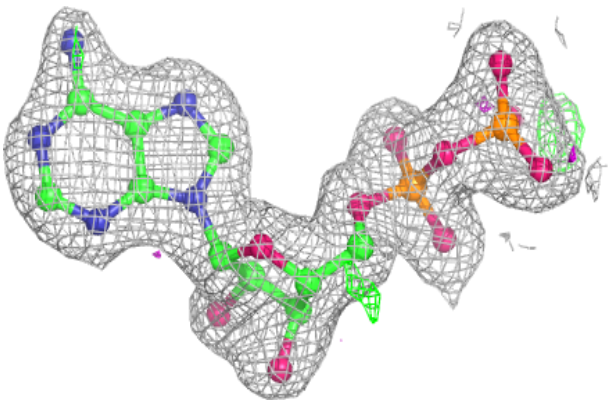
Electron density around ACP F 1292:

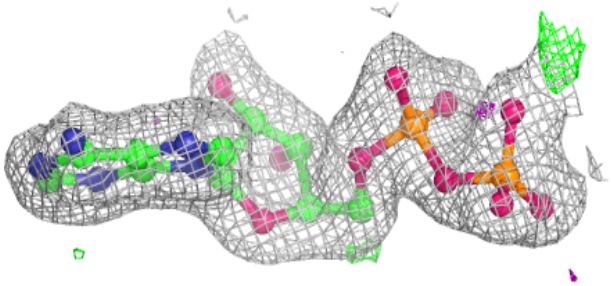
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

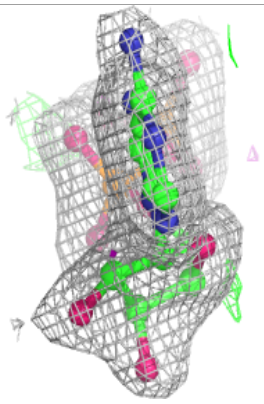


Electron density around ADP G 1292:

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

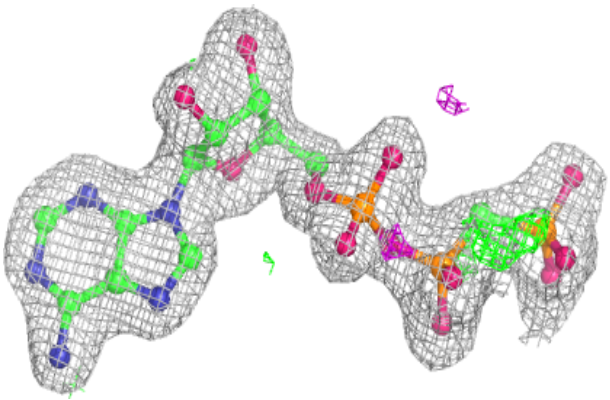


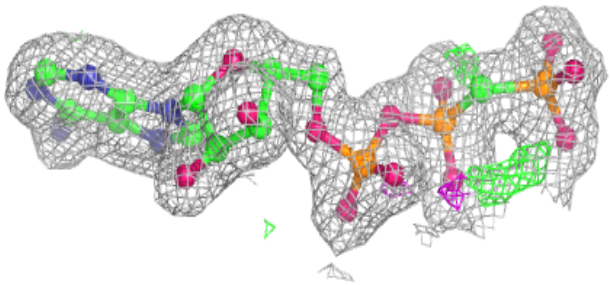


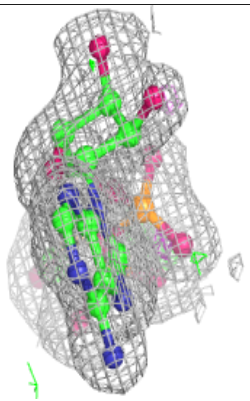


Electron density around ACP H 1292:

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

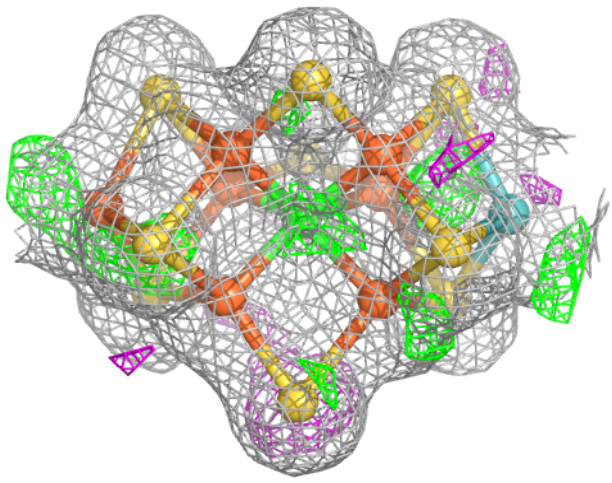


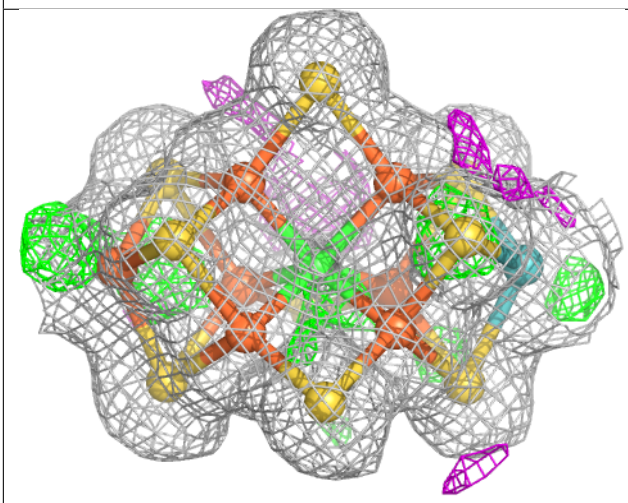


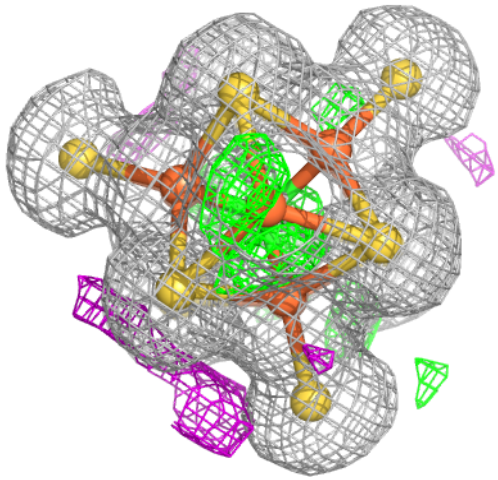


Electron density around ICS A 1496:

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

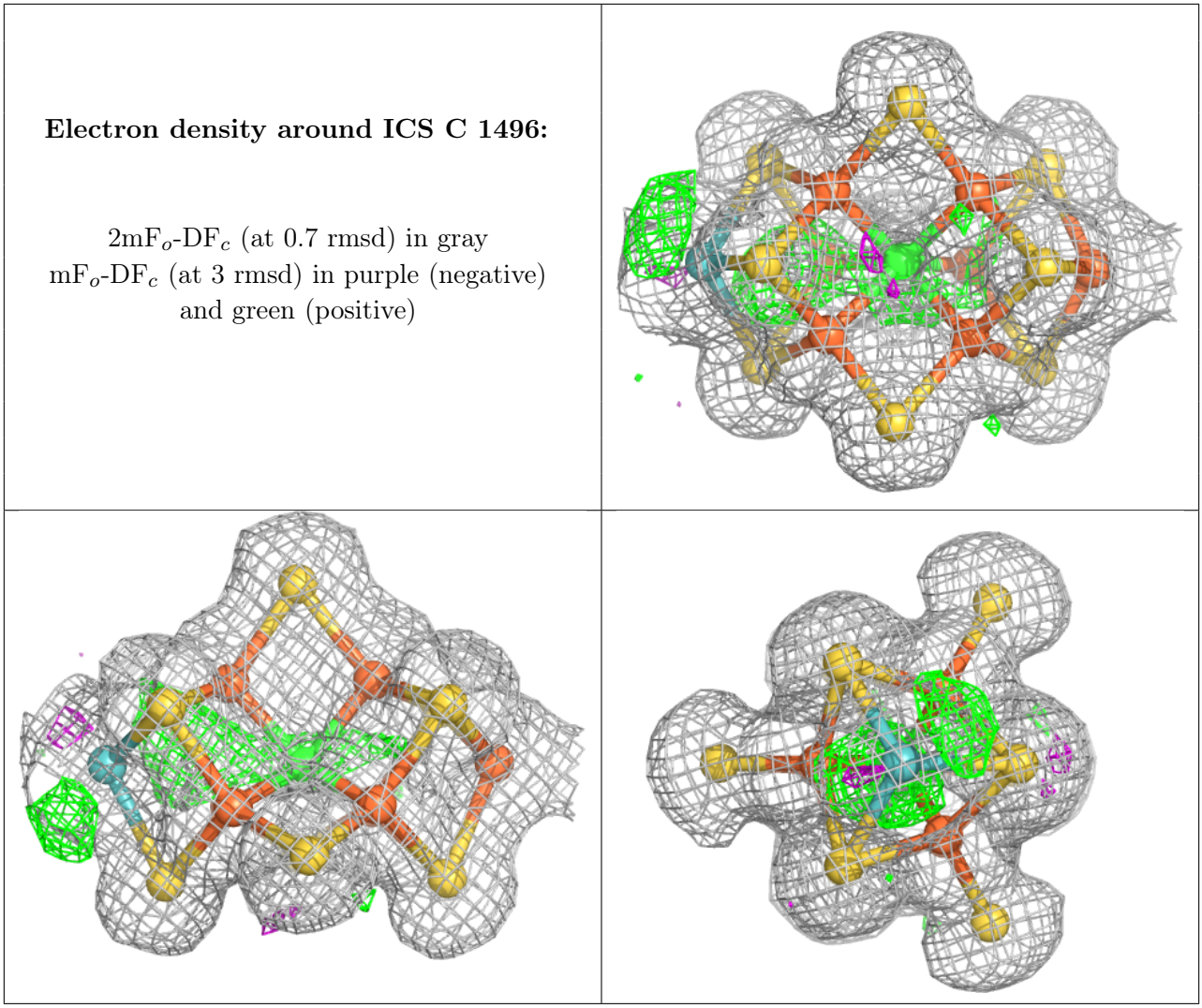






Electron density around ICS C 1496:

$2mF_o$-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.