



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:39 am BST

PDB ID : 2AFH
Title : Crystal Structure of Nucleotide-Free Av2-Av1 Complex
Authors : Tezcan, F.A.; Kaiser, J.T.; Mustafi, D.; Walton, M.Y.; Howard, J.B.; Rees, D.C.
Deposited on : 2005-07-25
Resolution : 2.10 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 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 : 2.11
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) : 2.11

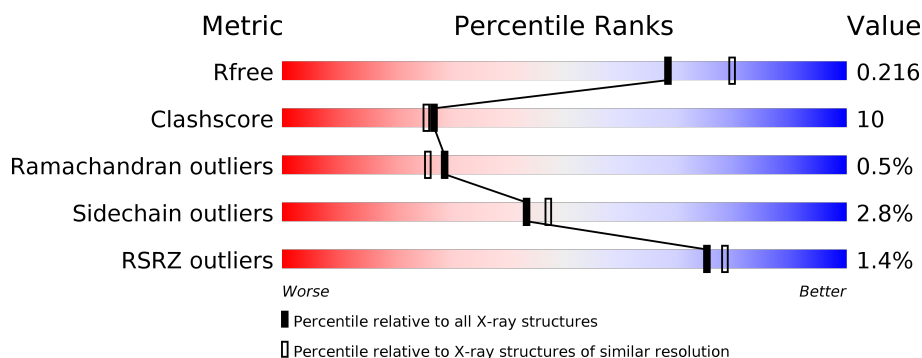
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div style="width: 81%;"></div> <div style="width: 15%;"></div> <div style="width: 4%;"></div> </div> <div>81% 15% .</div>
1	C	491	<div> <div style="width: 81%;"></div> <div style="width: 14%;"></div> <div style="width: 5%;"></div> </div> <div>81% 14% . .</div>
2	B	522	<div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div>87% 12% .</div>
2	D	522	<div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div>87% 12% .</div>
3	E	289	<div> <div style="width: 5%;"></div> <div style="width: 62%;"></div> <div style="width: 36%;"></div> <div style="width: 5%;"></div> </div> <div>5% 62% 36% .</div>
3	F	289	<div> <div style="width: 6%;"></div> <div style="width: 66%;"></div> <div style="width: 28%;"></div> <div style="width: 5%;"></div> </div> <div>6% 66% 28% 5% .</div>

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
11	PG4	E	5007	-	-	X	-
12	1PE	B	5017	-	-	X	-
12	1PE	C	5013	-	-	X	-
13	PEG	D	5020	-	-	X	-
14	P6G	D	5009	-	X	-	-
6	PGE	A	5015	-	-	X	-
6	PGE	D	5010	-	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 22638 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	8	0	0
			3782	2405	645	708	24			
1	C	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			

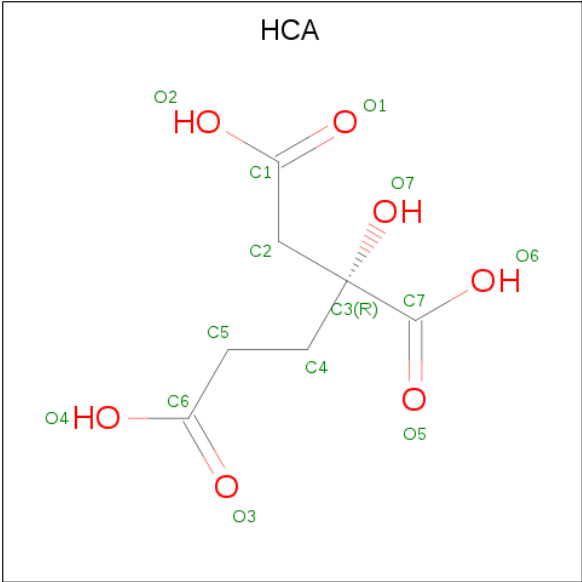
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	6	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

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

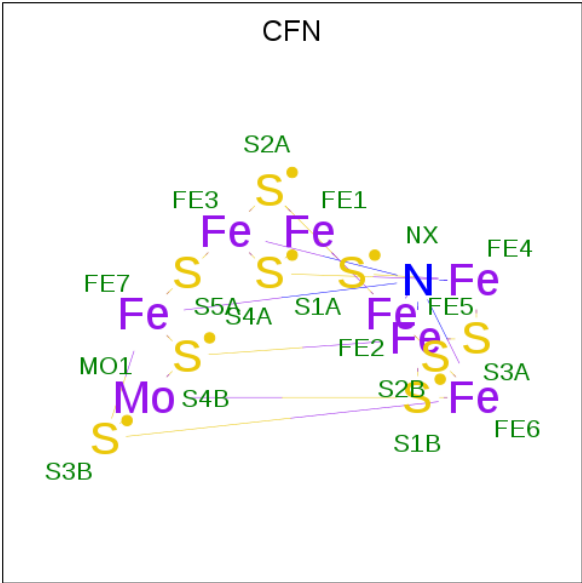
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	289	Total	C	N	O	S	0	0	0
			2187	1364	369	433	21			
3	F	286	Total	C	N	O	S	4	0	0
			2161	1349	366	425	21			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



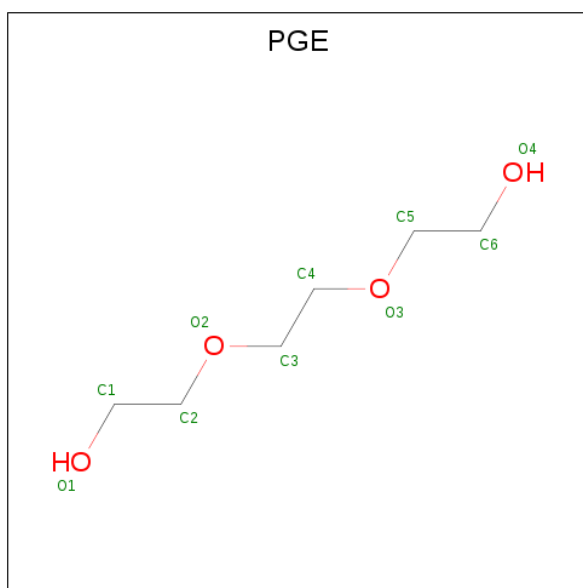
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE(7)-MO-S(9)-N CLUSTER (three-letter code: CFN) (formula: Fe₇MoNS₉).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		

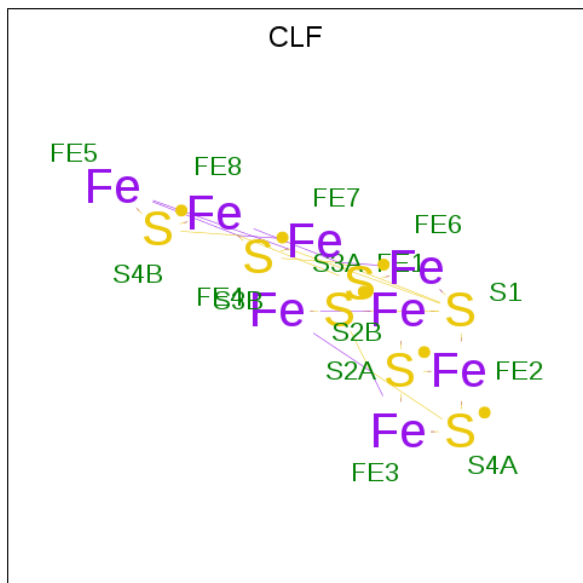
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

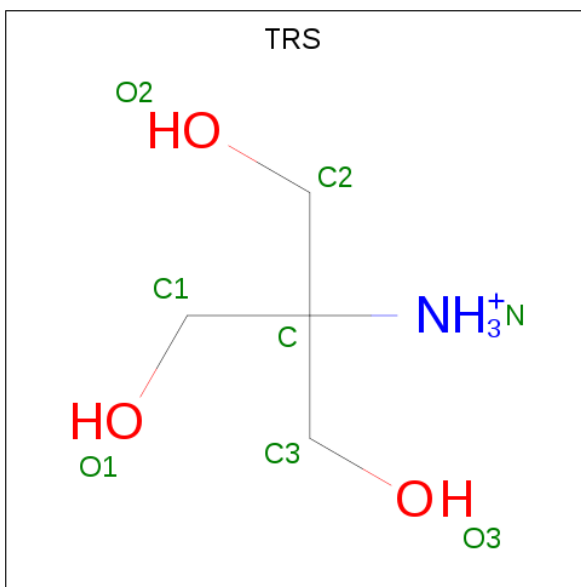
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		

- Molecule 9 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



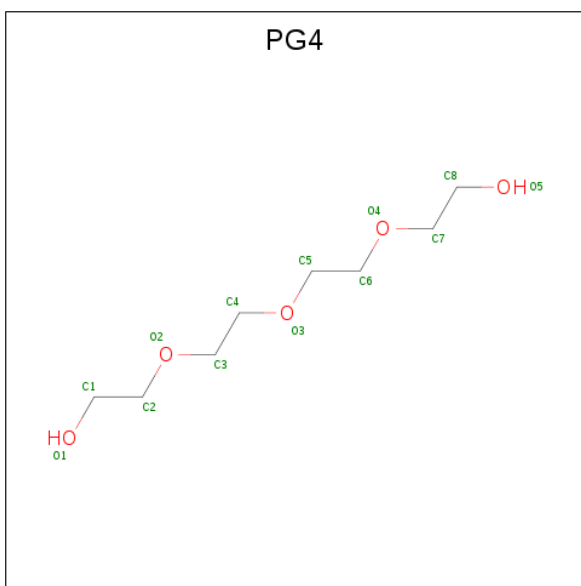
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			15	8	7		
9	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $\text{C}_4\text{H}_{12}\text{NO}_3$).



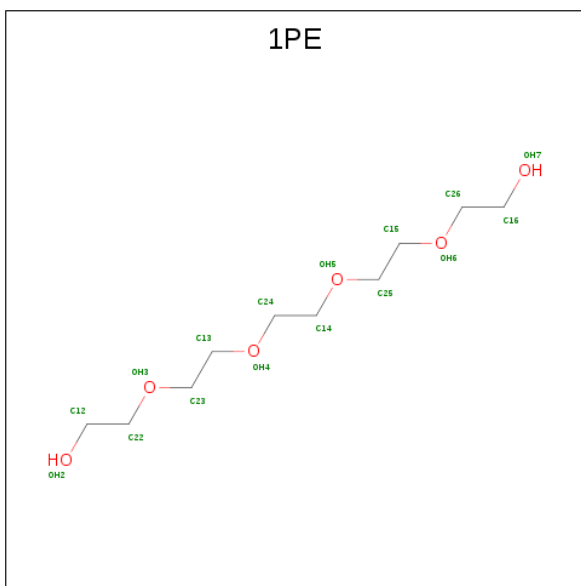
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			8	4	1	3		
10	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



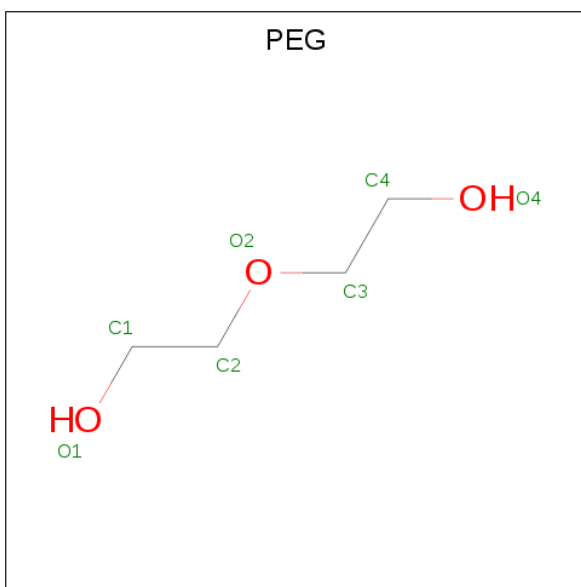
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			13	8	5		
11	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



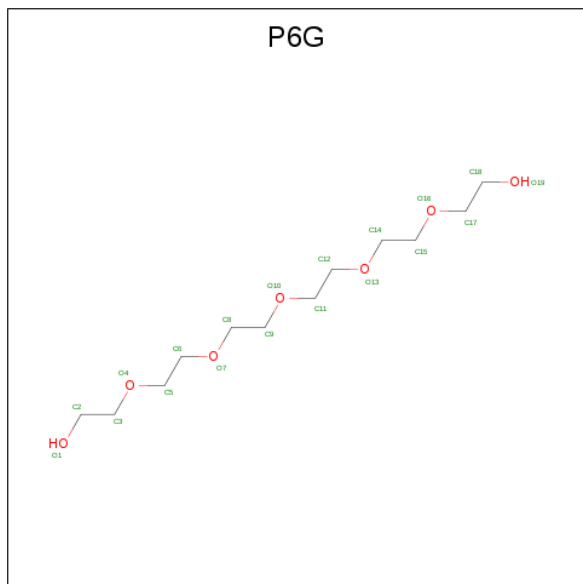
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			16	10	6		
12	C	1	Total	C	O	0	0
			16	10	6		

- Molecule 13 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



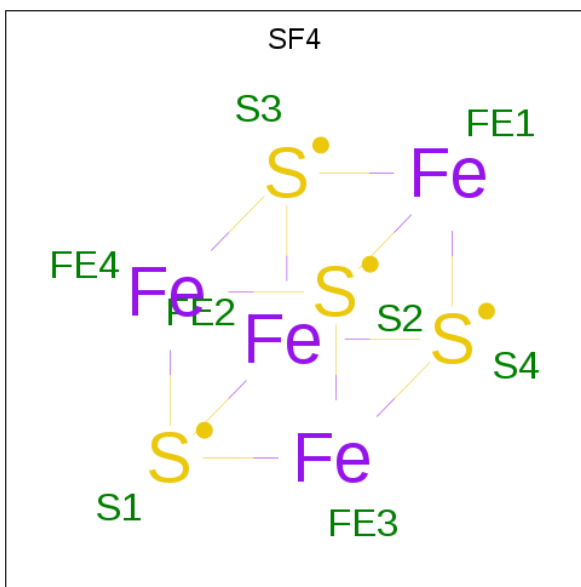
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			7	4	3		
13	D	1	Total	C	O	0	0
			7	4	3		
13	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 14 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			19	12	7		

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

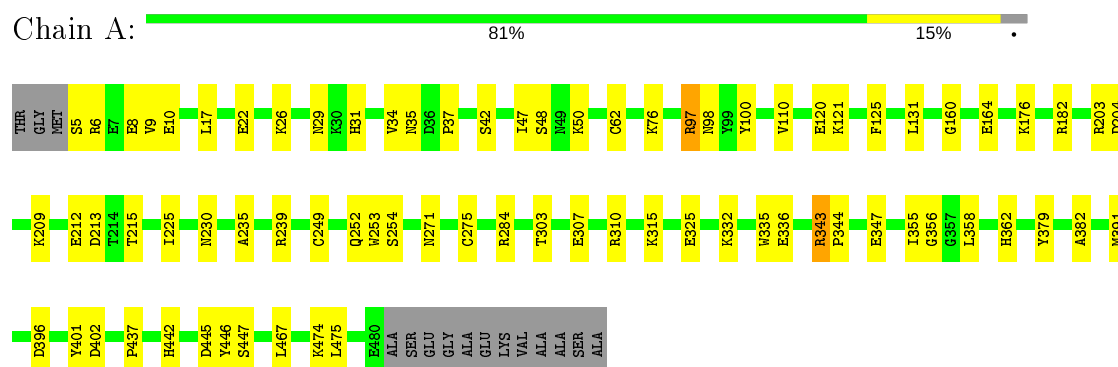
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	355	Total	O	0	0
			355	355		
16	B	594	Total	O	0	0
			594	594		
16	C	362	Total	O	0	0
			362	362		
16	D	527	Total	O	0	0
			527	527		
16	E	115	Total	O	0	0
			115	115		
16	F	118	Total	O	0	0
			118	118		

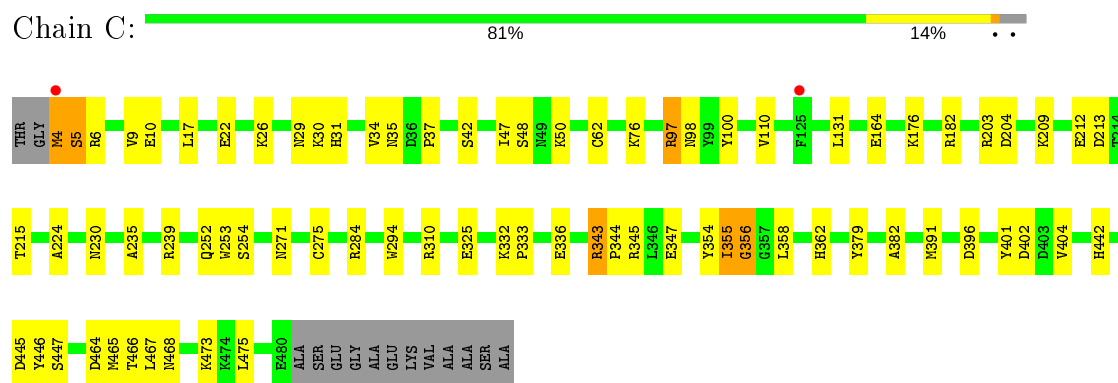
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

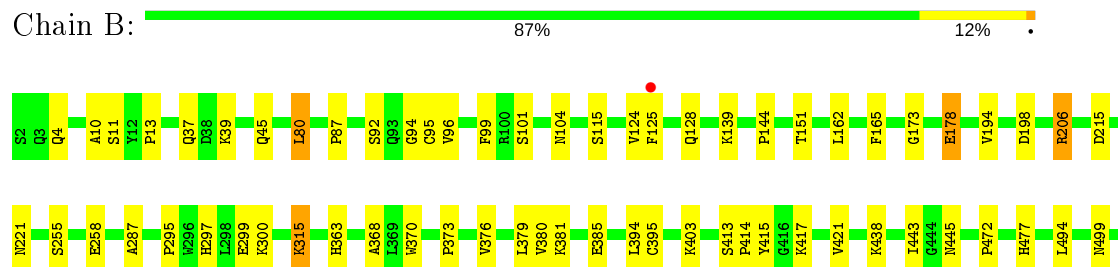
- Molecule 1: Nitrogenase molybdenum-iron protein



- Molecule 1: Nitrogenase molybdenum-iron protein

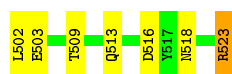
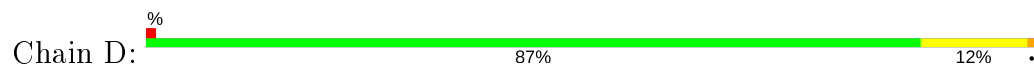


- Molecule 2: Nitrogenase molybdenum-iron protein





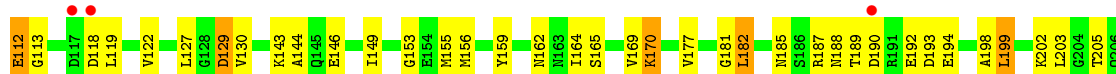
• Molecule 2: Nitrogenase molybdenum-iron protein



• Molecule 3: Nitrogenase iron protein 1



• Molecule 3: Nitrogenase iron protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.91Å 75.89Å 223.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.28 – 2.10 43.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (43.28-2.10) 95.6 (43.28-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.221 0.167 , 0.216	Depositor DCC
R_{free} test set	8399 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22638	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFN, PGE, NA, SF4, CLF, 1PE, PG4, HCA, P6G, TRS, PEG, CA

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	0.55	0/3870	0.80	4/5219 (0.1%)
1	C	0.55	0/3878	0.80	4/5229 (0.1%)
2	B	0.63	0/4280	0.83	5/5786 (0.1%)
2	D	0.60	0/4280	0.83	5/5786 (0.1%)
3	E	0.48	0/2211	0.74	1/2977 (0.0%)
3	F	0.48	0/2185	0.76	1/2943 (0.0%)
All	All	0.57	0/20704	0.80	20/27940 (0.1%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	206	ARG	NE-CZ-NH1	-17.03	111.78	120.30
2	B	206	ARG	NE-CZ-NH2	-16.77	111.92	120.30
2	B	206	ARG	NE-CZ-NH1	14.63	127.62	120.30
2	D	206	ARG	NE-CZ-NH2	14.33	127.47	120.30
1	C	97	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	97	ARG	NE-CZ-NH2	-9.09	115.75	120.30
2	D	206	ARG	CD-NE-CZ	8.95	136.13	123.60
2	B	206	ARG	CD-NE-CZ	8.39	135.35	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	97	ARG	NE-CZ-NH1	7.67	124.14	120.30
2	B	368	ALA	N-CA-C	-6.18	94.30	111.00
2	D	368	ALA	N-CA-C	-5.90	95.06	111.00
2	B	4	GLN	N-CA-C	-5.57	95.96	111.00
2	D	4	GLN	N-CA-C	-5.57	95.96	111.00
1	C	356	GLY	N-CA-C	5.39	126.58	113.10
1	A	356	GLY	N-CA-C	5.29	126.32	113.10
3	E	255	ILE	N-CA-C	-5.25	96.82	111.00
1	A	76	LYS	N-CA-C	5.21	125.07	111.00
1	C	76	LYS	N-CA-C	5.15	124.91	111.00
3	F	207	MET	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	TYR	Sidechain
1	C	446	TYR	Sidechain

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	3782	0	3720	66	0
1	C	3790	0	3729	63	0
2	B	4174	0	4088	60	0
2	D	4174	0	4088	59	0
3	E	2187	0	2197	106	0
3	F	2161	0	2176	81	0
4	A	14	0	6	2	0
4	C	14	0	6	1	0
5	A	18	0	0	1	0
5	C	18	0	0	0	0
6	A	20	0	28	8	0
6	B	10	0	14	5	0
6	C	20	0	28	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	30	0	42	8	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
9	B	15	0	0	0	0
9	C	15	0	0	0	0
10	B	8	0	12	0	0
10	C	8	0	12	2	0
11	B	13	0	18	0	0
11	E	13	0	18	7	0
12	B	16	0	22	7	0
12	C	16	0	22	22	0
13	B	7	0	10	0	0
13	D	14	0	20	5	0
14	D	19	0	26	1	0
15	E	8	0	0	0	0
16	A	355	0	0	11	0
16	B	594	0	0	8	0
16	C	362	0	0	4	0
16	D	527	0	0	11	1
16	E	115	0	0	9	0
16	F	118	0	0	5	0
All	All	22638	0	20282	415	1

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 10.

All (415) 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)
1:A:160:GLY:HA3	3:E:140:ARG:HH21	1.16	1.06
1:A:303:THR:HG23	6:A:5015:PGE:H22	1.39	1.01
2:B:295:PRO:HB2	6:B:5005:PGE:H4	1.46	0.96
3:F:21:ASN:HD21	3:F:227:VAL:H	1.05	0.95
1:A:249:CYS:HB3	16:A:5292:HOH:O	1.65	0.94
2:B:477:HIS:H	2:D:499:ASN:HD21	1.04	0.94
2:D:292:LEU:HD12	16:D:5165:HOH:O	1.69	0.92
12:C:5013:1PE:C23	12:C:5013:1PE:H161	2.01	0.91
3:E:140:ARG:HH11	3:E:140:ARG:HG3	1.35	0.91
3:E:21:ASN:HD21	3:E:227:VAL:H	1.20	0.89
2:B:499:ASN:HD21	2:D:477:HIS:H	1.11	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:20:GLN:HE22	3:E:47:LEU:H	1.19	0.87
1:A:335:TRP:CH2	6:A:5015:PGE:H5	2.11	0.86
2:B:125:PHE:CE1	3:E:104:THR:HG23	2.10	0.85
1:A:121:LYS:HE3	16:A:5318:HOH:O	1.75	0.85
2:D:292:LEU:HB2	16:D:5518:HOH:O	1.75	0.84
1:C:473:LYS:HD3	6:C:5011:PGE:H12	1.58	0.84
3:E:141:GLU:O	3:E:143:LYS:HD2	1.77	0.84
3:E:187:ARG:HD3	16:E:5081:HOH:O	1.79	0.82
3:F:279:GLU:HA	3:F:282:VAL:HG23	1.63	0.81
1:A:35:ASN:ND2	1:A:391:MET:HG2	1.96	0.80
12:B:5017:1PE:H251	12:B:5017:1PE:H132	1.61	0.80
3:E:223:ARG:NH1	3:F:284:LYS:HB2	1.97	0.80
1:C:35:ASN:ND2	1:C:391:MET:HG2	1.97	0.80
12:C:5013:1PE:H161	12:C:5013:1PE:H231	1.65	0.78
2:D:414:PRO:O	2:D:417:LYS:HE3	1.82	0.78
3:F:39:ASP:OD1	3:F:41:LYS:HG3	1.82	0.77
3:F:281:ILE:HA	3:F:284:LYS:HD2	1.66	0.77
1:C:310:ARG:HD2	1:C:325:GLU:OE2	1.85	0.77
3:E:189:THR:HG21	16:E:5077:HOH:O	1.86	0.76
3:F:43:ASP:HB3	3:F:46:ARG:HH11	1.48	0.76
3:E:289:VAL:HG23	3:F:223:ARG:HH12	1.48	0.76
14:D:5009:P6G:H111	16:D:5316:HOH:O	1.85	0.75
1:A:160:GLY:HA3	3:E:140:ARG:NH2	1.98	0.75
2:B:125:PHE:HE1	3:E:104:THR:HA	1.51	0.75
1:A:307:GLU:HB2	6:A:5015:PGE:H1	1.69	0.74
3:F:187:ARG:HG2	3:F:192:GLU:OE1	1.88	0.74
1:A:239:ARG:HH11	1:A:252:GLN:HE21	1.36	0.73
1:A:310:ARG:HD2	1:A:325:GLU:OE2	1.88	0.73
1:C:239:ARG:HH11	1:C:252:GLN:HE21	1.37	0.73
3:F:8:TYR:HB3	3:F:164:ILE:HD13	1.69	0.73
3:F:21:ASN:ND2	3:F:227:VAL:H	1.83	0.73
12:B:5017:1PE:H141	16:B:5177:HOH:O	1.88	0.72
1:A:164:GLU:OE2	1:A:182:ARG:HD3	1.87	0.72
2:D:7:LYS:NZ	16:D:5309:HOH:O	2.20	0.72
3:E:139:ILE:HG23	3:E:177:VAL:HG21	1.72	0.72
2:B:414:PRO:O	2:B:417:LYS:HE3	1.90	0.72
3:E:140:ARG:HG3	3:E:140:ARG:NH1	1.92	0.72
12:C:5013:1PE:C16	12:C:5013:1PE:H221	2.20	0.71
1:C:4:MET:O	1:C:5:SER:HB3	1.89	0.71
1:C:164:GLU:OE2	1:C:182:ARG:HD3	1.90	0.71
2:D:413:SER:OG	13:D:5020:PEG:H42	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:5015:PGE:H12	16:A:5155:HOH:O	1.89	0.70
3:E:31:LYS:NZ	11:E:5007:PG4:H22	2.07	0.70
1:C:176:LYS:HE2	16:C:5347:HOH:O	1.92	0.70
1:C:294:TRP:CE2	10:C:5004:TRS:H12	2.26	0.70
3:F:4:GLN:NE2	3:F:122:VAL:HB	2.07	0.69
3:E:223:ARG:HH12	3:F:284:LYS:CB	2.05	0.69
3:F:41:LYS:HB2	3:F:43:ASP:OD2	1.91	0.69
1:C:47:ILE:HD12	1:C:48:SER:H	1.58	0.69
2:B:125:PHE:CE1	3:E:104:THR:HA	2.27	0.69
2:D:302:LYS:HD2	16:D:5165:HOH:O	1.91	0.69
1:A:42:SER:HA	1:A:391:MET:HE1	1.74	0.69
2:D:315:LYS:CD	6:D:5006:PGE:H6	2.23	0.69
1:C:345:ARG:HE	12:C:5013:1PE:H251	1.56	0.68
3:E:156:MET:HG2	16:E:5091:HOH:O	1.93	0.68
1:A:47:ILE:HD12	1:A:48:SER:H	1.58	0.68
3:E:45:THR:CG2	3:E:85:CYS:HB3	2.24	0.68
3:E:106:ILE:O	3:E:110:GLU:HG3	1.93	0.68
1:C:42:SER:HA	1:C:391:MET:HE1	1.75	0.68
2:D:523:ARG:HD2	16:D:5119:HOH:O	1.94	0.68
3:E:269:MET:CE	3:E:276:VAL:HG22	2.24	0.68
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.76	0.68
3:E:166:LYS:O	3:E:170:LYS:HG2	1.93	0.67
2:D:315:LYS:HD2	6:D:5006:PGE:H6	1.76	0.67
2:D:207:TYR:CD1	6:D:5010:PGE:H5	2.30	0.67
2:B:477:HIS:N	2:D:499:ASN:HD21	1.87	0.66
2:D:80:LEU:HD13	2:D:87:PRO:HG2	1.76	0.66
1:C:345:ARG:NE	12:C:5013:1PE:H251	2.10	0.66
3:F:279:GLU:HA	3:F:282:VAL:CG2	2.25	0.66
12:B:5017:1PE:H252	12:B:5017:1PE:H222	1.77	0.66
2:B:37:GLN:HE22	2:D:513:GLN:HE22	1.42	0.66
3:F:4:GLN:HE21	3:F:4:GLN:HA	1.60	0.66
3:F:20:GLN:HE22	3:F:47:LEU:H	1.42	0.65
1:A:31:HIS:HE1	16:A:5298:HOH:O	1.77	0.65
1:A:332:LYS:O	1:A:336:GLU:HG3	1.97	0.65
3:E:289:VAL:HG23	3:F:223:ARG:NH1	2.10	0.65
3:F:43:ASP:HB3	3:F:46:ARG:NH1	2.10	0.65
1:C:203:ARG:HD2	1:C:204:ASP:OD1	1.97	0.65
2:B:477:HIS:H	2:D:499:ASN:ND2	1.87	0.65
3:F:50:HIS:ND1	16:F:343:HOH:O	2.29	0.65
3:E:46:ARG:HG2	3:E:51:SER:O	1.97	0.65
2:B:315:LYS:HD2	6:B:5005:PGE:H2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ARG:HD2	16:B:5529:HOH:O	1.97	0.64
3:F:10:LYS:HG3	3:F:11:GLY:N	2.13	0.64
12:C:5013:1PE:H161	12:C:5013:1PE:H232	1.79	0.64
1:A:203:ARG:HD2	1:A:204:ASP:OD1	1.98	0.64
3:E:261:MET:HE2	3:E:261:MET:HA	1.79	0.64
3:E:45:THR:HG21	3:E:85:CYS:HB3	1.79	0.64
1:A:307:GLU:HB2	6:A:5015:PGE:C1	2.27	0.64
3:E:242:ALA:O	3:E:246:LYS:HG3	1.98	0.64
1:A:303:THR:CG2	6:A:5015:PGE:H22	2.22	0.63
3:E:170:LYS:HZ1	3:F:92:GLU:HB3	1.62	0.63
1:C:209:LYS:HD2	16:C:5337:HOH:O	1.97	0.63
3:E:20:GLN:HE22	3:E:47:LEU:N	1.95	0.63
3:F:198:ALA:O	3:F:202:LYS:HG3	1.99	0.63
1:C:332:LYS:O	1:C:336:GLU:HG3	1.99	0.63
3:E:106:ILE:HG21	3:E:143:LYS:HE3	1.79	0.62
3:E:140:ARG:CG	3:E:140:ARG:HH11	2.09	0.62
2:B:80:LEU:HD13	2:B:87:PRO:HG2	1.80	0.62
3:E:262:ASP:O	3:E:266:GLU:HG2	2.00	0.62
1:A:442:HIS:HB2	16:A:5267:HOH:O	1.98	0.61
3:F:32:LYS:HB3	3:F:119:LEU:HA	1.80	0.61
2:D:413:SER:HB2	13:D:5020:PEG:H22	1.83	0.61
3:F:95:VAL:HG13	3:F:96:GLY:H	1.63	0.61
1:C:5:SER:O	1:C:9:VAL:HG23	2.01	0.60
3:F:155:MET:HG3	3:F:156:MET:HE2	1.84	0.60
2:D:125:PHE:HB2	16:D:5470:HOH:O	2.01	0.60
2:D:295:PRO:HB3	16:D:5518:HOH:O	2.01	0.60
3:E:241:ARG:O	3:E:245:ARG:HG3	2.01	0.60
3:F:80:TYR:O	3:F:83:VAL:HG13	2.02	0.60
1:C:35:ASN:HD21	1:C:391:MET:HG2	1.66	0.60
1:C:473:LYS:HE2	6:C:5011:PGE:H52	1.84	0.60
1:A:35:ASN:HD21	1:A:391:MET:HG2	1.66	0.59
3:E:116:GLU:HB2	3:E:118:ASP:OD1	2.02	0.59
3:E:170:LYS:NZ	3:F:92:GLU:HB3	2.17	0.59
3:E:269:MET:HE3	3:E:276:VAL:HG22	1.83	0.58
3:F:155:MET:HG3	3:F:156:MET:CE	2.33	0.58
13:D:5020:PEG:H12	16:D:5183:HOH:O	2.02	0.58
2:B:125:PHE:HE1	3:E:104:THR:HG23	1.64	0.58
2:B:295:PRO:CB	6:B:5005:PGE:H4	2.28	0.58
3:F:162:ASN:HD21	3:F:259:ILE:H	1.52	0.58
3:E:248:VAL:HG11	11:E:5007:PG4:H21	1.85	0.57
1:C:42:SER:CA	1:C:391:MET:HE1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:CA	1:A:391:MET:HE1	2.32	0.57
2:B:39:LYS:HD2	16:B:5540:HOH:O	2.05	0.57
3:E:20:GLN:NE2	3:E:47:LEU:H	1.98	0.57
3:E:202:LYS:HE3	16:E:5089:HOH:O	2.04	0.57
12:B:5017:1PE:H132	12:B:5017:1PE:C25	2.33	0.57
1:A:160:GLY:CA	3:E:140:ARG:HH21	2.05	0.57
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.40	0.57
1:C:345:ARG:HG2	12:C:5013:1PE:H142	1.86	0.57
3:E:31:LYS:NZ	11:E:5007:PG4:H71	2.20	0.57
3:E:50:HIS:HE1	3:E:229:GLU:OE1	1.88	0.56
3:F:193:ASP:OD2	3:F:194:GLU:N	2.39	0.56
3:F:269:MET:HA	3:F:274:MET:O	2.05	0.56
1:C:343:ARG:HD3	1:C:347:GLU:OE1	2.05	0.56
1:C:31:HIS:HE1	16:C:5322:HOH:O	1.87	0.56
1:C:442:HIS:HB2	16:C:5278:HOH:O	2.04	0.56
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.88	0.56
2:B:363:HIS:NE2	12:C:5013:1PE:H162	2.21	0.56
3:E:32:LYS:HE2	3:E:118:ASP:HB2	1.88	0.56
3:F:21:ASN:HD21	3:F:227:VAL:N	1.90	0.56
1:A:239:ARG:HD2	1:A:252:GLN:NE2	2.21	0.56
1:C:294:TRP:CZ2	10:C:5004:TRS:H12	2.39	0.56
3:F:215:ASN:HA	3:F:218:GLN:NE2	2.20	0.56
1:A:9:VAL:CG1	1:A:34:VAL:HG22	2.36	0.55
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.87	0.55
3:E:145:GLN:OE1	3:E:176:SER:HB2	2.06	0.55
1:A:225:ILE:HG13	16:A:5292:HOH:O	2.05	0.55
2:B:499:ASN:ND2	2:D:477:HIS:H	1.93	0.55
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.42	0.55
12:C:5013:1PE:H221	12:C:5013:1PE:OH7	2.06	0.55
2:D:503:GLU:HG3	16:D:5510:HOH:O	2.06	0.55
1:A:125:PHE:HZ	3:F:58:MET:HG3	1.71	0.55
12:C:5013:1PE:C16	12:C:5013:1PE:H231	2.35	0.55
3:F:149:ILE:HB	3:F:182:LEU:HD12	1.88	0.55
2:B:513:GLN:HE22	2:D:37:GLN:HE22	1.54	0.55
3:E:288:GLU:O	3:E:289:VAL:HG13	2.06	0.55
1:A:31:HIS:HD2	1:A:402:ASP:OD2	1.91	0.54
1:C:239:ARG:HD2	1:C:252:GLN:NE2	2.22	0.54
1:C:31:HIS:HD2	1:C:402:ASP:OD2	1.90	0.54
12:C:5013:1PE:H221	12:C:5013:1PE:H161	1.90	0.54
2:D:381:LYS:O	2:D:385:GLU:HG3	2.07	0.54
3:F:52:LYS:NZ	16:F:395:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:5012:PGE:H22	16:A:5161:HOH:O	2.06	0.54
2:D:80:LEU:HD13	2:D:87:PRO:CG	2.38	0.53
1:C:9:VAL:CG1	1:C:34:VAL:HG22	2.38	0.53
3:E:98:ALA:O	3:E:102:VAL:HG23	2.09	0.53
3:E:269:MET:HE2	3:E:276:VAL:HG22	1.91	0.53
1:A:125:PHE:HE1	3:F:91:PRO:HA	1.75	0.52
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.90	0.52
1:A:125:PHE:CZ	3:F:58:MET:HG3	2.44	0.52
2:B:494:LEU:HD23	2:B:494:LEU:C	2.30	0.52
3:F:281:ILE:HG22	3:F:284:LYS:HD2	1.91	0.52
1:C:468:ASN:CB	12:C:5013:1PE:H151	2.39	0.52
1:C:4:MET:O	1:C:5:SER:CB	2.56	0.52
3:E:223:ARG:HH12	3:F:284:LYS:HB3	1.75	0.52
3:E:49:LEU:C	3:E:51:SER:H	2.13	0.52
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.91	0.52
3:F:260:THR:OG1	3:F:263:GLU:HG3	2.10	0.52
3:F:46:ARG:HB3	3:F:51:SER:O	2.10	0.52
3:E:153:GLY:HA3	3:E:192:GLU:HG3	1.92	0.51
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.93	0.51
3:E:100:ARG:HH11	3:E:100:ARG:HG2	1.75	0.51
3:E:281:ILE:HG13	3:E:289:VAL:HG21	1.92	0.51
1:A:343:ARG:HD3	1:A:347:GLU:OE1	2.11	0.50
3:E:223:ARG:NH1	3:F:284:LYS:CB	2.65	0.50
3:E:28:GLU:OE1	3:E:241:ARG:NE	2.31	0.50
3:E:57:ILE:CD1	3:E:105:ALA:HA	2.41	0.50
2:B:198:ASP:HB2	2:B:297:HIS:O	2.12	0.50
1:A:35:ASN:HD22	1:A:391:MET:HG2	1.74	0.50
3:E:100:ARG:O	3:E:104:THR:OG1	2.29	0.50
3:F:63:GLU:HB2	16:F:328:HOH:O	2.11	0.50
3:E:32:LYS:HD3	3:E:118:ASP:O	2.11	0.50
3:F:22:LEU:HD12	3:F:22:LEU:O	2.12	0.50
2:B:499:ASN:HD21	2:D:477:HIS:N	1.94	0.50
3:F:153:GLY:HA3	3:F:192:GLU:HG3	1.94	0.50
3:E:52:LYS:NZ	3:F:277:GLU:OE2	2.45	0.50
2:B:315:LYS:CD	6:B:5005:PGE:H3	2.41	0.49
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.94	0.49
1:A:467:LEU:HD23	1:A:467:LEU:O	2.13	0.49
3:E:43:ASP:HB3	16:E:5092:HOH:O	2.12	0.49
2:B:80:LEU:HD13	2:B:87:PRO:CG	2.42	0.49
1:C:22:GLU:CD	1:C:26:LYS:HE3	2.33	0.49
2:D:494:LEU:HD23	2:D:494:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:103:ILE:HD11	3:E:141:GLU:HG3	1.94	0.49
2:B:381:LYS:O	2:B:385:GLU:HG3	2.12	0.49
2:D:198:ASP:HB2	2:D:297:HIS:O	2.13	0.49
3:E:99:GLY:HA3	3:E:134:GLY:HA2	1.94	0.49
3:F:46:ARG:HH21	3:F:53:ALA:HA	1.77	0.49
1:A:176:LYS:HE2	16:A:5253:HOH:O	2.13	0.49
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.12	0.49
3:E:64:ALA:C	3:E:66:THR:H	2.15	0.48
1:A:249:CYS:CB	16:A:5292:HOH:O	2.39	0.48
2:D:151:THR:CG2	2:D:162:LEU:HD11	2.43	0.48
3:F:58:MET:HA	3:F:58:MET:CE	2.43	0.48
1:A:474:LYS:HB3	2:D:322:LEU:HD21	1.95	0.48
2:B:300:LYS:HD2	16:B:5528:HOH:O	2.14	0.48
1:A:97:ARG:NH2	1:A:447:SER:O	2.35	0.48
2:D:207:TYR:CE1	6:D:5010:PGE:H5	2.48	0.48
3:E:187:ARG:O	3:E:188:ASN:HB2	2.13	0.48
3:F:262:ASP:O	3:F:266:GLU:HG3	2.14	0.48
3:F:52:LYS:HG3	16:F:395:HOH:O	2.13	0.48
3:E:103:ILE:HG12	3:E:137:MET:HG2	1.95	0.48
3:E:31:LYS:HZ1	11:E:5007:PG4:H22	1.79	0.48
1:C:239:ARG:HH11	1:C:252:GLN:NE2	2.09	0.48
1:C:30:LYS:O	1:C:47:ILE:HG22	2.14	0.48
3:E:30:GLY:O	11:E:5007:PG4:H62	2.14	0.48
2:B:125:PHE:HE1	3:E:104:THR:CA	2.25	0.48
3:E:26:LEU:O	3:E:29:MET:HB3	2.12	0.47
1:C:213:ASP:OD2	1:C:215:THR:HG23	2.15	0.47
1:C:464:ASP:OD1	12:C:5013:1PE:H152	2.14	0.47
3:E:103:ILE:CD1	3:E:141:GLU:HG3	2.44	0.47
3:E:31:LYS:HZ2	11:E:5007:PG4:H71	1.79	0.47
3:F:165:SER:O	3:F:169:VAL:HG23	2.14	0.47
1:C:468:ASN:HB2	12:C:5013:1PE:H151	1.97	0.47
3:F:113:GLY:HA2	16:F:365:HOH:O	2.14	0.47
2:B:370:TRP:HA	2:B:394:LEU:O	2.15	0.47
2:D:502:LEU:HD22	2:D:523:ARG:HD3	1.96	0.47
1:A:343:ARG:N	1:A:344:PRO:HD2	2.30	0.47
1:C:37:PRO:HD3	1:C:396:ASP:HA	1.97	0.47
3:E:60:MET:HE1	3:E:75:VAL:HA	1.96	0.47
2:B:438:LYS:HB2	12:B:5017:1PE:H152	1.96	0.47
2:B:502:LEU:HD22	2:B:523:ARG:HD3	1.96	0.46
1:C:468:ASN:HB2	12:C:5013:1PE:C15	2.45	0.46
1:A:120:GLU:HG2	3:F:104:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:LYS:HE2	2:B:421:VAL:O	2.15	0.46
2:B:445:ASN:HB2	2:B:472:PRO:O	2.16	0.46
3:E:57:ILE:HD13	3:E:105:ALA:HA	1.95	0.46
3:E:64:ALA:O	3:E:66:THR:N	2.46	0.46
3:F:187:ARG:HG3	3:F:189:THR:OG1	2.15	0.46
3:F:76:LEU:HD11	3:F:84:LYS:HB3	1.97	0.46
1:C:97:ARG:NH2	1:C:447:SER:O	2.38	0.46
1:C:467:LEU:O	1:C:467:LEU:HD23	2.16	0.46
1:A:315:LYS:HE3	16:A:5331:HOH:O	2.15	0.46
2:D:376:VAL:O	2:D:380:VAL:HG23	2.15	0.46
2:B:194:VAL:HB	2:B:297:HIS:CG	2.50	0.46
1:C:35:ASN:HD22	1:C:391:MET:HG2	1.77	0.46
2:D:194:VAL:HB	2:D:297:HIS:CG	2.51	0.46
1:A:230:ASN:HA	1:A:235:ALA:H	1.80	0.46
3:E:159:TYR:CD2	3:E:261:MET:HE1	2.51	0.46
2:B:10:ALA:O	2:B:11:SER:C	2.54	0.46
3:E:186:SER:HB2	3:E:210:PHE:CZ	2.51	0.46
2:B:151:THR:CG2	2:B:162:LEU:HD11	2.46	0.45
2:D:403:LYS:HE2	2:D:421:VAL:O	2.16	0.45
3:E:202:LYS:HE2	16:E:5085:HOH:O	2.15	0.45
3:E:248:VAL:HG11	11:E:5007:PG4:C2	2.47	0.45
3:E:67:VAL:C	3:E:69:ASP:H	2.20	0.45
3:F:33:VAL:HG12	3:F:34:MET:N	2.32	0.45
3:E:49:LEU:C	3:E:51:SER:N	2.68	0.45
2:D:370:TRP:HA	2:D:394:LEU:O	2.17	0.45
2:B:417:LYS:HD2	12:C:5013:1PE:OH2	2.17	0.45
2:D:33:GLU:O	6:D:5008:PGE:H42	2.16	0.45
3:E:217:VAL:O	3:E:221:GLU:HG3	2.17	0.45
1:A:22:GLU:CD	1:A:26:LYS:HE3	2.37	0.45
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.99	0.45
1:C:230:ASN:HA	1:C:235:ALA:H	1.82	0.45
2:B:376:VAL:O	2:B:380:VAL:HG23	2.16	0.45
2:B:438:LYS:CB	12:B:5017:1PE:H152	2.47	0.45
1:A:335:TRP:CZ3	6:A:5015:PGE:H5	2.52	0.45
2:D:178:GLU:H	2:D:178:GLU:CD	2.19	0.45
3:E:50:HIS:HA	3:E:224:ARG:O	2.16	0.45
2:D:445:ASN:HB2	2:D:472:PRO:O	2.17	0.45
3:E:205:THR:OG1	3:E:206:GLN:N	2.48	0.44
1:C:473:LYS:CE	6:C:5011:PGE:H52	2.47	0.44
3:E:56:THR:OG1	3:E:59:GLU:CB	2.65	0.44
1:A:379:TYR:CD2	1:A:382:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:HD12	1:C:48:SER:N	2.30	0.44
3:E:100:ARG:HD2	16:E:5113:HOH:O	2.17	0.44
1:C:345:ARG:CZ	12:C:5013:1PE:H242	2.47	0.44
3:E:57:ILE:HD12	3:E:105:ALA:HB2	2.00	0.44
3:E:269:MET:HE3	3:E:276:VAL:HG13	1.99	0.44
1:A:37:PRO:HD3	1:A:396:ASP:HA	2.00	0.44
1:C:475:LEU:HD12	1:C:475:LEU:N	2.33	0.44
1:A:442:HIS:CG	4:A:2494:HCA:H52	2.51	0.44
3:F:181:GLY:HA2	3:F:205:THR:OG1	2.18	0.44
3:F:29:MET:CE	3:F:31:LYS:HE2	2.47	0.44
3:F:20:GLN:NE2	3:F:47:LEU:H	2.13	0.43
1:A:6:ARG:O	1:A:10:GLU:HG3	2.18	0.43
2:B:173:GLY:HA2	16:B:5438:HOH:O	2.18	0.43
3:F:130:VAL:O	3:F:130:VAL:HG13	2.18	0.43
2:B:415:TYR:CE1	12:C:5013:1PE:H222	2.53	0.43
12:B:5017:1PE:H241	16:B:5177:HOH:O	2.17	0.43
2:B:37:GLN:NE2	2:D:513:GLN:HE22	2.10	0.43
1:C:379:TYR:CD2	1:C:382:ALA:HB2	2.53	0.43
1:A:47:ILE:HD11	1:A:50:LYS:HE2	2.01	0.43
3:F:112:GLU:HA	3:F:112:GLU:OE1	2.19	0.43
2:D:42:GLU:OE2	13:D:5019:PEG:H31	2.19	0.43
1:C:343:ARG:N	1:C:344:PRO:HD2	2.34	0.43
3:E:56:THR:HG22	3:E:87:GLU:HB3	2.00	0.43
3:F:127:LEU:HD11	3:F:129:ASP:OD2	2.19	0.43
1:C:473:LYS:CD	6:C:5011:PGE:H12	2.40	0.43
2:D:128:GLN:OE1	2:D:165:PHE:HA	2.19	0.43
2:D:183:PHE:HE1	6:D:5010:PGE:H6	1.84	0.43
1:A:5:SER:HB3	1:A:8:GLU:CG	2.49	0.42
1:C:355:ILE:HG22	1:C:356:GLY:H	1.84	0.42
2:D:373:PRO:HG3	2:D:395:CYS:SG	2.59	0.42
3:E:101:GLY:HA3	16:E:5096:HOH:O	2.19	0.42
2:B:178:GLU:H	2:B:178:GLU:CD	2.22	0.42
2:B:373:PRO:HG3	2:B:395:CYS:SG	2.59	0.42
3:E:102:VAL:HG11	3:E:138:PRO:HG3	2.00	0.42
3:F:215:ASN:HA	3:F:218:GLN:HE22	1.84	0.42
1:A:239:ARG:HH11	1:A:252:GLN:NE2	2.11	0.42
1:C:224:ALA:HB3	1:C:271:ASN:HD22	1.84	0.42
12:C:5013:1PE:C22	12:C:5013:1PE:H161	2.50	0.42
2:D:10:ALA:O	2:D:11:SER:C	2.58	0.42
1:A:213:ASP:OD2	1:A:215:THR:HG23	2.19	0.42
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LEU:N	1:A:475:LEU:HD12	2.35	0.42
3:E:260:THR:OG1	3:E:263:GLU:HG3	2.18	0.42
3:F:187:ARG:O	3:F:188:ASN:HB2	2.19	0.42
3:E:224:ARG:HD2	3:F:282:VAL:CG1	2.50	0.42
3:F:4:GLN:HE22	3:F:122:VAL:CG1	2.33	0.42
2:B:139:LYS:HA	2:B:144:PRO:HD2	2.01	0.42
1:C:253:TRP:HA	1:C:254:SER:HA	1.73	0.42
3:E:45:THR:OG1	3:E:54:GLN:NE2	2.50	0.42
2:D:32:GLU:O	2:D:33:GLU:C	2.58	0.42
1:A:442:HIS:ND1	4:A:2494:HCA:H52	2.35	0.42
1:C:17:LEU:HD11	1:C:29:ASN:HD22	1.85	0.42
1:C:332:LYS:HB3	1:C:333:PRO:CD	2.49	0.42
2:D:35:TYR:CE1	6:D:5008:PGE:H32	2.54	0.42
2:B:379:LEU:HD21	2:B:443:ILE:HG21	2.02	0.42
2:B:414:PRO:CB	12:C:5013:1PE:H132	2.49	0.42
1:A:271:ASN:HA	1:A:271:ASN:HD22	1.65	0.42
1:A:9:VAL:HG12	1:A:34:VAL:HG22	2.01	0.42
2:D:124:VAL:HB	16:D:5453:HOH:O	2.20	0.42
2:B:128:GLN:OE1	2:B:165:PHE:HA	2.20	0.41
1:C:62:CYS:HB3	2:D:94:GLY:HA3	2.02	0.41
3:F:199:LEU:HD22	3:F:203:LEU:HG	2.02	0.41
3:F:146:GLU:HG2	3:F:253:LEU:HD11	2.01	0.41
1:A:442:HIS:HA	5:A:2496:CFN:S4B	2.59	0.41
3:E:15:LYS:HB3	3:E:15:LYS:HE3	1.81	0.41
2:B:45:GLN:NE2	16:B:5497:HOH:O	2.46	0.41
2:D:509:THR:HG21	2:D:518:ASN:HD22	1.86	0.41
3:E:3:ARG:HD2	16:E:5090:HOH:O	2.20	0.41
1:C:6:ARG:O	1:C:10:GLU:HG3	2.20	0.41
2:D:118:MET:HE1	2:D:158:ILE:HD11	2.02	0.41
3:F:214:ASP:OD1	3:F:216:VAL:HG12	2.21	0.41
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.55	0.41
3:F:66:THR:OG1	3:F:68:GLU:HG2	2.21	0.41
1:A:5:SER:HB3	1:A:8:GLU:HG3	2.03	0.41
2:B:363:HIS:CE1	12:C:5013:1PE:H162	2.55	0.41
2:D:215:ASP:N	2:D:215:ASP:OD1	2.53	0.41
3:E:27:ALA:C	3:E:29:MET:N	2.74	0.41
3:F:95:VAL:HG22	3:F:96:GLY:N	2.36	0.41
2:B:101:SER:HA	2:B:104:ASN:HD22	1.84	0.41
1:C:47:ILE:HD11	1:C:50:LYS:HE2	2.03	0.41
3:E:215:ASN:HA	3:E:218:GLN:NE2	2.35	0.41
3:F:225:MET:HE3	3:F:229:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:TYR:O	3:F:83:VAL:CG1	2.67	0.41
1:A:467:LEU:HD23	1:A:467:LEU:C	2.40	0.41
2:B:124:VAL:HG13	3:E:103:ILE:HG21	2.02	0.41
1:C:442:HIS:CG	4:C:3494:HCA:H52	2.55	0.41
2:D:101:SER:HA	2:D:104:ASN:HD22	1.84	0.41
3:E:50:HIS:CE1	3:E:229:GLU:OE1	2.72	0.41
3:E:95:VAL:HG13	3:F:170:LYS:HG2	2.02	0.41
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.55	0.41
1:C:464:ASP:OD2	12:C:5013:1PE:H262	2.21	0.41
3:E:75:VAL:HG13	3:E:86:VAL:HG23	2.03	0.41
3:F:144:ALA:O	3:F:177:VAL:HG22	2.20	0.41
3:F:155:MET:HE3	3:F:159:TYR:HB2	2.02	0.41
1:A:253:TRP:HA	1:A:254:SER:HA	1.69	0.41
1:C:284:ARG:HG2	1:C:284:ARG:HH11	1.87	0.41
2:D:509:THR:O	2:D:516:ASP:HA	2.21	0.41
3:E:4:GLN:HB3	3:E:143:LYS:O	2.21	0.41
3:F:95:VAL:HG13	3:F:96:GLY:N	2.34	0.41
1:A:209:LYS:HD2	16:A:5316:HOH:O	2.21	0.40
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.86	0.40
1:A:17:LEU:HD11	1:A:29:ASN:HD22	1.86	0.40
2:B:523:ARG:NH1	16:B:5532:HOH:O	1.80	0.40
2:D:183:PHE:CE1	6:D:5010:PGE:H6	2.55	0.40
3:E:230:TYR:O	3:F:285:THR:HG23	2.21	0.40
3:F:68:GLU:H	3:F:68:GLU:CD	2.24	0.40
2:D:413:SER:HB2	13:D:5020:PEG:C2	2.48	0.40
3:E:57:ILE:HD12	3:E:105:ALA:CB	2.51	0.40
3:F:76:LEU:O	3:F:77:LYS:HD3	2.20	0.40
1:A:5:SER:O	1:A:6:ARG:C	2.60	0.40
1:A:42:SER:HB3	1:A:391:MET:HE2	2.03	0.40
2:B:413:SER:HA	2:B:414:PRO:HD3	1.97	0.40
2:B:509:THR:HG21	2:B:518:ASN:HD22	1.86	0.40
1:C:465:MET:HG3	1:C:466:THR:N	2.36	0.40
3:E:127:LEU:HD11	3:E:129:ASP:OD1	2.21	0.40
2:B:299:GLU:OE1	6:B:5005:PGE:H62	2.22	0.40
2:D:231:GLU:HB3	2:D:237:PHE:CZ	2.56	0.40

All (1) 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)
16:D:5299:HOH:O	16:D:5382:HOH:O[3_545]	2.19	0.01

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	474/491 (96%)	450 (95%)	23 (5%)	1 (0%)	47	49
1	C	475/491 (97%)	447 (94%)	26 (6%)	2 (0%)	34	32
2	B	520/522 (100%)	504 (97%)	15 (3%)	1 (0%)	47	49
2	D	520/522 (100%)	504 (97%)	15 (3%)	1 (0%)	47	49
3	E	287/289 (99%)	267 (93%)	17 (6%)	3 (1%)	15	11
3	F	284/289 (98%)	265 (93%)	14 (5%)	5 (2%)	8	4
All	All	2560/2604 (98%)	2437 (95%)	110 (4%)	13 (0%)	29	26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	64	ALA
3	F	190	ASP
3	F	282	VAL
2	B	255	SER
2	D	255	SER
3	E	72	LEU
3	F	129	ASP
1	C	5	SER
3	F	53	ALA
3	F	285	THR
3	E	65	GLY
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	406/414 (98%)	398 (98%)	8 (2%)	55	60
1	C	407/414 (98%)	399 (98%)	8 (2%)	55	60
2	B	454/454 (100%)	445 (98%)	9 (2%)	55	60
2	D	454/454 (100%)	447 (98%)	7 (2%)	65	71
3	E	233/233 (100%)	218 (94%)	15 (6%)	17	14
3	F	230/233 (99%)	216 (94%)	14 (6%)	18	16
All	All	2184/2202 (99%)	2123 (97%)	61 (3%)	43	47

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	131	LEU
1	A	212	GLU
1	A	343	ARG
1	A	362	HIS
1	A	401	TYR
1	A	437	PRO
1	A	445	ASP
2	B	13	PRO
2	B	80	LEU
2	B	92	SER
2	B	178	GLU
2	B	206	ARG
2	B	215	ASP
2	B	258	GLU
2	B	315	LYS
2	B	523	ARG
1	C	4	MET
1	C	98	ASN
1	C	131	LEU
1	C	212	GLU
1	C	343	ARG
1	C	362	HIS
1	C	401	TYR
1	C	445	ASP
2	D	80	LEU
2	D	92	SER

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Mol	Chain	Res	Type
2	D	178	GLU
2	D	215	ASP
2	D	258	GLU
2	D	315	LYS
2	D	523	ARG
3	E	44	SER
3	E	68	GLU
3	E	69	ASP
3	E	83	VAL
3	E	104	THR
3	E	115	TYR
3	E	117	ASP
3	E	118	ASP
3	E	126	VAL
3	E	140	ARG
3	E	152	SER
3	E	185	ASN
3	E	199	LEU
3	E	213	ARG
3	E	281	ILE
3	F	4	GLN
3	F	46	ARG
3	F	58	MET
3	F	83	VAL
3	F	112	GLU
3	F	118	ASP
3	F	143	LYS
3	F	170	LYS
3	F	182	LEU
3	F	185	ASN
3	F	199	LEU
3	F	215	ASN
3	F	225	MET
3	F	276	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	31	HIS
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	49	ASN
1	A	252	GLN
1	A	271	ASN
1	A	476	GLN
2	B	37	GLN
2	B	45	GLN
2	B	104	ASN
2	B	130	ASN
2	B	499	ASN
2	B	518	ASN
1	C	14	GLN
1	C	29	ASN
1	C	31	HIS
1	C	35	ASN
1	C	49	ASN
1	C	252	GLN
1	C	271	ASN
1	C	476	GLN
2	D	37	GLN
2	D	45	GLN
2	D	104	ASN
2	D	130	ASN
2	D	499	ASN
2	D	518	ASN
3	E	20	GLN
3	E	21	ASN
3	E	50	HIS
3	E	54	GLN
3	E	55	ASN
3	E	107	ASN
3	E	185	ASN
3	E	201	ASN
3	E	215	ASN
3	E	218	GLN
3	E	257	ASN
3	F	4	GLN
3	F	20	GLN
3	F	21	ASN
3	F	55	ASN
3	F	107	ASN
3	F	162	ASN
3	F	163	ASN

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Mol	Chain	Res	Type
3	F	185	ASN
3	F	201	ASN
3	F	218	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 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	$\# Z > 2$
13	PEG	D	5019	-	6,6,6	1.03	0	5,5,5	0.32	0
6	PGE	B	5005	-	9,9,9	1.16	0	8,8,8	0.57	0
13	PEG	B	5018	-	6,6,6	1.07	1 (16%)	5,5,5	0.36	0
10	TRS	C	5004	-	7,7,7	0.37	0	9,9,9	1.32	0
5	CFN	A	2496	1	18,30,30	1.61	3 (16%)	-		
14	P6G	D	5009	-	18,18,18	1.76	10 (55%)	17,17,17	0.68	0
6	PGE	C	5011	-	9,9,9	1.53	4 (44%)	8,8,8	0.49	0
11	PG4	E	5007	-	12,12,12	1.45	2 (16%)	11,11,11	0.55	0
11	PG4	B	5014	-	12,12,12	1.35	1 (8%)	11,11,11	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGE	D	5008	-	9,9,9	1.21	0	8,8,8	0.35	0
12	1PE	C	5013	-	15,15,15	1.69	6 (40%)	14,14,14	0.65	0
9	CLF	C	3498	1,2	0,24,24	0.00	-	-	-	-
12	1PE	B	5017	-	15,15,15	1.78	7 (46%)	14,14,14	0.60	0
4	HCA	C	3494	-	4,13,13	2.07	1 (25%)	4,18,18	1.85	1 (25%)
13	PEG	D	5020	-	6,6,6	1.37	2 (33%)	5,5,5	0.38	0
6	PGE	A	5012	-	9,9,9	1.22	0	8,8,8	0.32	0
5	CFN	C	3496	1	18,30,30	1.90	6 (33%)	-	-	-
4	HCA	A	2494	-	4,13,13	2.47	2 (50%)	4,18,18	1.97	2 (50%)
6	PGE	C	5016	-	9,9,9	1.49	4 (44%)	8,8,8	0.49	0
6	PGE	D	5006	-	9,9,9	1.09	0	8,8,8	0.45	0
9	CLF	B	2498	1,2	0,24,24	0.00	-	-	-	-
6	PGE	A	5015	-	9,9,9	1.65	4 (44%)	8,8,8	0.52	0
10	TRS	B	5003	-	7,7,7	0.52	0	9,9,9	1.24	1 (11%)
15	SF4	E	3290	3	0,12,12	0.00	-	-	-	-
6	PGE	D	5010	-	9,9,9	1.58	4 (44%)	8,8,8	0.56	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
13	PEG	D	5019	-	-	3/4/4/4	-
6	PGE	B	5005	-	-	2/7/7/7	-
9	CLF	C	3498	1,2	-	-	0/12/10/10
10	TRS	C	5004	-	-	8/9/9/9	-
14	P6G	D	5009	-	-	15/16/16/16	-
6	PGE	C	5011	-	-	1/7/7/7	-
11	PG4	E	5007	-	-	5/10/10/10	-
11	PG4	B	5014	-	-	1/10/10/10	-
6	PGE	D	5008	-	-	4/7/7/7	-
12	1PE	C	5013	-	-	8/13/13/13	-
13	PEG	B	5018	-	-	3/4/4/4	-
12	1PE	B	5017	-	-	8/13/13/13	-
4	HCA	C	3494	-	-	1/7/17/17	-
13	PEG	D	5020	-	-	2/4/4/4	-
6	PGE	A	5012	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	A	2494	-	-	0/7/17/17	-
6	PGE	C	5016	-	-	2/7/7/7	-
6	PGE	D	5006	-	-	5/7/7/7	-
9	CLF	B	2498	1,2	-	-	0/12/10/10
6	PGE	A	5015	-	-	4/7/7/7	-
10	TRS	B	5003	-	-	2/9/9/9	-
15	SF4	E	3290	3	-	-	0/6/5/5
6	PGE	D	5010	-	-	6/7/7/7	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2494	HCA	O7-C3	4.23	1.49	1.43
4	C	3494	HCA	O7-C3	3.91	1.49	1.43
5	C	3496	CFN	S1B-FE6	-3.30	2.23	2.29
5	C	3496	CFN	S2A-FE2	-3.26	2.23	2.29
5	A	2496	CFN	S1B-FE6	-3.13	2.23	2.29
5	A	2496	CFN	S4B-FE7	-2.93	2.23	2.29
12	B	5017	1PE	OH5-C25	2.66	1.53	1.42
5	C	3496	CFN	S4B-FE7	-2.65	2.24	2.29
12	B	5017	1PE	OH6-C15	2.61	1.53	1.42
5	C	3496	CFN	S3B-FE7	-2.61	2.24	2.29
6	A	5015	PGE	O3-C5	2.58	1.53	1.42
14	D	5009	P6G	O7-C8	2.49	1.52	1.42
12	B	5017	1PE	OH3-C22	2.45	1.52	1.42
5	C	3496	CFN	S4A-FE4	-2.45	2.24	2.29
4	A	2494	HCA	C2-C3	-2.44	1.51	1.54
14	D	5009	P6G	O4-C5	2.42	1.52	1.42
6	A	5015	PGE	O2-C3	2.39	1.52	1.42
12	B	5017	1PE	OH6-C26	2.38	1.52	1.42
12	B	5017	1PE	OH4-C13	2.37	1.52	1.42
12	C	5013	1PE	OH6-C15	2.36	1.52	1.42
14	D	5009	P6G	O16-C17	2.36	1.52	1.42
12	C	5013	1PE	OH6-C26	2.35	1.52	1.42
12	C	5013	1PE	OH3-C23	2.35	1.52	1.42
14	D	5009	P6G	O7-C6	2.33	1.52	1.42
12	C	5013	1PE	OH5-C14	2.30	1.52	1.42
6	A	5015	PGE	O3-C4	2.29	1.52	1.42
12	C	5013	1PE	OH4-C13	2.29	1.52	1.42
14	D	5009	P6G	O16-C15	2.28	1.51	1.42
6	D	5010	PGE	O2-C3	2.28	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3496	CFN	S4A-FE3	-2.27	2.25	2.29
6	D	5010	PGE	O2-C2	2.27	1.51	1.42
11	E	5007	PG4	O2-C3	2.26	1.51	1.42
6	C	5016	PGE	O2-C2	2.25	1.51	1.42
13	D	5020	PEG	O2-C3	2.25	1.51	1.42
13	D	5020	PEG	O2-C2	2.25	1.51	1.42
14	D	5009	P6G	O13-C14	2.24	1.51	1.42
6	D	5010	PGE	O3-C4	2.24	1.51	1.42
6	D	5010	PGE	O3-C5	2.24	1.51	1.42
5	A	2496	CFN	S5A-FE3	2.22	2.30	2.24
6	C	5011	PGE	O2-C3	2.22	1.51	1.42
6	C	5011	PGE	O2-C2	2.21	1.51	1.42
6	C	5011	PGE	O3-C5	2.17	1.51	1.42
6	C	5016	PGE	O2-C3	2.17	1.51	1.42
6	A	5015	PGE	O2-C2	2.15	1.51	1.42
12	C	5013	1PE	OH4-C24	2.15	1.51	1.42
14	D	5009	P6G	O10-C9	2.14	1.51	1.42
6	C	5016	PGE	O3-C5	2.12	1.51	1.42
6	C	5016	PGE	O3-C4	2.09	1.51	1.42
11	B	5014	PG4	O4-C7	2.08	1.51	1.42
6	C	5011	PGE	O3-C4	2.07	1.51	1.42
14	D	5009	P6G	O4-C3	2.07	1.51	1.42
14	D	5009	P6G	O10-C11	2.06	1.51	1.42
12	B	5017	1PE	OH3-C23	2.05	1.50	1.42
14	D	5009	P6G	O13-C12	2.05	1.50	1.42
11	E	5007	PG4	O3-C4	2.04	1.50	1.42
13	B	5018	PEG	O2-C2	2.03	1.50	1.42
12	B	5017	1PE	OH5-C14	2.01	1.50	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	HCA	C4-C5-C6	2.83	115.67	111.39
4	A	2494	HCA	C4-C3-C7	-2.73	106.72	111.52
10	B	5003	TRS	O3-C3-C	-2.25	103.86	111.00
4	A	2494	HCA	C4-C5-C6	2.06	114.52	111.39

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	5004	TRS	C1-C-C2-O2

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Mol	Chain	Res	Type	Atoms
10	C	5004	TRS	C3-C-C2-O2
10	C	5004	TRS	N-C-C2-O2
10	C	5004	TRS	C2-C-C3-O3
14	D	5009	P6G	C15-C14-O13-C12
12	C	5013	1PE	C24-C14-OH5-C25
14	D	5009	P6G	C9-C8-O7-C6
11	E	5007	PG4	C5-C6-O4-C7
13	D	5020	PEG	C4-C3-O2-C2
6	A	5015	PGE	O2-C3-C4-O3
12	C	5013	1PE	OH6-C15-C25-OH5
14	D	5009	P6G	O13-C14-C15-O16
11	E	5007	PG4	C1-C2-O2-C3
13	D	5019	PEG	O1-C1-C2-O2
12	B	5017	1PE	OH2-C12-C22-OH3
6	A	5012	PGE	O3-C5-C6-O4
11	E	5007	PG4	O3-C5-C6-O4
6	C	5016	PGE	C1-C2-O2-C3
13	D	5019	PEG	O2-C3-C4-O4
13	B	5018	PEG	O1-C1-C2-O2
6	D	5008	PGE	O3-C5-C6-O4
13	D	5020	PEG	O2-C3-C4-O4
14	D	5009	P6G	O7-C8-C9-O10
6	B	5005	PGE	O1-C1-C2-O2
6	C	5016	PGE	O1-C1-C2-O2
12	B	5017	1PE	C13-C23-OH3-C22
6	D	5006	PGE	O1-C1-C2-O2
6	D	5010	PGE	O1-C1-C2-O2
11	E	5007	PG4	O2-C3-C4-O3
14	D	5009	P6G	C14-C15-O16-C17
13	B	5018	PEG	O2-C3-C4-O4
14	D	5009	P6G	O1-C2-C3-O4
12	B	5017	1PE	OH7-C16-C26-OH6
12	C	5013	1PE	OH7-C16-C26-OH6
6	A	5015	PGE	O3-C5-C6-O4
12	B	5017	1PE	OH5-C14-C24-OH4
12	C	5013	1PE	OH2-C12-C22-OH3
14	D	5009	P6G	O10-C11-C12-O13
14	D	5009	P6G	C2-C3-O4-C5
14	D	5009	P6G	C8-C9-O10-C11
14	D	5009	P6G	C11-C12-O13-C14
6	D	5010	PGE	C6-C5-O3-C4
12	C	5013	1PE	OH5-C14-C24-OH4

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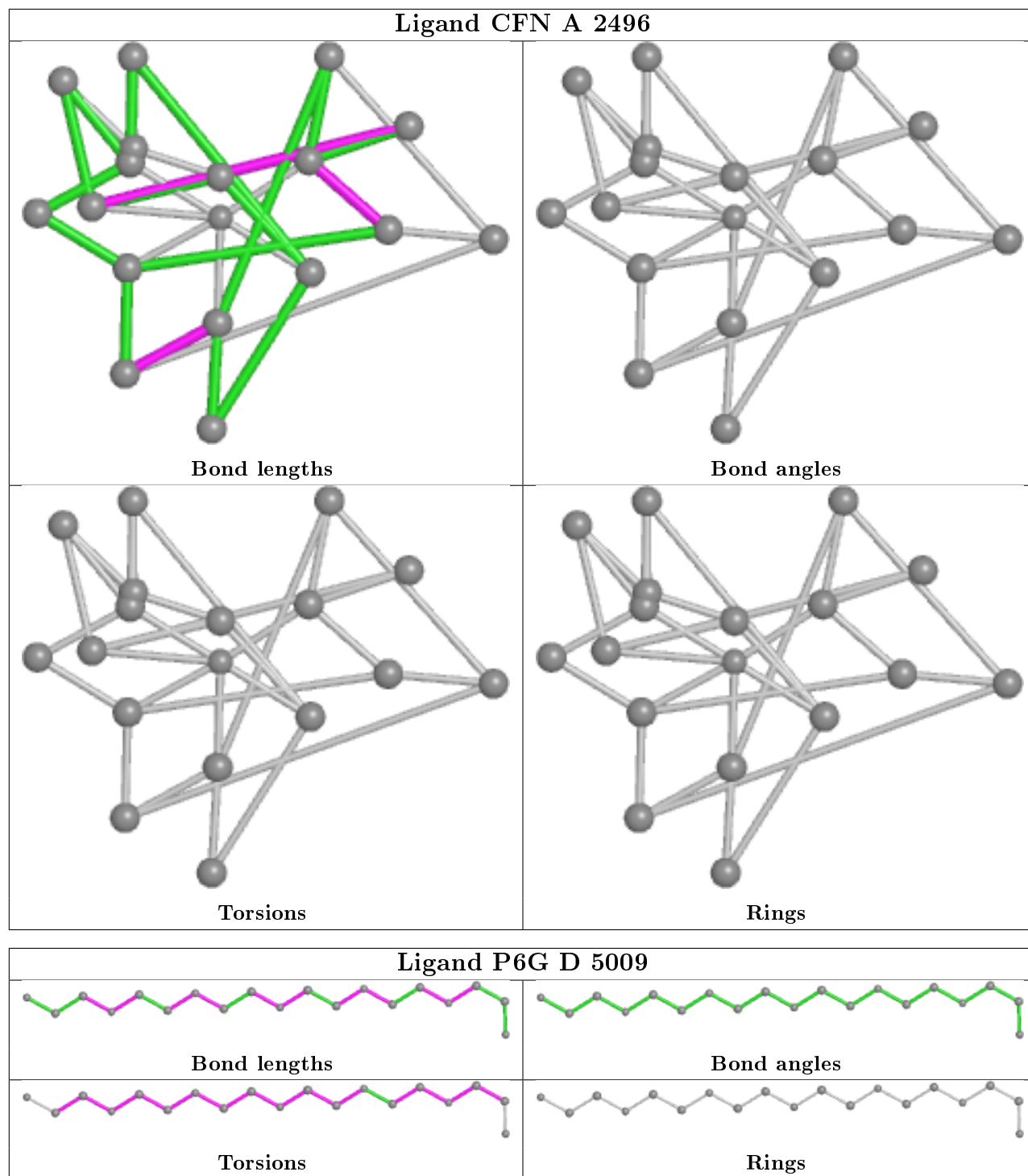
Mol	Chain	Res	Type	Atoms
6	A	5015	PGE	C3-C4-O3-C5
6	D	5008	PGE	C6-C5-O3-C4
10	C	5004	TRS	N-C-C1-O1
10	C	5004	TRS	C1-C-C3-O3
12	B	5017	1PE	C16-C26-OH6-C15
12	C	5013	1PE	C25-C15-OH6-C26
6	D	5006	PGE	C6-C5-O3-C4
14	D	5009	P6G	O16-C17-C18-O19
14	D	5009	P6G	C18-C17-O16-C15
11	E	5007	PG4	C4-C3-O2-C2
12	C	5013	1PE	C16-C26-OH6-C15
6	C	5011	PGE	C3-C4-O3-C5
6	A	5015	PGE	C4-C3-O2-C2
6	D	5010	PGE	C3-C4-O3-C5
14	D	5009	P6G	C12-C11-O10-C9
14	D	5009	P6G	C6-C5-O4-C3
12	B	5017	1PE	OH4-C13-C23-OH3
6	D	5010	PGE	O2-C3-C4-O3
12	B	5017	1PE	C25-C15-OH6-C26
13	D	5019	PEG	C4-C3-O2-C2
10	C	5004	TRS	C2-C-C1-O1
10	B	5003	TRS	C3-C-C1-O1
10	B	5003	TRS	C3-C-C2-O2
6	A	5012	PGE	C4-C3-O2-C2
14	D	5009	P6G	O4-C5-C6-O7
12	C	5013	1PE	C14-C24-OH4-C13
6	D	5006	PGE	C3-C4-O3-C5
6	D	5010	PGE	O3-C5-C6-O4
6	B	5005	PGE	O2-C3-C4-O3
10	C	5004	TRS	N-C-C3-O3
12	B	5017	1PE	C14-C24-OH4-C13
6	D	5008	PGE	O1-C1-C2-O2
6	D	5006	PGE	C1-C2-O2-C3
11	B	5014	PG4	O2-C3-C4-O3
13	B	5018	PEG	C4-C3-O2-C2
4	C	3494	HCA	C7-C3-C4-C5
6	D	5006	PGE	O2-C3-C4-O3
6	D	5008	PGE	C4-C3-O2-C2
6	D	5010	PGE	C4-C3-O2-C2
6	A	5012	PGE	O1-C1-C2-O2

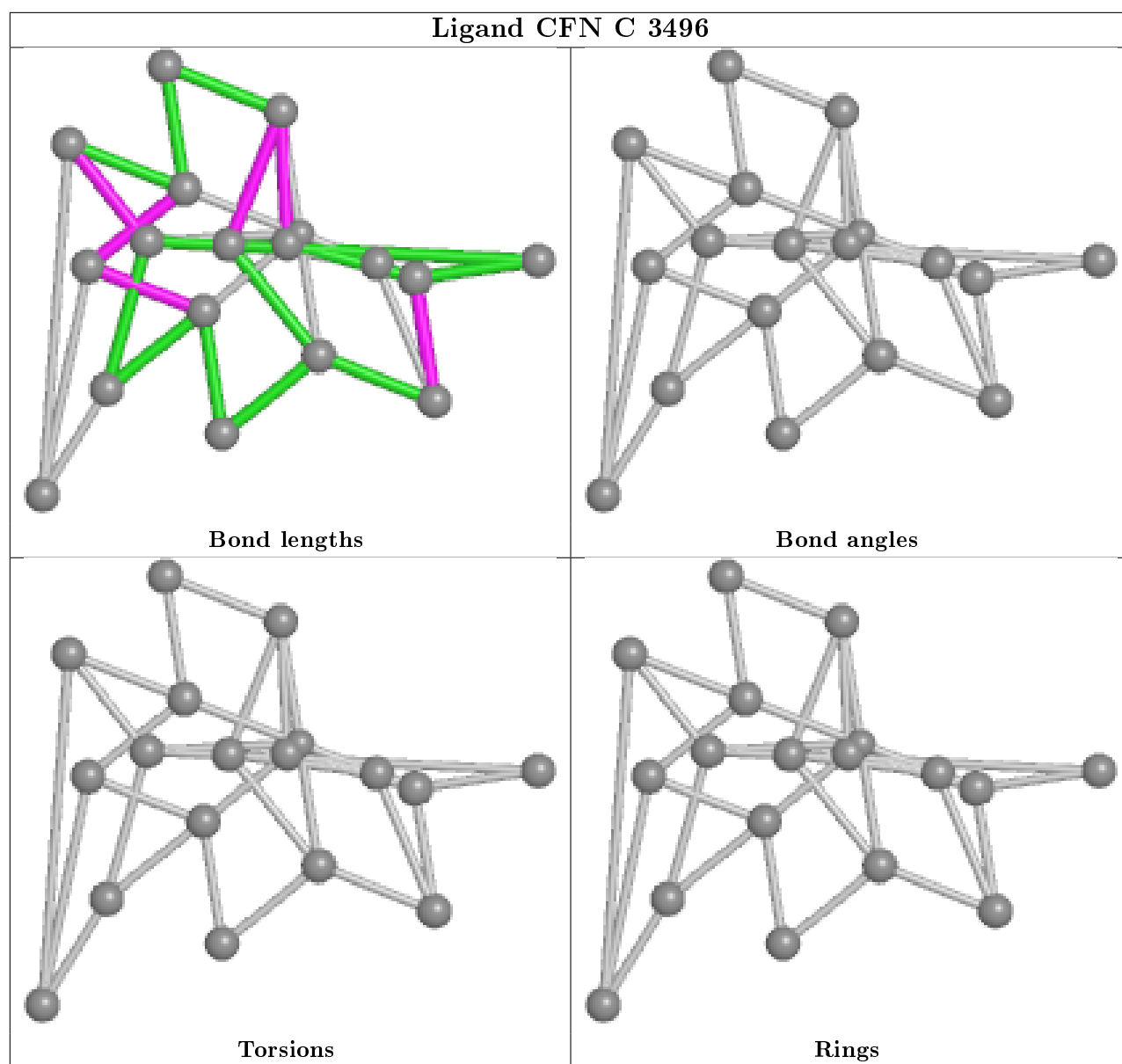
There are no ring outliers.

17 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	5019	PEG	1	0
6	B	5005	PGE	5	0
10	C	5004	TRS	2	0
5	A	2496	CFN	1	0
14	D	5009	P6G	1	0
6	C	5011	PGE	4	0
11	E	5007	PG4	7	0
6	D	5008	PGE	2	0
12	C	5013	1PE	22	0
12	B	5017	1PE	7	0
4	C	3494	HCA	1	0
13	D	5020	PEG	4	0
6	A	5012	PGE	1	0
4	A	2494	HCA	2	0
6	D	5006	PGE	2	0
6	A	5015	PGE	7	0
6	D	5010	PGE	4	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, 95th 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	476/491 (96%)	-0.44	0 100 100	12, 22, 40, 66	2 (0%)
1	C	477/491 (97%)	-0.43	2 (0%) 92 93	13, 22, 41, 64	0
2	B	522/522 (100%)	-0.60	1 (0%) 95 95	10, 16, 32, 55	1 (0%)
2	D	522/522 (100%)	-0.56	3 (0%) 89 91	10, 18, 35, 53	0
3	E	289/289 (100%)	0.02	14 (4%) 30 36	20, 35, 65, 85	0
3	F	286/289 (98%)	-0.05	16 (5%) 24 29	19, 35, 67, 84	1 (0%)
All	All	2572/2604 (98%)	-0.40	36 (1%) 75 78	10, 22, 49, 85	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	66	THR	7.6
2	B	125	PHE	6.4
3	E	42	ALA	5.6
3	F	276	VAL	4.8
3	E	65	GLY	4.7
1	C	125	PHE	4.3
3	F	1	ALA	4.2
3	F	273	ILE	4.2
2	D	215	ASP	4.1
1	C	4	MET	3.8
3	E	67	VAL	3.5
3	F	277	GLU	3.4
3	F	284	LYS	3.4
3	E	41	LYS	3.4
3	F	190	ASP	3.4
2	D	214	ASP	3.3
3	F	271	PHE	3.2
3	E	172	ALA	3.1
3	E	68	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	272	GLY	2.7
3	E	173	ASN	2.7
3	E	1	ALA	2.5
3	F	117	ASP	2.4
3	E	64	ALA	2.4
2	D	125	PHE	2.4
3	E	70	LEU	2.4
3	F	282	VAL	2.4
3	F	118	ASP	2.4
3	F	280	SER	2.4
3	E	62	ALA	2.4
3	E	72	LEU	2.2
3	F	73	GLU	2.1
3	F	281	ILE	2.1
3	F	275	GLU	2.1
3	E	61	ALA	2.0
3	F	278	ASP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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(\AA^2)	Q<0.9
8	NA	B	2492	1/1	0.43	0.13	40,40,40,40	0
6	PGE	A	5015	10/10	0.76	0.33	44,48,52,61	0
11	PG4	E	5007	13/13	0.79	0.21	43,48,56,57	0
6	PGE	D	5010	10/10	0.81	0.28	39,46,53,58	0
10	TRS	C	5004	8/8	0.82	0.27	44,47,50,50	0
6	PGE	C	5016	10/10	0.83	0.34	40,49,53,62	0

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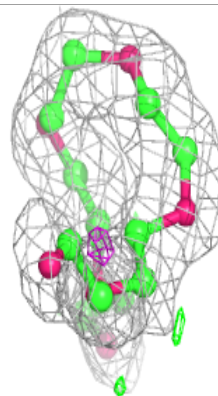
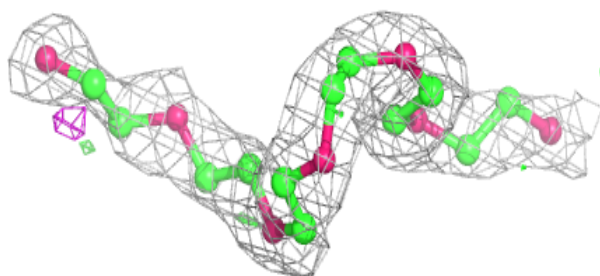
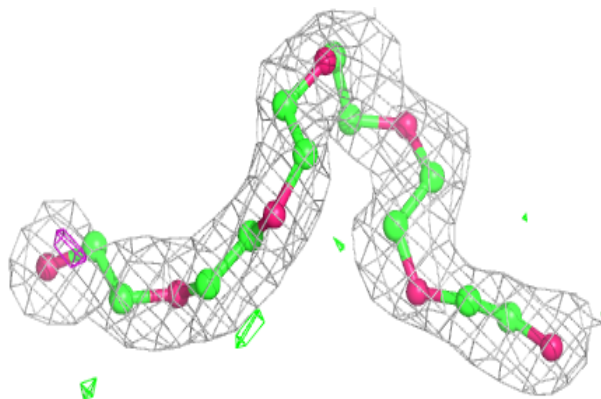
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	1PE	C	5013	16/16	0.84	0.24	36,45,50,55	0
6	PGE	A	5012	10/10	0.86	0.33	40,47,58,58	0
13	PEG	D	5020	7/7	0.86	0.29	33,38,45,50	0
13	PEG	D	5019	7/7	0.87	0.16	46,52,59,65	0
6	PGE	C	5011	10/10	0.88	0.20	37,46,52,56	0
12	1PE	B	5017	16/16	0.89	0.31	22,44,51,57	0
14	P6G	D	5009	19/19	0.90	0.12	24,38,48,51	0
6	PGE	D	5006	10/10	0.90	0.13	29,41,45,47	0
6	PGE	D	5008	10/10	0.93	0.15	29,44,51,62	0
13	PEG	B	5018	7/7	0.93	0.10	28,30,46,49	0
6	PGE	B	5005	10/10	0.94	0.11	26,30,45,48	0
11	PG4	B	5014	13/13	0.94	0.10	26,34,40,47	0
10	TRS	B	5003	8/8	0.95	0.16	22,28,37,45	0
9	CLF	B	2498	15/15	0.96	0.09	3,15,16,36	2
4	HCA	A	2494	14/14	0.96	0.16	12,17,22,23	0
9	CLF	C	3498	15/15	0.97	0.07	18,21,24,38	0
4	HCA	C	3494	14/14	0.98	0.14	15,17,21,21	0
15	SF4	E	3290	8/8	0.98	0.05	25,27,28,30	0
7	CA	B	2491	1/1	0.99	0.05	25,25,25,25	0
5	CFN	A	2496	18/18	0.99	0.08	15,18,19,20	0
5	CFN	C	3496	18/18	0.99	0.10	14,18,22,22	0
7	CA	D	2490	1/1	0.99	0.03	24,24,24,24	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.

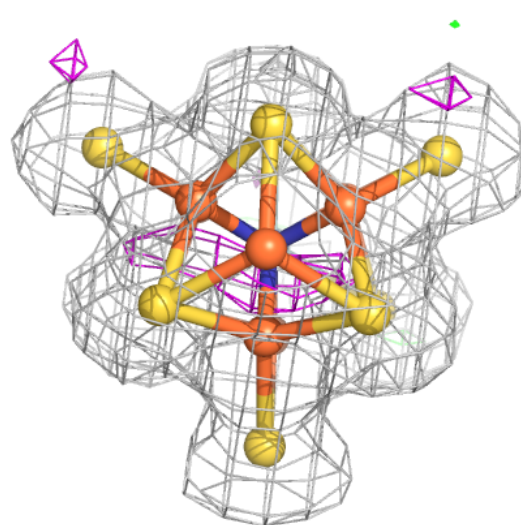
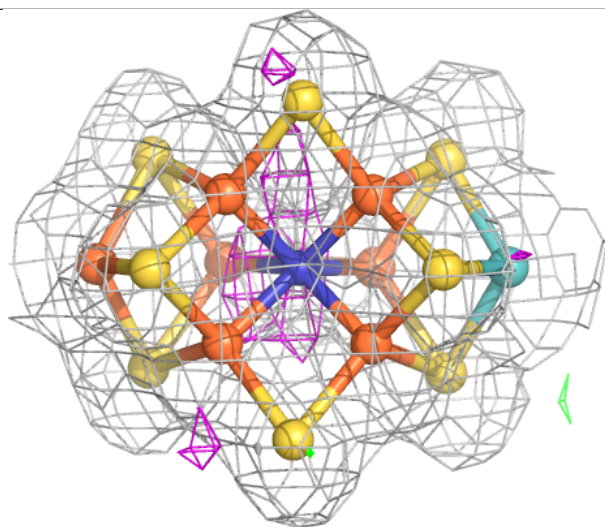
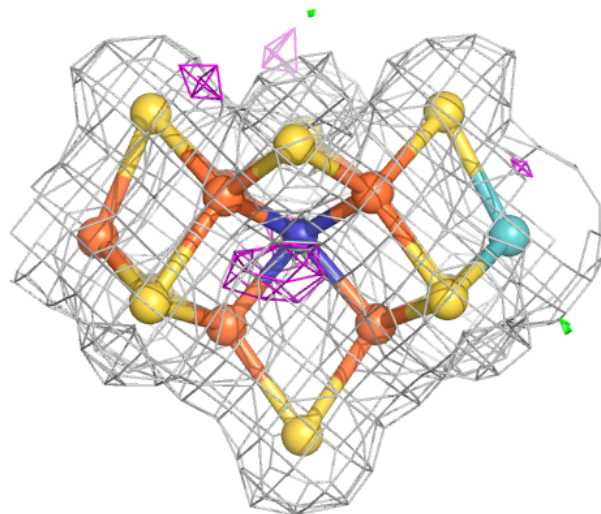
Electron density around P6G D 5009:

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



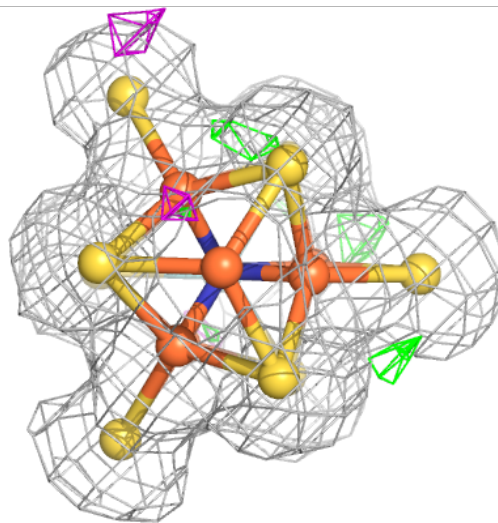
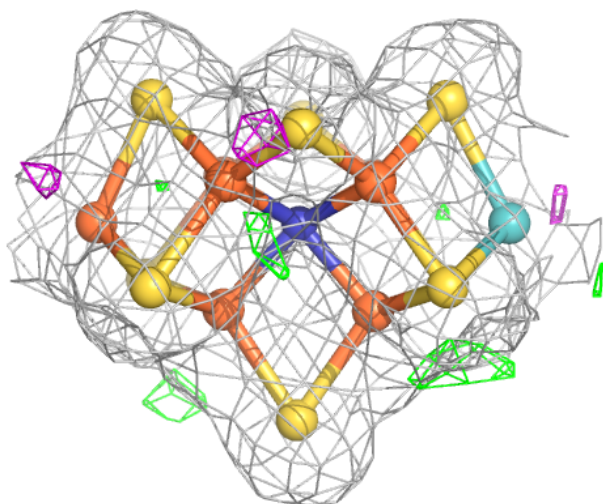
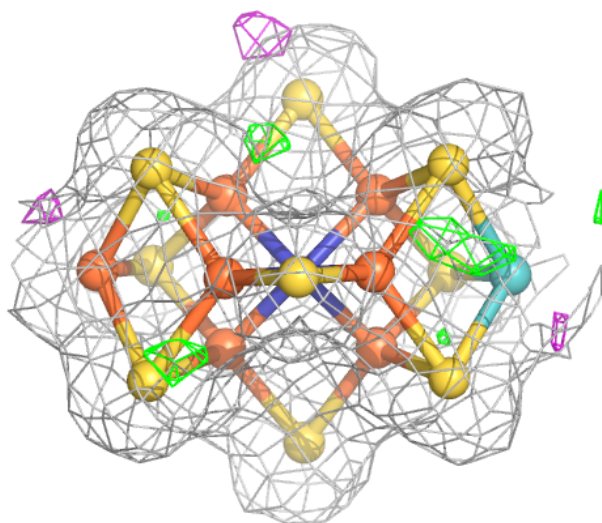
Electron density around CFN A 2496:

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



Electron density around CFN C 3496:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.