



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:08 am BST

PDB ID : 6FEA  
Title : A. vinelandii vanadium nitrogenase, turnover state  
Authors : Sippel, D.; Einsle, O.  
Deposited on : 2017-12-31  
Resolution : 1.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

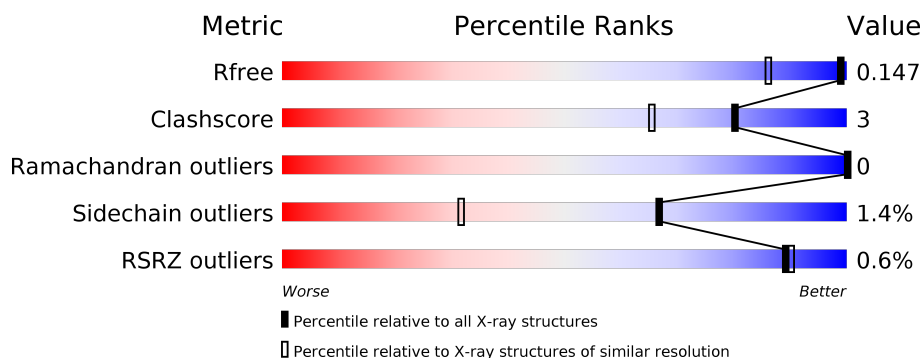
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	<div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	D	474	<div> <div>84%</div> <div>11%</div> <div>••</div> </div>
2	B	475	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>••</div> </div>
2	E	475	<div> <div>85%</div> <div>10%</div> <div>••</div> </div>
3	C	113	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>••</div> </div>
3	F	113	<div> <div>4%</div> <div>73%</div> <div>20%</div> <div>•••</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 19493 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 protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	8	0
			3764	2403	643	692	26			
1	D	461	Total	C	N	O	S	0	8	0
			3764	2403	643	692	26			

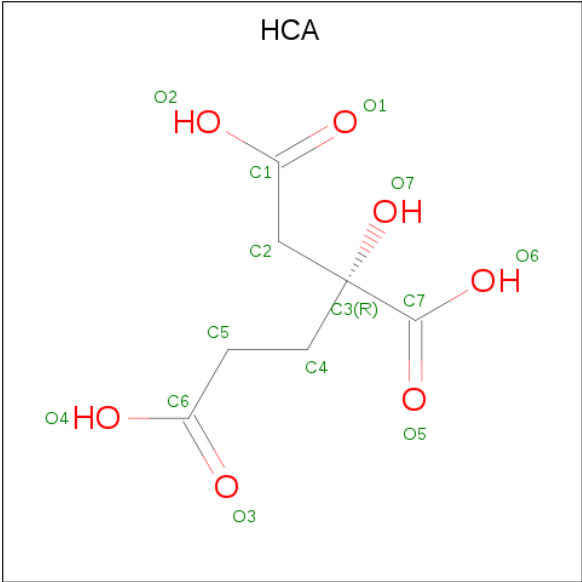
- Molecule 2 is a protein called Vanadium nitrogenase beta subunit, vnfK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	0	2	0
			3644	2315	626	682	21			
2	E	464	Total	C	N	O	S	0	4	0
			3659	2323	628	687	21			

- Molecule 3 is a protein called Vanadium nitrogenase, delta subunit, VnfG.

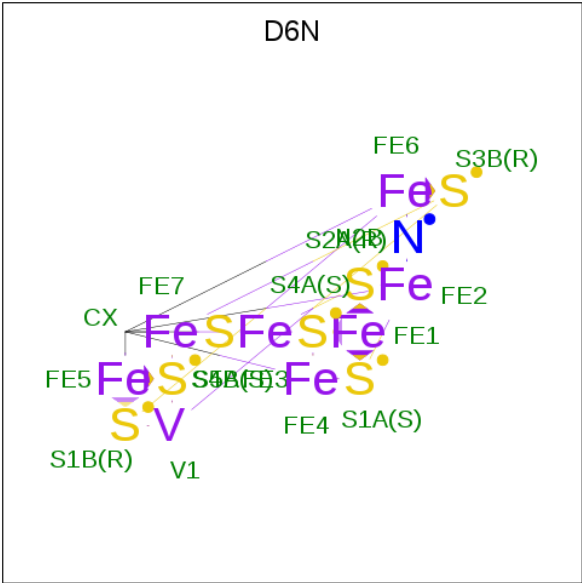
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	113	Total	C	N	O	S	0	1	0
			953	598	171	181	3			
3	F	111	Total	C	N	O	S	0	2	0
			947	594	172	179	2			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>7</sub>).



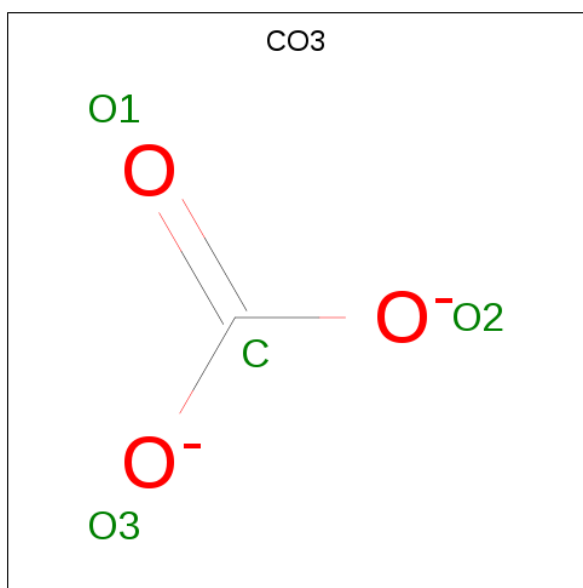
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FeV (three-letter code: D6N) (formula: CFe<sub>7</sub>NS<sub>7</sub>V).



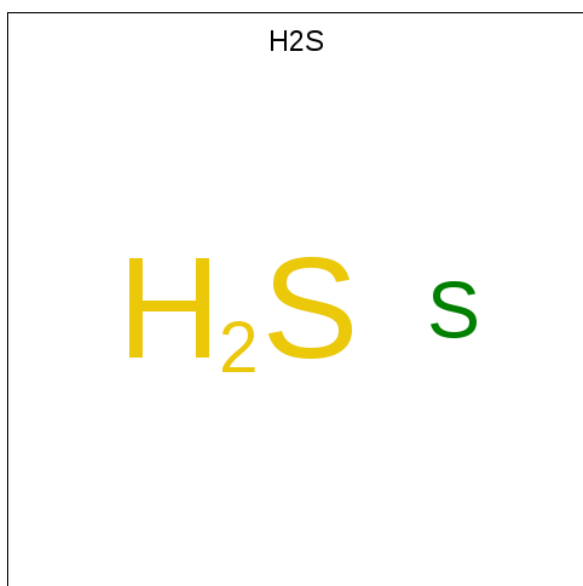
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	S	V	0	0
			17	1	7	1	7	1		
5	D	1	Total	C	Fe	N	S	V	0	0
			17	1	7	1	7	1		

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	S	0	0
			1	1		

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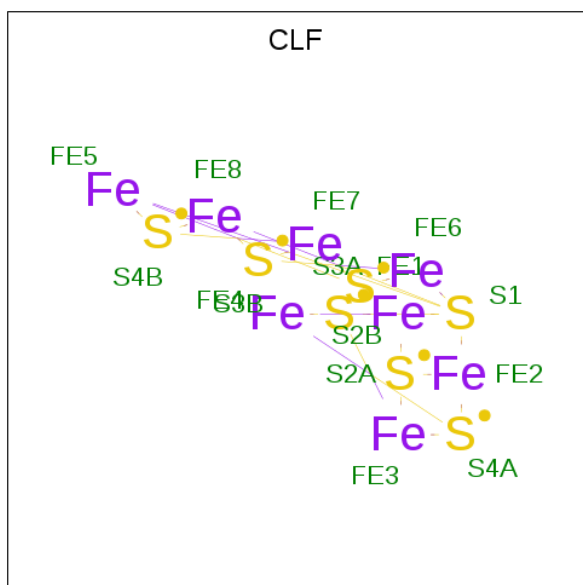
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total S 1 1	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Zn 1 1	0	0
8	A	1	Total Zn 1 1	0	0

- Molecule 9 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe<sub>8</sub>S<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Fe S 16 9 7	0	1
9	D	1	Total Fe S 16 9 7	0	1

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Mg 2 2	0	0
10	C	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total 1	Mg 1	0	0

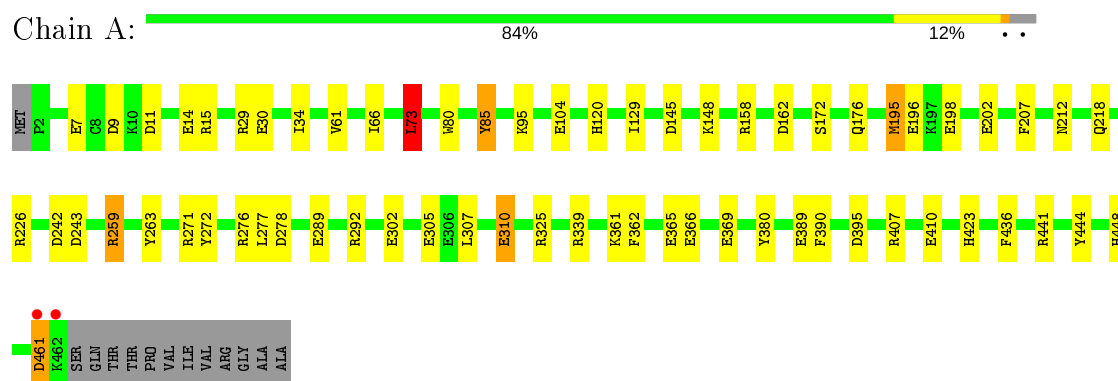
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	580	Total 580	O 580	0	0
11	B	562	Total 562	O 562	0	0
11	C	178	Total 178	O 178	0	0
11	D	570	Total 570	O 570	0	0
11	E	607	Total 607	O 607	0	0
11	F	155	Total 155	O 155	0	0

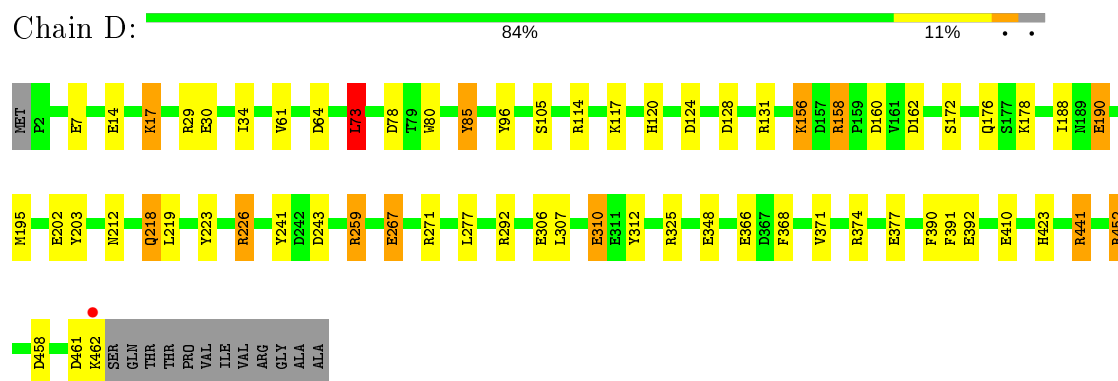
### 3 Residue-property plots

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.

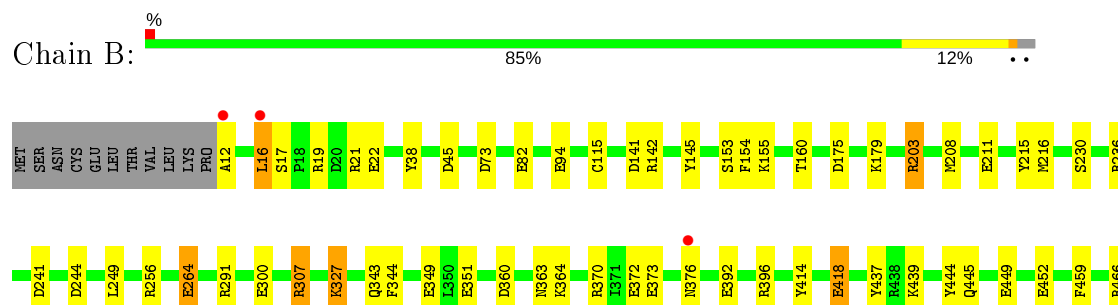
#### • Molecule 1: Nitrogenase protein alpha chain



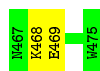
#### • Molecule 1: Nitrogenase protein alpha chain



#### • Molecule 2: Vanadium nitrogenase beta subunit, vnfK

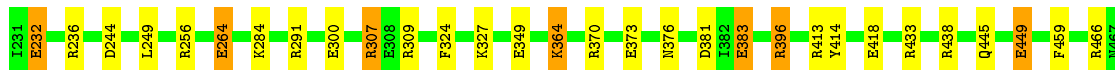






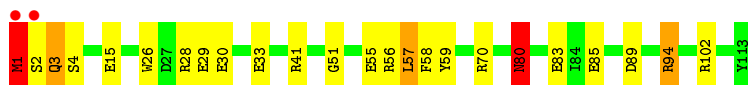
- Molecule 2: Vanadium nitrogenase beta subunit, vnfK

Chain E: 85% 10% ..



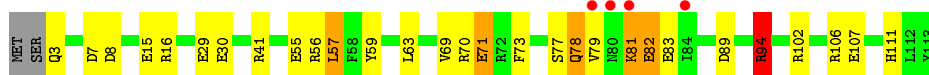
- Molecule 3: Vanadium nitrogenase, delta subunit, VnfG

Chain C: 2% 79% 17% ..



- Molecule 3: Vanadium nitrogenase, delta subunit, VnfG

Chain F: 4% 73% 20% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.61Å 79.75Å 107.16Å 84.05° 72.44° 75.25°	Depositor
Resolution (Å)	102.12 – 1.20 48.38 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (102.12-1.20) 99.6 (48.38-1.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.117 , 0.145 0.119 , 0.147	Depositor DCC
$R_{free}$ test set	35693 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	19493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, D6N, CLF, MG, H2S, HCA, CO3

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	1.45	34/3859 (0.9%)	1.31	31/5213 (0.6%)
1	D	1.40	33/3859 (0.9%)	1.30	40/5213 (0.8%)
2	B	1.50	43/3722 (1.2%)	1.41	42/5039 (0.8%)
2	E	1.50	42/3737 (1.1%)	1.33	35/5059 (0.7%)
3	C	1.59	14/973 (1.4%)	1.33	12/1315 (0.9%)
3	F	1.92	21/967 (2.2%)	1.66	27/1307 (2.1%)
All	All	1.50	187/17117 (1.1%)	1.35	187/23146 (0.8%)

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	D	0	1
2	B	0	1
2	E	0	2
3	F	0	1
All	All	0	6

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	82	GLU	CD-OE2	24.46	1.52	1.25
1	D	172	SER	CB-OG	-22.46	1.13	1.42
2	E	418	GLU	CD-OE1	17.38	1.44	1.25
1	D	366	GLU	CB-CG	-13.29	1.26	1.52
1	A	14	GLU	CD-OE2	12.82	1.39	1.25
1	A	461	ASP	CG-OD2	12.28	1.53	1.25
1	D	310	GLU	CD-OE1	11.65	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	GLU	CA-C	11.63	1.83	1.52
2	E	12	ALA	N-CA	10.72	1.67	1.46
2	B	449	GLU	CD-OE2	10.65	1.37	1.25
2	B	264	GLU	CD-OE1	10.58	1.37	1.25
2	B	466	ARG	CZ-NH1	10.53	1.46	1.33
2	E	133	ARG	CD-NE	10.29	1.64	1.46
3	C	56	ARG	CD-NE	-10.22	1.29	1.46
2	B	300	GLU	CD-OE1	9.94	1.36	1.25
2	B	264	GLU	CG-CD	9.79	1.66	1.51
2	B	469	GLU	CD-OE2	9.78	1.36	1.25
3	F	15	GLU	CD-OE2	9.55	1.36	1.25
2	B	12	ALA	N-CA	9.35	1.65	1.46
2	B	418	GLU	CD-OE2	9.31	1.35	1.25
2	E	396	ARG	NE-CZ	-9.23	1.21	1.33
2	E	449	GLU	CD-OE2	9.23	1.35	1.25
1	D	7	GLU	CD-OE2	9.05	1.35	1.25
1	A	14	GLU	CD-OE1	9.03	1.35	1.25
2	E	181	GLN	CD-OE1	9.01	1.43	1.24
2	E	469	GLU	CD-OE2	9.00	1.35	1.25
1	A	198	GLU	CD-OE1	8.64	1.35	1.25
1	A	195	MET	CA-CB	-8.57	1.35	1.53
1	A	30	GLU	CD-OE1	8.56	1.35	1.25
2	E	373	GLU	CD-OE1	-8.29	1.16	1.25
1	A	310	GLU	CD-OE1	8.24	1.34	1.25
3	F	55	GLU	CD-OE2	8.12	1.34	1.25
2	B	392[A]	GLU	CD-OE2	-8.10	1.16	1.25
2	B	392[B]	GLU	CD-OE2	-8.10	1.16	1.25
1	A	195	MET	CG-SD	8.03	2.02	1.81
1	A	289	GLU	CD-OE2	7.94	1.34	1.25
2	B	211	GLU	CG-CD	-7.93	1.40	1.51
2	E	230	SER	CB-OG	-7.88	1.32	1.42
1	D	195	MET	CB-CG	-7.86	1.26	1.51
1	A	366	GLU	CB-CG	-7.84	1.37	1.52
2	E	376	ASN	C-O	7.84	1.38	1.23
1	D	14	GLU	CG-CD	7.72	1.63	1.51
1	D	105	SER	CB-OG	-7.72	1.32	1.42
1	A	302	GLU	CG-CD	7.71	1.63	1.51
2	E	466	ARG	CZ-NH1	7.67	1.43	1.33
1	D	410	GLU	CD-OE2	7.63	1.34	1.25
2	E	418	GLU	CG-CD	7.62	1.63	1.51
1	A	104	GLU	CD-OE1	7.59	1.33	1.25
3	C	15	GLU	CD-OE2	7.56	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	264[A]	GLU	CD-OE1	7.51	1.33	1.25
2	E	264[B]	GLU	CD-OE1	7.51	1.33	1.25
1	A	14	GLU	CG-CD	7.49	1.63	1.51
1	A	202	GLU	CD-OE2	7.46	1.33	1.25
2	B	414	TYR	CG-CD1	-7.46	1.29	1.39
2	B	372	GLU	CD-OE2	-7.42	1.17	1.25
2	E	232	GLU	CD-OE1	7.42	1.33	1.25
2	E	300	GLU	CD-OE1	7.42	1.33	1.25
1	D	7	GLU	CD-OE1	7.30	1.33	1.25
1	A	365	GLU	CD-OE2	7.30	1.33	1.25
2	E	133	ARG	CZ-NH1	7.27	1.42	1.33
1	A	172	SER	CB-OG	-7.22	1.32	1.42
3	F	78	GLN	CA-C	7.16	1.71	1.52
1	A	7	GLU	CD-OE1	7.16	1.33	1.25
1	D	366	GLU	CG-CD	7.15	1.62	1.51
2	B	376	ASN	N-CA	7.11	1.60	1.46
2	E	418	GLU	CD-OE2	7.06	1.33	1.25
2	B	82	GLU	CG-CD	7.02	1.62	1.51
2	B	230	SER	CB-OG	-6.99	1.33	1.42
2	B	300	GLU	CD-OE2	6.99	1.33	1.25
2	B	373	GLU	CD-OE2	6.98	1.33	1.25
1	D	348	GLU	CD-OE2	-6.95	1.18	1.25
2	B	307	ARG	CG-CD	6.94	1.69	1.51
1	D	306	GLU	CD-OE2	6.91	1.33	1.25
1	D	190	GLU	CD-OE2	6.85	1.33	1.25
3	F	83	GLU	C-O	-6.80	1.10	1.23
2	B	203	ARG	CD-NE	6.76	1.57	1.46
1	A	195	MET	CB-CG	-6.75	1.29	1.51
3	F	15	GLU	CD-OE1	6.71	1.33	1.25
2	B	363	ASN	CB-CG	6.68	1.66	1.51
2	B	452	GLU	CD-OE2	6.66	1.32	1.25
2	E	300	GLU	CG-CD	6.64	1.61	1.51
2	E	449	GLU	CG-CD	-6.63	1.42	1.51
3	F	71	GLU	CG-CD	-6.62	1.42	1.51
1	D	292	ARG	CZ-NH2	6.60	1.41	1.33
3	F	78	GLN	CD-OE1	6.58	1.38	1.24
1	A	73	LEU	CG-CD1	6.56	1.76	1.51
2	E	232	GLU	CD-OE2	-6.55	1.18	1.25
1	A	7	GLU	CD-OE2	6.51	1.32	1.25
3	F	59	TYR	CE1-CZ	-6.47	1.30	1.38
1	A	361	LYS	CD-CE	-6.47	1.35	1.51
2	B	414	TYR	CD1-CE1	6.45	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	17	SER	CB-OG	-6.39	1.33	1.42
1	D	267	GLU	CG-CD	6.38	1.61	1.51
2	E	203	ARG	CD-NE	6.38	1.57	1.46
3	C	85	GLU	CD-OE2	6.36	1.32	1.25
2	E	414	TYR	CZ-OH	6.35	1.48	1.37
3	F	56	ARG	CD-NE	-6.33	1.35	1.46
1	D	392	GLU	CD-OE2	6.32	1.32	1.25
2	E	142	ARG	CA-CB	6.29	1.67	1.53
1	A	410	GLU	CD-OE2	6.29	1.32	1.25
1	D	312	TYR	CE1-CZ	-6.28	1.30	1.38
1	D	17	LYS	CB-CG	-6.28	1.35	1.52
1	D	267	GLU	CD-OE1	-6.27	1.18	1.25
3	F	70	ARG	CZ-NH1	6.24	1.41	1.33
1	D	306	GLU	CD-OE1	6.24	1.32	1.25
2	B	418	GLU	CG-CD	-6.22	1.42	1.51
2	E	236	ARG	CG-CD	6.19	1.67	1.51
2	E	396	ARG	CD-NE	6.19	1.56	1.46
1	D	348	GLU	CD-OE1	-6.17	1.18	1.25
3	F	41	ARG	CZ-NH1	6.16	1.41	1.33
2	E	284	LYS	CE-NZ	-6.15	1.33	1.49
2	E	307	ARG	CB-CG	-6.14	1.35	1.52
2	E	468	LYS	CE-NZ	6.10	1.64	1.49
3	C	29	GLU	CG-CD	6.03	1.60	1.51
1	A	172	SER	CA-CB	-6.01	1.44	1.52
1	D	14	GLU	CD-OE2	6.00	1.32	1.25
2	B	418	GLU	CD-OE1	5.96	1.32	1.25
1	D	267	GLU	CD-OE2	-5.96	1.19	1.25
2	B	343	GLN	CD-OE1	5.94	1.37	1.24
1	D	366	GLU	CD-OE1	-5.94	1.19	1.25
1	A	80	TRP	CE3-CZ3	5.91	1.48	1.38
3	F	83	GLU	CD-OE2	5.90	1.32	1.25
2	E	349	GLU	CD-OE1	-5.89	1.19	1.25
2	B	351	GLU	CD-OE2	5.89	1.32	1.25
2	E	383	GLU	CD-OE1	5.87	1.32	1.25
2	E	44	LYS	CE-NZ	5.85	1.63	1.49
2	B	22	GLU	CG-CD	-5.82	1.43	1.51
2	E	17	SER	CB-OG	-5.82	1.34	1.42
2	E	414	TYR	CD1-CE1	5.80	1.48	1.39
2	B	327	LYS	CE-NZ	5.79	1.63	1.49
2	B	363	ASN	CG-OD1	5.78	1.36	1.24
1	A	366	GLU	CD-OE1	-5.77	1.19	1.25
2	B	307	ARG	CB-CG	-5.76	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	55	GLU	CD-OE1	5.76	1.31	1.25
2	B	466	ARG	CZ-NH2	5.76	1.40	1.33
2	B	154	PHE	CG-CD1	-5.72	1.30	1.38
2	E	256	ARG	CZ-NH2	-5.72	1.25	1.33
3	C	59	TYR	CD1-CE1	-5.72	1.30	1.39
3	F	30	GLU	CB-CG	-5.72	1.41	1.52
2	B	351	GLU	CD-OE1	-5.71	1.19	1.25
1	A	263	TYR	CE2-CZ	-5.70	1.31	1.38
1	A	461	ASP	CG-OD1	5.69	1.38	1.25
2	B	38	TYR	CE2-CZ	-5.69	1.31	1.38
1	A	441	ARG	CD-NE	-5.68	1.36	1.46
1	A	305	GLU	CD-OE1	5.67	1.31	1.25
3	F	3	GLN	CD-NE2	5.64	1.47	1.32
2	B	396	ARG	NE-CZ	-5.63	1.25	1.33
3	C	55	GLU	CD-OE2	5.58	1.31	1.25
2	E	38	TYR	CE2-CZ	-5.58	1.31	1.38
2	B	155	LYS	CB-CG	-5.57	1.37	1.52
2	E	19	ARG	CB-CG	-5.57	1.37	1.52
3	F	106	ARG	CD-NE	-5.56	1.36	1.46
3	F	29	GLU	CD-OE1	5.54	1.31	1.25
3	C	33	GLU	CD-OE2	5.54	1.31	1.25
1	D	218	GLN	CD-OE1	5.53	1.36	1.24
3	C	30	GLU	CD-OE2	5.52	1.31	1.25
1	D	203	TYR	CD1-CE1	5.50	1.47	1.39
2	B	264	GLU	CD-OE2	5.48	1.31	1.25
2	E	466	ARG	CZ-NH2	5.47	1.40	1.33
2	E	381	ASP	CA-CB	-5.47	1.42	1.53
3	F	55	GLU	CD-OE1	5.46	1.31	1.25
3	F	73	PHE	CG-CD2	-5.46	1.30	1.38
1	D	30	GLU	CD-OE1	5.45	1.31	1.25
1	D	34	ILE	C-O	5.43	1.33	1.23
2	B	256	ARG	CZ-NH2	-5.40	1.26	1.33
1	D	226	ARG	CZ-NH1	5.34	1.40	1.33
1	D	96	TYR	CG-CD2	-5.34	1.32	1.39
3	C	3	GLN	N-CA	5.30	1.56	1.46
2	E	13	GLU	CG-CD	5.30	1.59	1.51
1	A	34	ILE	C-O	5.30	1.33	1.23
2	E	17	SER	CA-CB	-5.26	1.45	1.52
2	B	142	ARG	CB-CG	-5.25	1.38	1.52
1	A	369	GLU	CD-OE2	5.24	1.31	1.25
1	D	223	TYR	CG-CD1	-5.24	1.32	1.39
3	F	107	GLU	CD-OE1	-5.23	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	TRP	CZ2-CH2	-5.21	1.27	1.37
1	A	380	TYR	CG-CD2	-5.18	1.32	1.39
3	C	51	GLY	C-O	5.17	1.31	1.23
2	B	349	GLU	CD-OE2	5.15	1.31	1.25
1	A	366	GLU	CG-CD	5.13	1.59	1.51
3	F	106	ARG	NE-CZ	5.11	1.39	1.33
3	C	58	PHE	CD1-CE1	5.09	1.49	1.39
3	C	2	SER	N-CA	5.07	1.56	1.46
1	D	202	GLU	CD-OE2	5.06	1.31	1.25
2	B	145	TYR	CG-CD1	-5.06	1.32	1.39
3	C	80	ASN	CG-OD1	5.04	1.35	1.24
1	A	272	TYR	CE1-CZ	5.02	1.45	1.38

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	466	ARG	NE-CZ-NH2	-23.73	108.43	120.30
3	F	56	ARG	NE-CZ-NH2	-16.57	112.01	120.30
3	F	56	ARG	NE-CZ-NH1	16.05	128.32	120.30
2	B	466	ARG	NE-CZ-NH1	15.96	128.28	120.30
2	B	418	GLU	OE1-CD-OE2	15.34	141.71	123.30
1	D	325	ARG	NE-CZ-NH1	15.25	127.92	120.30
2	E	133	ARG	NE-CZ-NH2	-12.99	113.80	120.30
2	E	466	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	A	148	LYS	CD-CE-NZ	-12.91	82.01	111.70
2	E	381	ASP	CB-CG-OD2	-12.47	107.08	118.30
2	B	307	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	A	243	ASP	CB-CG-OD2	-11.82	107.67	118.30
1	D	325	ARG	NE-CZ-NH2	-11.69	114.46	120.30
2	E	466	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	D	310	GLU	OE1-CD-OE2	10.65	136.07	123.30
1	A	73	LEU	CB-CG-CD1	10.46	128.78	111.00
2	E	291	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	292	ARG	NE-CZ-NH2	-10.27	115.17	120.30
2	B	291	ARG	NE-CZ-NH1	10.03	125.31	120.30
2	E	291	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	E	396	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	A	461	ASP	CB-CG-OD1	-9.83	109.45	118.30
2	B	307	ARG	NE-CZ-NH1	-9.71	115.45	120.30
3	F	102	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	D	292	ARG	NE-CZ-NH2	-9.63	115.49	120.30
2	E	469	GLU	OE1-CD-OE2	-9.44	111.97	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	28	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	325	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	D	195	MET	CG-SD-CE	-9.04	85.74	100.20
1	D	243	ASP	CB-CG-OD2	-9.03	110.17	118.30
2	E	101	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	A	145	ASP	CB-CG-OD1	8.84	126.25	118.30
3	F	94[A]	ARG	NE-CZ-NH2	8.71	124.66	120.30
3	F	94[B]	ARG	NE-CZ-NH2	8.71	124.66	120.30
3	C	28	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	259	ARG	NE-CZ-NH1	8.45	124.52	120.30
2	B	370	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	259	ARG	NE-CZ-NH2	-8.41	116.09	120.30
3	C	57	LEU	CA-CB-CG	-8.22	96.39	115.30
2	B	141	ASP	CB-CG-OD2	-7.97	111.13	118.30
2	B	469	GLU	OE1-CD-OE2	-7.96	113.75	123.30
2	B	418	GLU	CG-CD-OE1	-7.93	102.44	118.30
2	B	16	LEU	CB-CG-CD1	7.92	124.46	111.00
1	D	64	ASP	CB-CG-OD1	7.90	125.41	118.30
1	D	259	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	E	123	ASP	CB-CG-OD1	7.65	125.19	118.30
1	D	114	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	30	GLU	OE1-CD-OE2	7.56	132.37	123.30
2	E	433	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	461	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	D	458	ASP	CB-CG-OD1	7.51	125.06	118.30
1	D	223	TYR	CG-CD1-CE1	7.48	127.29	121.30
3	C	70	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	390	PHE	CB-CG-CD2	-7.40	115.62	120.80
2	B	291	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	B	449	GLU	OE1-CD-OE2	7.34	132.11	123.30
2	B	211	GLU	OE1-CD-OE2	7.33	132.10	123.30
1	D	156	LYS	CD-CE-NZ	7.32	128.53	111.70
1	D	73	LEU	CB-CG-CD1	7.31	123.43	111.00
1	A	362	PHE	CB-CG-CD1	7.29	125.91	120.80
1	A	292	ARG	NE-CZ-NH1	7.28	123.94	120.30
3	F	41	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	E	244	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	162	ASP	CB-CG-OD2	7.12	124.71	118.30
1	D	310	GLU	CG-CD-OE1	-7.10	104.10	118.30
2	B	208	MET	CG-SD-CE	-7.10	88.84	100.20
1	A	95	LYS	CD-CE-NZ	7.07	127.96	111.70
3	F	57	LEU	CB-CG-CD2	-7.04	99.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	TYR	CB-CG-CD1	6.96	125.17	121.00
1	A	15	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	B	179	LYS	CD-CE-NZ	-6.95	95.73	111.70
2	E	208	MET	CG-SD-CE	-6.92	89.13	100.20
1	A	325	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	E	211	GLU	OE1-CD-OE2	6.89	131.57	123.30
1	A	271	ARG	NE-CZ-NH2	-6.89	116.86	120.30
2	B	444	TYR	CG-CD2-CE2	-6.89	115.79	121.30
3	C	57	LEU	CB-CG-CD1	6.87	122.69	111.00
2	E	414	TYR	CZ-CE2-CD2	-6.87	113.62	119.80
3	F	57	LEU	CA-CB-CG	-6.84	99.56	115.30
3	F	106	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	172	SER	N-CA-CB	6.75	120.62	110.50
3	C	1	MET	CG-SD-CE	6.70	110.92	100.20
3	F	8	ASP	CB-CG-OD2	-6.67	112.30	118.30
2	B	241	ASP	CB-CG-OD1	6.66	124.30	118.30
2	E	381	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	278	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	158	ARG	NE-CZ-NH1	6.56	123.58	120.30
3	C	57	LEU	CB-CG-CD2	-6.54	99.88	111.00
2	E	167	LYS	CD-CE-NZ	-6.52	96.71	111.70
2	B	244	ASP	CB-CG-OD2	-6.52	112.44	118.30
3	F	70	ARG	NE-CZ-NH1	6.50	123.55	120.30
3	F	79	VAL	CG1-CB-CG2	6.47	121.26	110.90
1	A	7	GLU	OE1-CD-OE2	6.45	131.04	123.30
2	E	309	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	D	78	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	276	ARG	NE-CZ-NH1	6.33	123.47	120.30
3	F	89	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	D	128	ASP	CB-CG-OD2	-6.26	112.66	118.30
3	F	69	VAL	CG1-CB-CG2	6.23	120.87	110.90
1	A	407	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	B	264	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	D	34	ILE	CG1-CB-CG2	6.20	125.05	111.40
2	B	444	TYR	CZ-CE2-CD2	6.11	125.30	119.80
2	B	175	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	390	PHE	CB-CG-CD1	6.04	125.02	120.80
3	F	102	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	E	324	PHE	CB-CG-CD1	6.02	125.01	120.80
1	D	162	ASP	CB-CG-OD2	5.98	123.68	118.30
2	B	344	PHE	CB-CG-CD2	-5.98	116.62	120.80
2	B	236	ARG	NE-CZ-NH1	-5.94	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	459	PHE	CB-CG-CD1	5.94	124.96	120.80
3	F	83	GLU	OE1-CD-OE2	5.91	130.40	123.30
2	E	324	PHE	CB-CG-CD2	-5.91	116.66	120.80
2	B	360	ASP	CB-CG-OD1	5.89	123.61	118.30
1	D	377	GLU	OE1-CD-OE2	5.87	130.34	123.30
2	E	133	ARG	CD-NE-CZ	-5.87	115.39	123.60
2	B	468	LYS	CD-CE-NZ	5.84	125.14	111.70
1	D	271	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	207	PHE	CB-CG-CD2	5.83	124.88	120.80
1	D	441	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	195	MET	CG-SD-CE	-5.81	90.91	100.20
2	B	145	TYR	CB-CG-CD2	-5.81	117.52	121.00
2	E	61	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	242	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	461	ASP	CB-CG-OD2	5.77	123.49	118.30
1	D	131	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	226	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	241	TYR	CB-CG-CD1	5.72	124.43	121.00
2	E	414	TYR	CE1-CZ-CE2	5.71	128.93	119.80
1	D	7	GLU	OE1-CD-OE2	5.68	130.12	123.30
2	E	133	ARG	NH1-CZ-NH2	5.67	125.64	119.40
3	F	69	VAL	CA-CB-CG1	5.66	119.39	110.90
2	B	19	ARG	CD-NE-CZ	5.66	131.52	123.60
3	C	41	ARG	NE-CZ-NH1	-5.63	117.48	120.30
2	E	249	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	A	172	SER	CB-CA-C	5.61	120.75	110.10
1	D	390	PHE	CB-CG-CD2	-5.59	116.89	120.80
3	F	78	GLN	CA-C-O	5.57	131.81	120.10
2	B	94	GLU	OE1-CD-OE2	5.55	129.97	123.30
3	F	16	ARG	NE-CZ-NH1	-5.55	117.53	120.30
2	B	437	TYR	CG-CD2-CE2	5.54	125.73	121.30
2	B	459	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	E	307	ARG	CG-CD-NE	-5.50	100.25	111.80
3	C	56	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	E	217	ASP	CB-CG-OD1	5.47	123.23	118.30
1	D	226	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	391	PHE	CB-CG-CD2	5.46	124.62	120.80
1	D	452	ARG	NE-CZ-NH1	-5.46	117.57	120.30
3	F	7	ASP	CB-CG-OD2	-5.43	113.41	118.30
2	B	307	ARG	CB-CG-CD	-5.42	97.50	111.60
2	B	211	GLU	CG-CD-OE1	-5.41	107.48	118.30
2	B	160	THR	OG1-CB-CG2	-5.38	97.62	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	102	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	374	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	D	128	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	124	ASP	CB-CG-OD1	5.36	123.12	118.30
3	C	102	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	292	ARG	CD-NE-CZ	5.31	131.04	123.60
2	E	370	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	B	45	ASP	CB-CG-OD1	5.28	123.05	118.30
3	F	94[A]	ARG	NE-CZ-NH1	-5.28	117.66	120.30
3	F	94[B]	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	E	29	TYR	CB-CG-CD1	5.25	124.15	121.00
3	F	82	GLU	CA-CB-CG	5.25	124.95	113.40
2	B	21	ARG	NE-CZ-NH1	-5.24	117.68	120.30
2	B	73	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	196	GLU	CA-CB-CG	-5.23	101.89	113.40
2	B	82	GLU	CG-CD-OE2	5.23	128.75	118.30
1	A	339	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	C	26	TRP	CD1-NE1-CE2	5.20	113.68	109.00
1	D	160	ASP	CB-CG-OD2	-5.19	113.63	118.30
3	C	89	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	292	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	F	77	SER	C-N-CA	5.18	134.65	121.70
1	A	15	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	E	413	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	E	204	TYR	CD1-CE1-CZ	-5.09	115.22	119.80
2	B	249	LEU	CB-CG-CD2	-5.08	102.36	111.00
2	B	414	TYR	CG-CD2-CE2	5.08	125.36	121.30
1	A	162	ASP	CB-CG-OD1	-5.07	113.74	118.30
2	B	439	LYS	CD-CE-NZ	-5.06	100.07	111.70
2	B	82	GLU	CG-CD-OE1	-5.05	108.20	118.30
2	E	438	ARG	NE-CZ-NH1	5.05	122.82	120.30
3	F	63	LEU	CB-CG-CD2	-5.04	102.44	111.00
3	F	59	TYR	CZ-CE2-CD2	-5.03	115.27	119.80
3	F	83	GLU	N-CA-C	-5.01	97.46	111.00
2	E	70	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	ASP	Sidechain
2	B	445	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	D	441	ARG	Sidechain
2	E	445	GLN	Sidechain
2	E	449	GLU	Sidechain
3	F	82	GLU	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	3764	0	3673	28	0
1	D	3764	0	3673	20	0
2	B	3644	0	3616	7	0
2	E	3659	0	3625	15	0
3	C	953	0	916	13	0
3	F	947	0	909	7	0
4	A	14	0	6	1	0
4	D	14	0	6	1	0
5	A	17	0	0	1	0
5	D	17	0	0	1	0
6	A	4	0	0	0	0
6	D	4	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	1	0
9	A	16	0	0	0	0
9	D	16	0	0	0	0
10	B	2	0	0	0	0
10	C	1	0	0	0	0
10	F	1	0	0	0	0
11	A	580	0	0	5	0
11	B	562	0	0	6	0
11	C	178	0	0	1	1
11	D	570	0	0	4	1
11	E	607	0	0	6	1
11	F	155	0	0	2	1
All	All	19493	0	16424	89	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:ALA:N	2:E:12:ALA:CA	1.67	1.56
1:A:73:LEU:CG	1:A:73:LEU:CD1	1.76	1.55
1:A:195:MET:CG	1:A:195:MET:SD	2.02	1.48
2:E:13:GLU:CA	2:E:13:GLU:C	1.83	1.47
1:D:190:GLU:HG2	11:D:737:HOH:O	1.69	0.91
2:B:264:GLU:HG3	11:B:994:HOH:O	1.73	0.89
1:A:73:LEU:CD1	11:B:701:HOH:O	2.22	0.88
1:A:73:LEU:CD2	1:A:73:LEU:CD1	2.53	0.87
2:E:383:GLU:OE1	2:E:396:ARG:NH1	2.09	0.85
1:A:73:LEU:HD11	11:B:701:HOH:O	1.77	0.84
1:D:120:HIS:HD2	1:D:158:ARG:HH11	1.28	0.82
2:E:327:LYS:HE3	11:E:681:HOH:O	1.80	0.81
1:A:120:HIS:HD2	1:A:158:ARG:HH11	1.25	0.80
1:D:226:ARG:HD3	1:D:307[A]:LEU:HD13	1.63	0.79
8:B:503:ZN:ZN	11:B:607:HOH:O	1.32	0.77
1:A:226:ARG:HD3	1:A:307[A]:LEU:HD13	1.64	0.77
2:B:327:LYS:NZ	11:B:601:HOH:O	1.95	0.73
1:A:195:MET:CE	1:A:195:MET:CG	2.66	0.73
1:A:277:LEU:HD13	3:C:57:LEU:HD11	1.71	0.72
1:A:310:GLU:HG3	11:A:872:HOH:O	1.90	0.71
1:A:195:MET:CB	1:A:195:MET:SD	2.78	0.71
1:A:73:LEU:CD1	1:A:73:LEU:HG	2.12	0.69
1:D:226:ARG:NH2	1:D:310:GLU:OE2	2.23	0.69
2:B:418:GLU:HG3	11:B:939:HOH:O	1.94	0.67
3:F:81:LYS:HD2	3:F:81:LYS:O	1.95	0.67
1:A:11:ASP:OD2	11:A:601:HOH:O	2.13	0.66
2:E:13:GLU:N	2:E:13:GLU:C	2.45	0.66
1:D:120:HIS:HE1	11:D:685:HOH:O	1.81	0.63
1:A:120:HIS:HE1	11:A:662:HOH:O	1.83	0.62
1:D:120:HIS:CD2	1:D:158:ARG:HH11	2.14	0.60
2:E:13:GLU:C	2:E:13:GLU:CB	2.70	0.59
3:C:80:ASN:C	3:C:80:ASN:HD22	2.07	0.58
2:E:177:HIS:HE1	11:E:1012:HOH:O	1.86	0.58
1:D:307[B]:LEU:HD23	1:D:307[B]:LEU:C	2.25	0.56
1:D:176:GLN:OE1	5:D:501:D6N:N2B	2.39	0.56
3:F:111:HIS:HD2	11:F:425:HOH:O	1.89	0.56
3:F:81:LYS:C	3:F:81:LYS:HD2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:C	1:A:73:LEU:HD22	2.27	0.55
2:E:232:GLU:OE2	11:E:602:HOH:O	2.18	0.54
2:E:264[B]:GLU:OE1	11:E:601:HOH:O	2.18	0.54
3:F:78:GLN:O	3:F:78:GLN:HG3	2.09	0.52
3:F:94[A]:ARG:HG3	3:F:94[A]:ARG:HH21	1.73	0.51
1:D:277:LEU:HD13	3:F:57:LEU:HD11	1.93	0.51
1:A:444:TYR:CE1	1:A:448[B]:HIS:HD2	2.29	0.51
2:E:383:GLU:HG3	11:E:606:HOH:O	2.10	0.51
2:E:383:GLU:CD	2:E:396:ARG:HH12	2.09	0.50
3:C:80:ASN:HD21	3:C:83:GLU:HG3	1.77	0.49
1:A:307[B]:LEU:HD23	1:A:307[B]:LEU:C	2.33	0.48
1:D:452:ARG:HD3	11:D:670:HOH:O	2.12	0.48
1:D:117:LYS:NZ	11:D:611:HOH:O	2.46	0.48
1:A:395[B]:ASP:OD1	11:A:602:HOH:O	2.20	0.48
3:C:80:ASN:ND2	3:C:83:GLU:H	2.13	0.47
1:A:226:ARG:NH2	1:A:310:GLU:OE2	2.47	0.47
1:A:444:TYR:CE1	1:A:448[B]:HIS:CD2	3.03	0.47
1:D:73:LEU:HD22	1:D:73:LEU:C	2.34	0.47
2:B:115:CYS:HB3	2:B:153:SER:OG	2.16	0.46
3:C:1:MET:CG	3:C:4:SER:H	2.30	0.44
1:A:423:HIS:HB3	4:A:501:HCA:O5	2.18	0.44
1:A:66:ILE:HG13	1:A:129:ILE:HG21	1.99	0.44
3:C:1:MET:HB3	3:C:4:SER:CB	2.48	0.43
1:D:212:ASN:HD21	1:D:218:GLN:NE2	2.16	0.43
1:A:176:GLN:OE1	5:A:502:D6N:N2B	2.51	0.43
2:E:364:LYS:NZ	11:E:604:HOH:O	2.28	0.43
3:C:1:MET:HB3	3:C:4:SER:HB3	2.01	0.43
3:F:94[A]:ARG:HG3	11:F:346:HOH:O	2.17	0.43
1:A:212:ASN:HD21	1:A:218:GLN:NE2	2.17	0.42
1:A:61:VAL:HG22	1:A:85:TYR:CE2	2.54	0.42
1:A:120:HIS:CD2	1:A:158:ARG:HD2	2.54	0.42
1:D:368:PHE:HA	1:D:371:VAL:HG12	2.02	0.42
2:E:115:CYS:HB3	2:E:153:SER:OG	2.18	0.42
3:C:1:MET:HG3	3:C:4:SER:H	1.85	0.41
1:D:423:HIS:HB3	4:D:502:HCA:O6	2.20	0.41
3:C:80:ASN:HD22	3:C:83:GLU:H	1.67	0.41
3:C:94:ARG:HD3	11:C:393:HOH:O	2.20	0.41
1:D:188:ILE:HD13	1:D:267:GLU:HB3	2.02	0.41
2:E:203:ARG:HH11	2:E:203:ARG:HD3	1.60	0.41
1:D:61:VAL:HG22	1:D:85:TYR:CE2	2.56	0.41
1:A:9:ASP:OD2	1:A:389:GLU:OE2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ASN:ND2	3:C:83:GLU:HG3	2.34	0.41
2:B:307:ARG:CG	2:B:307:ARG:NH1	2.83	0.41
1:D:212:ASN:HD21	1:D:218:GLN:HE21	1.68	0.41
1:A:448[A]:HIS:HD2	11:A:822:HOH:O	2.04	0.40
1:D:120:HIS:CD2	1:D:158:ARG:HD2	2.55	0.40
2:B:215:TYR:HA	2:B:216:MET:HA	1.89	0.40
3:C:57:LEU:HD12	3:C:57:LEU:HA	1.93	0.40
1:D:219:LEU:HD23	1:D:219:LEU:C	2.42	0.40
2:B:203:ARG:HH11	2:B:203:ARG:HD3	1.61	0.40
3:C:1:MET:HG3	3:C:3:GLN:N	2.37	0.40
2:E:215:TYR:HA	2:E:216:MET:HA	1.89	0.40

All (2) 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)
11:C:440:HOH:O	11:D:1015:HOH:O[1_644]	1.92	0.28
11:E:1091:HOH:O	11:F:434:HOH:O[1_545]	2.01	0.19

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/474 (98%)	457 (98%)	10 (2%)	0	100	100
1	D	467/474 (98%)	457 (98%)	10 (2%)	0	100	100
2	B	464/475 (98%)	454 (98%)	10 (2%)	0	100	100
2	E	466/475 (98%)	457 (98%)	9 (2%)	0	100	100
3	C	112/113 (99%)	107 (96%)	5 (4%)	0	100	100
3	F	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
All	All	2087/2124 (98%)	2040 (98%)	47 (2%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/404 (100%)	397 (99%)	5 (1%)	71	37
1	D	402/404 (100%)	394 (98%)	8 (2%)	55	17
2	B	389/398 (98%)	387 (100%)	2 (0%)	88	67
2	E	391/398 (98%)	387 (99%)	4 (1%)	76	47
3	C	103/102 (101%)	100 (97%)	3 (3%)	42	7
3	F	102/102 (100%)	98 (96%)	4 (4%)	32	4
All	All	1789/1808 (99%)	1763 (98%)	26 (2%)	67	29

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	73	LEU
1	A	85	TYR
1	A	259	ARG
1	A	436	PHE
2	B	16	LEU
2	B	364	LYS
3	C	1	MET
3	C	80	ASN
3	C	94	ARG
1	D	17	LYS
1	D	29	ARG
1	D	73	LEU
1	D	85	TYR
1	D	156	LYS
1	D	178	LYS
1	D	259	ARG
1	D	462	LYS
2	E	16	LEU

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Mol	Chain	Res	Type
2	E	208	MET
2	E	307	ARG
2	E	364	LYS
3	F	71	GLU
3	F	81	LYS
3	F	94[A]	ARG
3	F	94[B]	ARG

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

Mol	Chain	Res	Type
1	A	120	HIS
1	A	218	GLN
2	B	54	GLN
3	C	46	GLN
3	C	80	ASN
1	D	120	HIS
1	D	218	GLN
2	E	54	GLN
2	E	402	GLN
3	F	46	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 18 ligands modelled in this entry, 2 are modelled with single atom and 6 are monoatomic - leaving 10 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	$\# Z  > 2$
6	CO3	D	503	5	0,3,3	0.00	-	0,3,3	0.00	-
5	D6N	D	501	1,4,6	6,28,28	1.46	1 (16%)	-		
4	HCA	A	501	5	4,13,13	1.54	1 (25%)	4,18,18	1.16	0
9	CLF	D	505[B]	2	0,24,24	0.00	-	-		
6	CO3	A	503	5	0,3,3	0.00	-	0,3,3	0.00	-
9	CLF	A	506[A]	2	0,24,24	0.00	-	-		
4	HCA	D	502	5	4,13,13	1.85	1 (25%)	4,18,18	0.89	0
9	CLF	D	505[A]	2	0,24,24	0.00	-	-		
9	CLF	A	506[B]	2	0,24,24	0.00	-	-		
5	D6N	A	502	1,4,6	6,28,28	1.56	1 (16%)	-		

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	501	5	-	0/7/17/17	-
9	CLF	D	505[B]	2	-	-	0/12/10/10
9	CLF	A	506[A]	2	-	-	0/12/10/10
4	HCA	D	502	5	-	0/7/17/17	-
9	CLF	D	505[A]	2	-	-	0/12/10/10
9	CLF	A	506[B]	2	-	-	0/12/10/10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	502	HCA	C2-C3	-3.38	1.50	1.54
5	A	502	D6N	S4B-FE7	-2.61	2.22	2.31
5	D	501	D6N	S4B-FE7	-2.45	2.23	2.31
4	A	501	HCA	O7-C3	2.25	1.46	1.43

There are no bond angle outliers.

There are no chirality outliers.

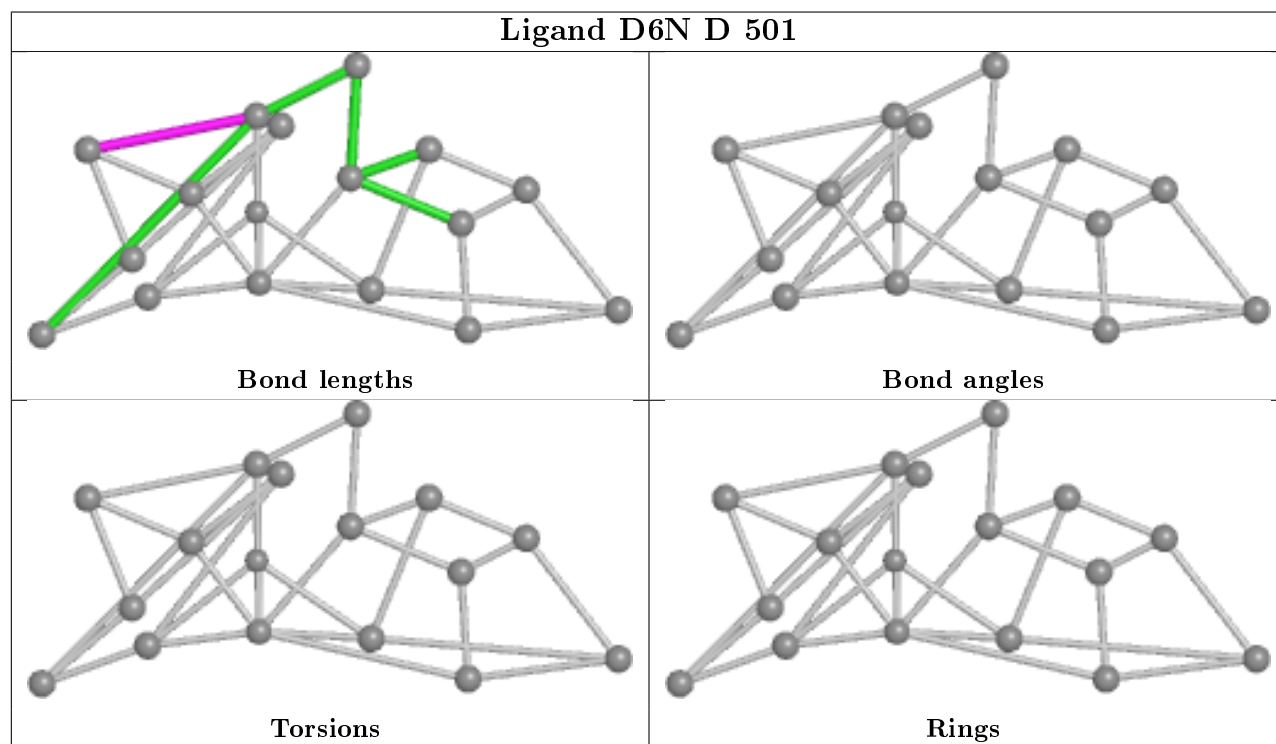
There are no torsion outliers.

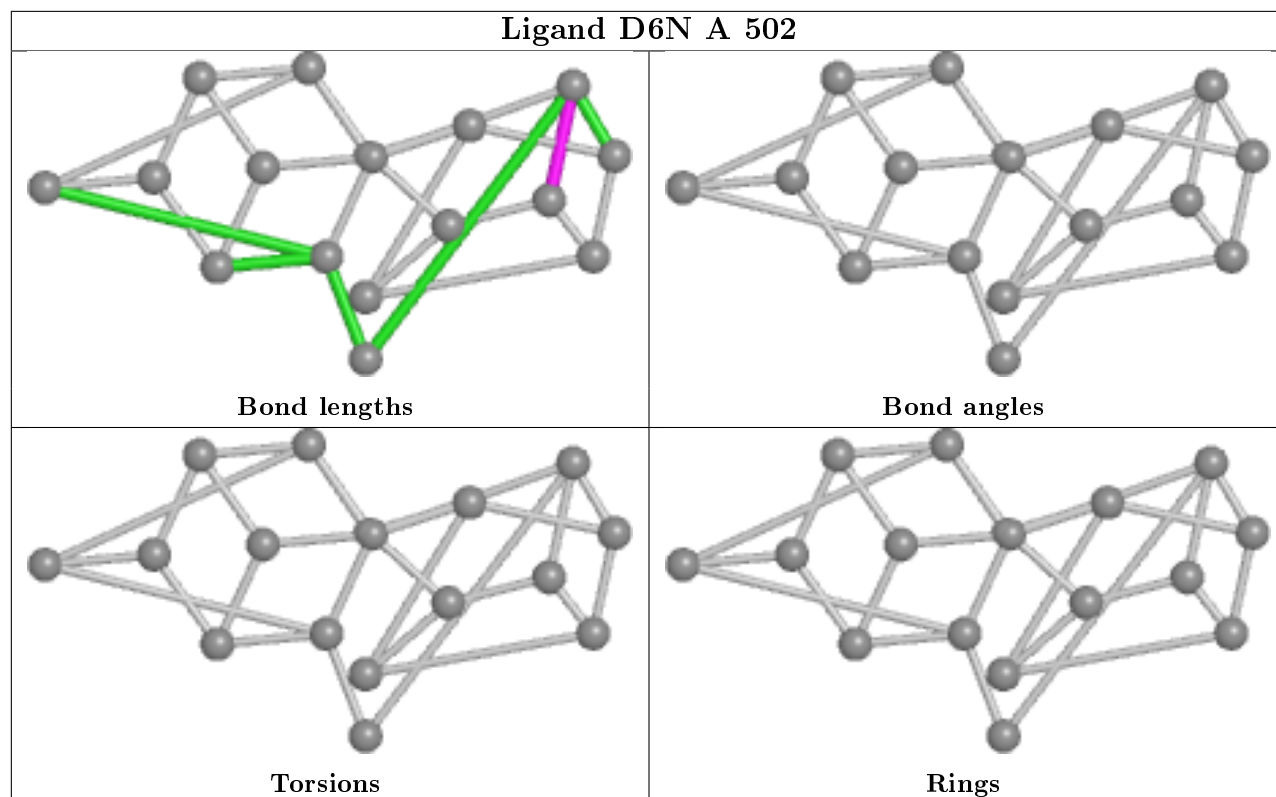
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	D6N	1	0
4	A	501	HCA	1	0
4	D	502	HCA	1	0
5	A	502	D6N	1	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	461/474 (97%)	-0.69	2 (0%) 92 92	9, 13, 24, 60	0
1	D	461/474 (97%)	-0.68	1 (0%) 95 94	7, 12, 24, 67	0
2	B	464/475 (97%)	-0.58	3 (0%) 89 90	8, 13, 27, 56	0
2	E	464/475 (97%)	-0.54	1 (0%) 95 94	7, 11, 24, 48	0
3	C	113/113 (100%)	-0.33	2 (1%) 68 68	12, 17, 36, 74	0
3	F	111/113 (98%)	-0.34	4 (3%) 42 41	11, 17, 52, 82	0
All	All	2074/2124 (97%)	-0.59	13 (0%) 89 90	7, 12, 28, 82	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	MET	4.4
2	B	12	ALA	4.2
3	F	79	VAL	3.9
3	F	84	ILE	3.9
2	B	376	ASN	3.8
2	E	12	ALA	3.3
1	D	462	LYS	3.2
3	C	2	SER	3.2
3	F	80	ASN	2.5
1	A	462	LYS	2.2
3	F	81	LYS	2.1
2	B	16	LEU	2.1
1	A	461	ASP	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

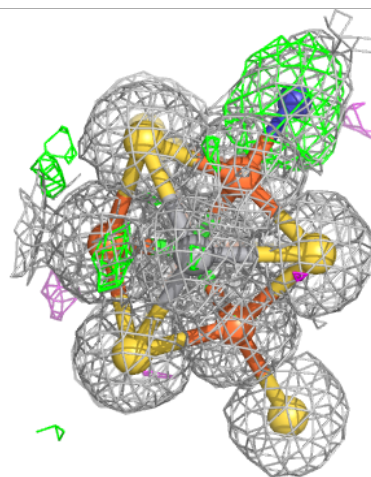
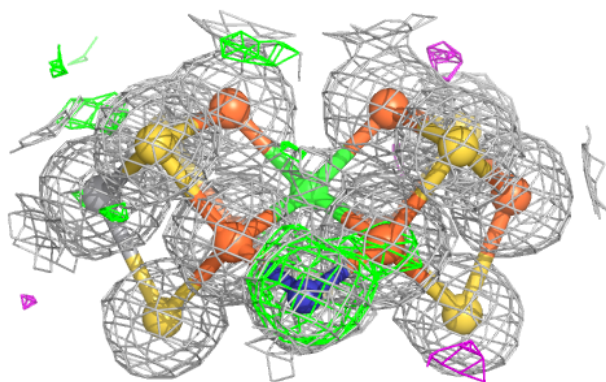
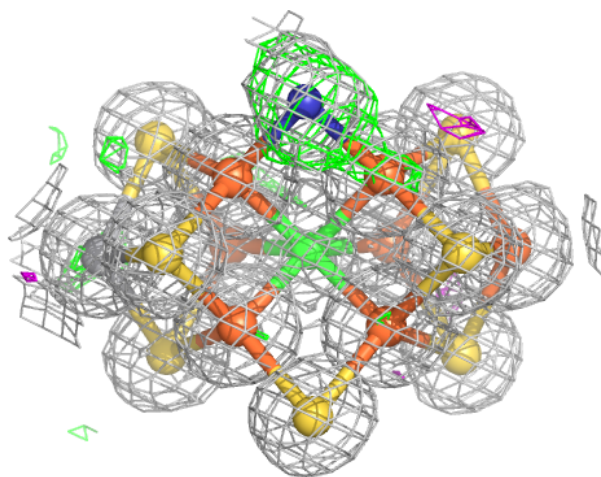
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	HCA	A	501	14/14	0.99	0.04	7,9,13,14	0
4	HCA	D	502	14/14	0.99	0.07	6,7,12,13	0
8	ZN	B	503	1/1	1.00	0.06	22,22,22,22	1
7	H2S	A	504	1/1	1.00	0.04	17,17,17,17	0
10	MG	B	501	1/1	1.00	0.03	10,10,10,10	0
10	MG	C	201	1/1	1.00	0.08	17,17,17,17	0
8	ZN	A	505	1/1	1.00	0.04	16,16,16,16	1
7	H2S	D	504	1/1	1.00	0.03	16,16,16,16	0
6	CO3	D	503	4/4	1.00	0.06	7,7,8,8	0
10	MG	B	502	1/1	1.00	0.03	9,9,9,9	0
9	CLF	D	505[B]	15/15	1.00	0.04	7,7,8,13	1
10	MG	F	201	1/1	1.00	0.07	15,15,15,15	0
6	CO3	A	503	4/4	1.00	0.05	9,9,9,9	0
9	CLF	A	506[A]	15/15	1.00	0.04	7,9,10,10	1
5	D6N	D	501	17/17	1.00	0.05	5,7,8,8	0
9	CLF	D	505[A]	15/15	1.00	0.04	5,7,8,8	1
9	CLF	A	506[B]	15/15	1.00	0.04	9,9,10,18	1
5	D6N	A	502	17/17	1.00	0.04	6,9,9,9	0

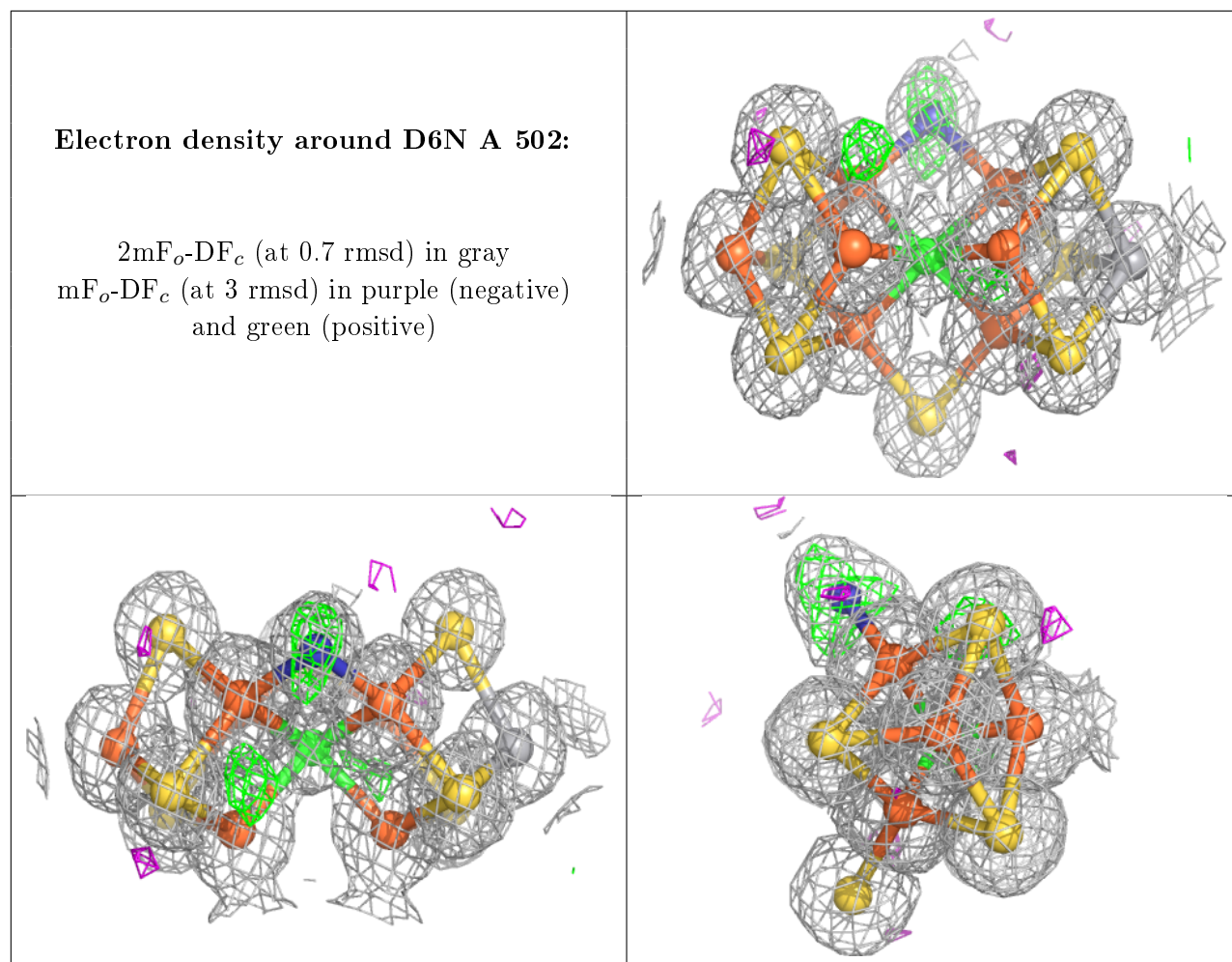
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around D6N D 501:**

$2mF_o-DF_c$  (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.