



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2026 – 11:02 am BST

PDB ID : 6FEA / pdb_00006fea
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

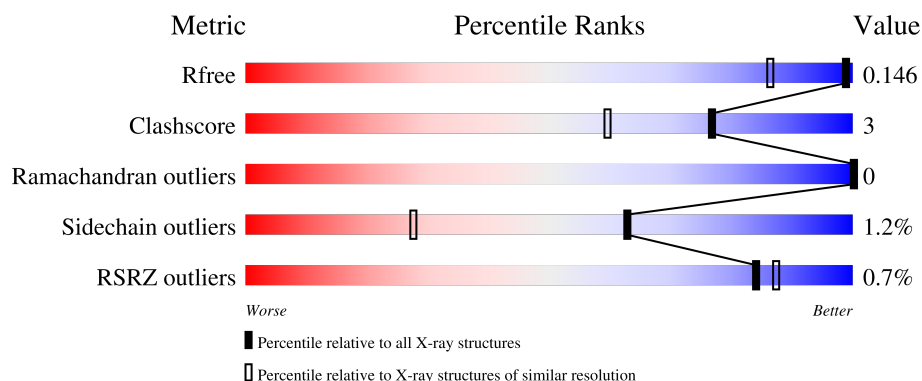
1 Overall quality at a glance

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}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 84% 11% ..
1	D	474	 85% 11% ..
2	B	475	 87% 9% ..
2	E	475	 87% 9% ..
3	C	113	 86% 11% ..

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Mol	Chain	Length	Quality of chain
3	F	113	5% 75% 18% 5%

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			

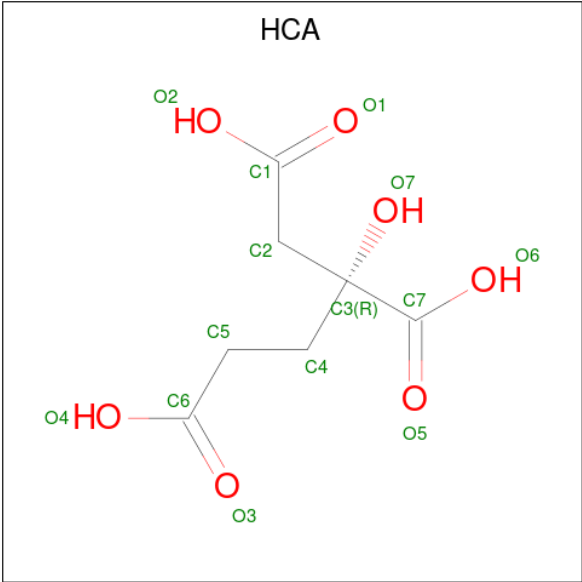
- Molecule 2 is a protein called Vanadium nitrogenase beta subunit, vnfK.

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.

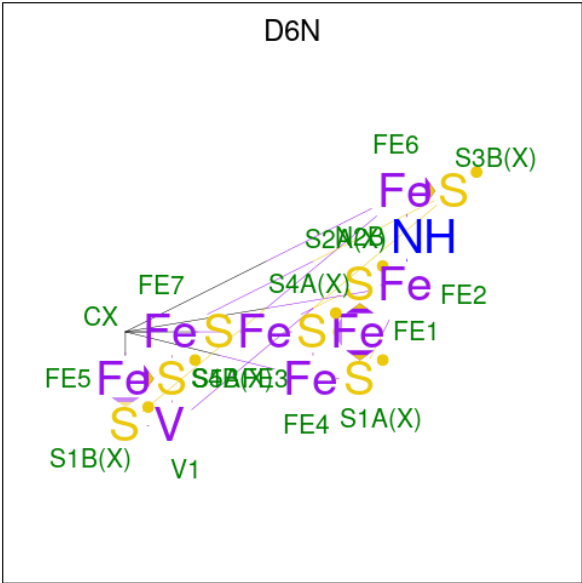
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	113	Total	C	N	O	S	0	1	0
			953	598	171	181	3			
3	F	111	Total	C	N	O	S	0	2	0
			947	594	172	179	2			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



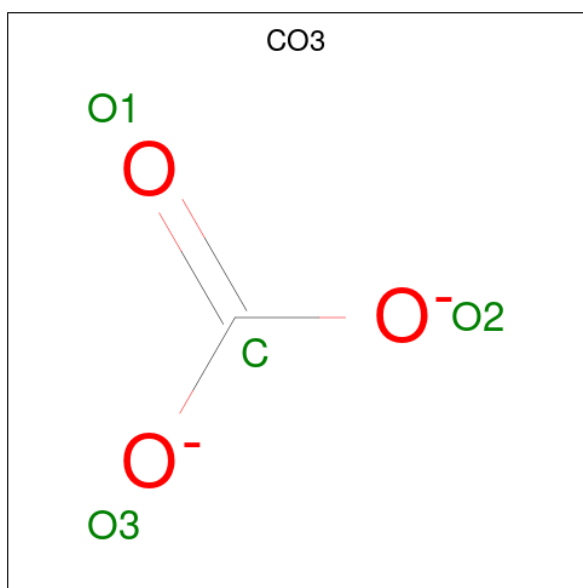
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FeV (CCD ID: D6N) (formula: $\text{CHFe}_7\text{NS}_7\text{V}$).



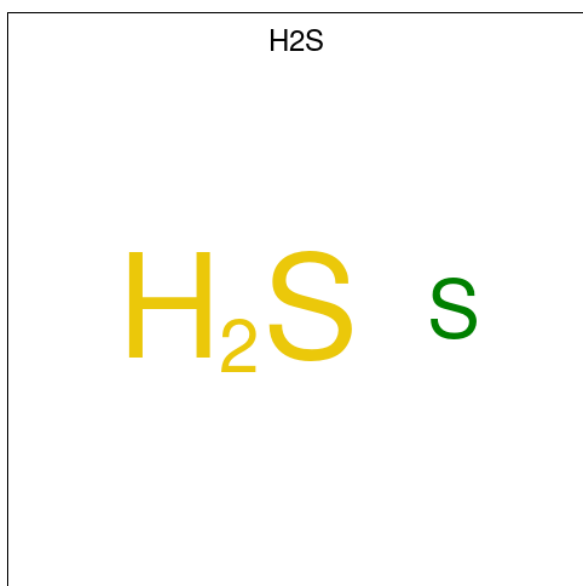
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	S	V	0	0
			17	1	7	1	7	1		
5	D	1	Total	C	Fe	N	S	V	0	0
			17	1	7	1	7	1		

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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 (CCD ID: H2S) (formula: H_2S).



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

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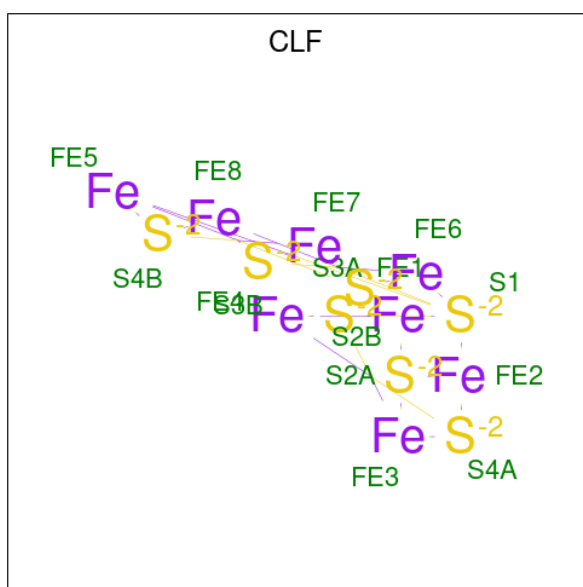
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total S 1 1	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 9 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



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 (CCD ID: 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

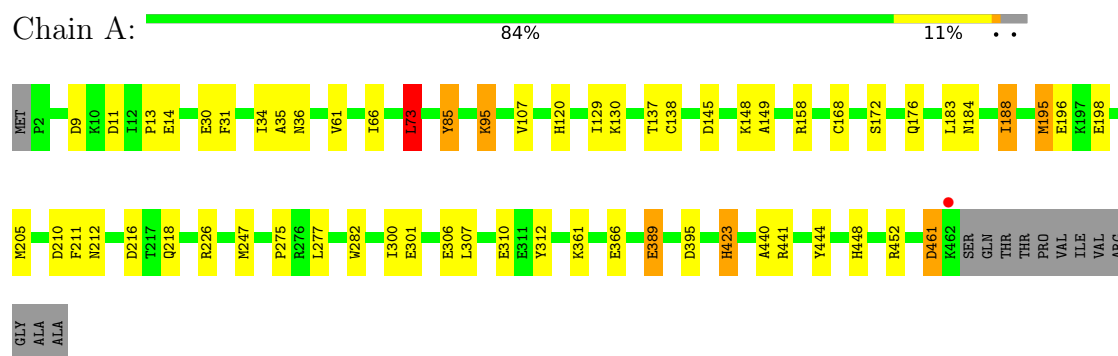
- Molecule 11 is water.

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

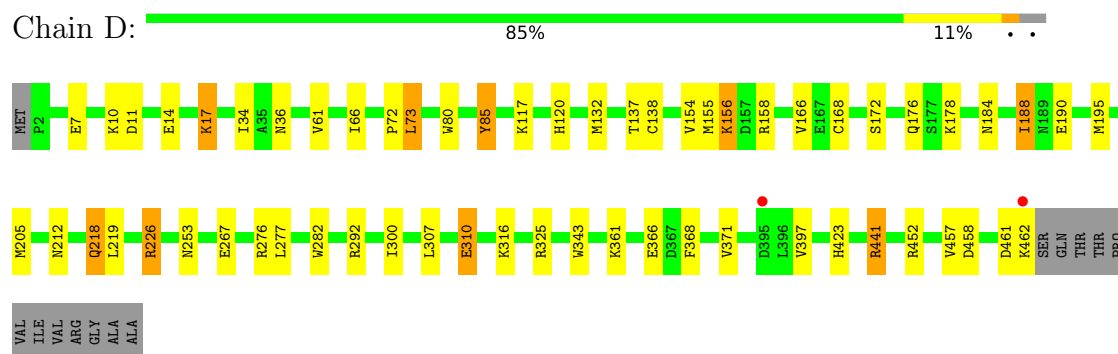
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

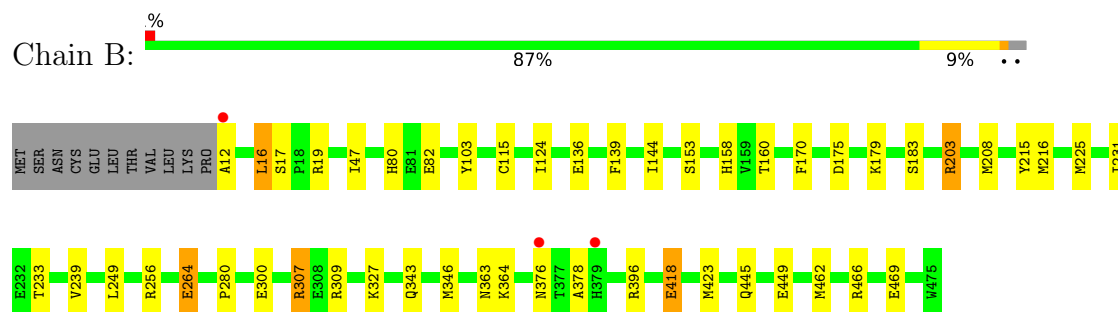
• Molecule 1: Nitrogenase protein alpha chain



• Molecule 1: Nitrogenase protein alpha chain

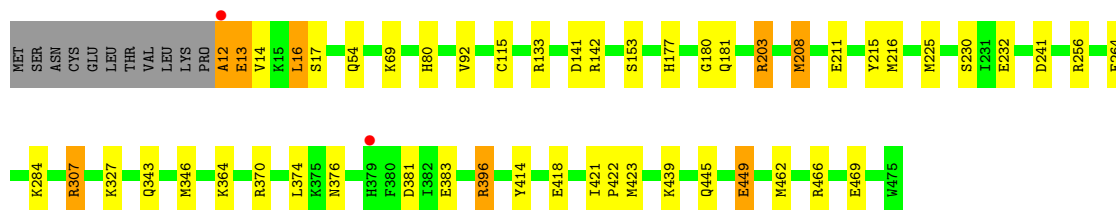


• Molecule 2: Vanadium nitrogenase beta subunit, vnfK



• Molecule 2: Vanadium nitrogenase beta subunit, vnfK

Chain E:  87% 9% . .



- Molecule 3: Vanadium nitrogenase, delta subunit, VnfG

Chain C:  86% 11% . .



- Molecule 3: Vanadium nitrogenase, delta subunit, VnfG

Chain F:  75% 18% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.61Å 79.75Å 107.16Å 84.05° 72.44° 75.25°	Depositor
Resolution (Å)	102.12 – 1.20 102.12 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (102.12-1.20) 99.6 (102.12-1.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.117 , 0.145 0.119 , 0.146	Depositor DCC
R_{free} test set	35693 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	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	0.98	EDS
Total number of atoms	19493	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: D6N, ZN, H2S, CO3, MG, HCA, CLF

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	1.68	41/3859 (1.1%)	1.36	12/5213 (0.2%)
1	D	1.58	33/3859 (0.9%)	1.33	12/5213 (0.2%)
2	B	1.75	40/3722 (1.1%)	1.47	17/5039 (0.3%)
2	E	1.75	37/3737 (1.0%)	1.37	18/5059 (0.4%)
3	C	1.84	12/973 (1.2%)	1.38	3/1315 (0.2%)
3	F	2.16	30/967 (3.1%)	1.65	16/1307 (1.2%)
All	All	1.73	193/17117 (1.1%)	1.40	78/23146 (0.3%)

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 (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	GLU	CA-C	25.45	1.83	1.52
1	A	461	ASP	CG-OD2	14.87	1.53	1.25
1	D	172	SER	CB-OG	-14.55	1.13	1.42
3	F	82	GLU	CD-OE2	14.32	1.52	1.25
3	F	78	GLN	CA-C	14.03	1.71	1.52
2	E	133	ARG	CD-NE	12.63	1.64	1.46
3	C	56	ARG	CD-NE	-12.27	1.29	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	12	ALA	N-CA	11.34	1.67	1.46
3	F	83	GLU	C-O	-11.17	1.10	1.24
1	A	195	MET	CA-CB	-11.07	1.35	1.53
2	B	376	ASN	N-CA	11.04	1.60	1.46
2	E	396	ARG	NE-CZ	-10.91	1.21	1.33
2	E	376	ASN	C-O	10.86	1.38	1.24
2	E	181	GLN	CD-OE1	10.64	1.43	1.23
2	E	418	GLU	CD-OE1	10.22	1.44	1.25
2	B	466	ARG	CZ-NH1	9.99	1.46	1.32
2	B	12	ALA	N-CA	9.89	1.65	1.46
2	B	462	MET	SD-CE	-9.35	1.56	1.79
2	E	225	MET	SD-CE	-8.83	1.57	1.79
3	C	3	GLN	N-CA	8.76	1.56	1.46
1	D	195	MET	CB-CG	-8.75	1.26	1.52
1	D	366	GLU	CB-CG	-8.52	1.26	1.52
1	A	195	MET	CG-SD	8.51	2.02	1.80
3	C	2	SER	N-CA	8.44	1.56	1.46
2	B	203	ARG	CD-NE	8.35	1.57	1.46
1	D	34	ILE	C-O	8.33	1.33	1.24
3	C	2	SER	CA-C	7.96	1.63	1.52
2	E	203	ARG	CD-NE	7.88	1.57	1.46
3	F	78	GLN	CD-OE1	7.83	1.38	1.23
2	E	462	MET	SD-CE	-7.80	1.60	1.79
2	E	423	MET	SD-CE	-7.66	1.60	1.79
2	E	396	ARG	CD-NE	7.66	1.56	1.46
1	A	14	GLU	CD-OE2	7.58	1.39	1.25
1	A	195	MET	CB-CG	-7.57	1.29	1.52
3	F	56	ARG	CD-NE	-7.54	1.35	1.46
1	A	34	ILE	C-O	7.44	1.33	1.24
2	B	144	ILE	CA-C	-7.40	1.43	1.52
2	E	466	ARG	CZ-NH1	7.33	1.43	1.32
2	E	346	MET	SD-CE	-7.25	1.61	1.79
1	A	205	MET	SD-CE	-7.21	1.61	1.79
1	D	168	CYS	CA-CB	7.20	1.64	1.53
2	E	142	ARG	CA-CB	7.17	1.67	1.53
1	A	73	LEU	CG-CD1	7.14	1.76	1.52
1	D	458	ASP	N-CA	-7.14	1.37	1.46
2	B	343	GLN	CD-OE1	7.09	1.37	1.23
2	E	133	ARG	CZ-NH1	6.97	1.42	1.32
3	F	75	TRP	CA-C	-6.96	1.43	1.52
3	F	44	THR	N-CA	6.94	1.54	1.46
1	D	310	GLU	CD-OE1	6.90	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	363	ASN	CG-OD1	6.90	1.36	1.23
1	A	461	ASP	CG-OD1	6.89	1.38	1.25
2	E	381	ASP	CA-CB	-6.86	1.42	1.53
2	E	142	ARG	CA-C	-6.78	1.44	1.52
1	A	441	ARG	CD-NE	-6.76	1.36	1.46
2	B	16	LEU	CA-C	-6.72	1.44	1.52
1	D	34	ILE	C-N	-6.67	1.24	1.33
2	B	396	ARG	NE-CZ	-6.66	1.25	1.33
1	D	218	GLN	CD-OE1	6.62	1.36	1.23
2	B	233	THR	CA-C	-6.62	1.46	1.53
3	F	106	ARG	CD-NE	-6.61	1.36	1.46
2	E	17	SER	CA-CB	-6.61	1.45	1.54
1	A	168	CYS	CA-C	-6.59	1.44	1.52
2	B	47	ILE	CA-C	-6.57	1.46	1.52
3	F	83	GLU	CA-C	6.56	1.61	1.52
1	D	166	VAL	CA-CB	6.52	1.62	1.54
3	F	3	GLN	CD-NE2	6.52	1.47	1.33
1	A	188	ILE	CB-CG1	6.48	1.66	1.53
2	B	376	ASN	C-O	6.44	1.32	1.24
3	F	79	VAL	C-O	6.41	1.31	1.23
2	B	225	MET	SD-CE	-6.37	1.63	1.79
3	F	84	ILE	C-O	-6.37	1.16	1.24
1	A	13	PRO	N-CA	-6.36	1.39	1.47
1	A	312	TYR	N-CA	-6.35	1.38	1.46
2	B	449	GLU	CD-OE2	6.33	1.37	1.25
1	D	205	MET	SD-CE	-6.32	1.63	1.79
1	D	292	ARG	CZ-NH2	6.29	1.41	1.33
3	F	4	SER	C-O	6.29	1.32	1.23
1	A	34	ILE	C-N	-6.28	1.25	1.33
2	B	264	GLU	CD-OE1	6.28	1.37	1.25
1	D	361	LYS	CA-CB	6.28	1.63	1.53
2	B	346	MET	SD-CE	-6.26	1.63	1.79
2	B	136	GLU	N-CA	6.25	1.53	1.46
1	D	300	ILE	N-CA	-6.20	1.38	1.46
1	A	306	GLU	CA-C	6.17	1.60	1.52
1	A	282	TRP	C-O	6.10	1.30	1.23
3	C	64	ALA	CA-C	-6.08	1.45	1.52
3	F	80	ASN	CA-C	-6.07	1.44	1.53
1	A	34	ILE	N-CA	-6.05	1.38	1.46
3	C	80	ASN	CG-OD1	6.05	1.35	1.23
3	F	106	ARG	NE-CZ	6.04	1.39	1.33
2	E	256	ARG	CZ-NH2	-6.03	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	65	MET	CA-C	6.03	1.60	1.52
3	F	70	ARG	CZ-NH1	6.01	1.41	1.32
2	B	124	ILE	CA-CB	6.00	1.61	1.54
3	F	82	GLU	CA-C	5.97	1.61	1.52
1	A	36	ASN	CG-OD1	5.96	1.34	1.23
1	A	172	SER	CA-CB	-5.96	1.44	1.53
3	C	51	GLY	C-O	5.93	1.31	1.23
3	F	41	ARG	CZ-NH1	5.93	1.41	1.32
2	B	300	GLU	CD-OE1	5.91	1.36	1.25
2	E	141	ASP	N-CA	5.90	1.53	1.46
3	F	84	ILE	N-CA	5.86	1.53	1.46
2	B	264	GLU	CG-CD	5.84	1.66	1.52
1	A	107	VAL	C-O	5.82	1.30	1.24
2	B	469	GLU	CD-OE2	5.82	1.36	1.25
1	A	361	LYS	CD-CE	-5.79	1.35	1.52
2	B	378	ALA	C-O	-5.78	1.16	1.23
2	B	170	PHE	C-N	-5.76	1.26	1.33
2	B	183	SER	N-CA	-5.76	1.38	1.46
2	E	370	ARG	NE-CZ	5.76	1.39	1.33
2	B	363	ASN	CB-CG	5.74	1.66	1.52
3	F	91	LEU	C-N	-5.72	1.26	1.33
1	A	301	GLU	CA-C	5.72	1.60	1.52
2	B	256	ARG	CZ-NH2	-5.71	1.26	1.33
3	F	75	TRP	CA-CB	5.70	1.62	1.53
2	E	13	GLU	N-CA	-5.69	1.39	1.46
1	D	461	ASP	CG-OD2	5.69	1.36	1.25
3	F	15	GLU	CD-OE2	5.69	1.36	1.25
1	A	31	PHE	N-CA	5.66	1.53	1.46
1	D	188	ILE	CB-CG1	5.63	1.64	1.53
2	B	307	ARG	CG-CD	5.62	1.69	1.52
1	D	17	LYS	CB-CG	-5.62	1.35	1.52
2	E	307	ARG	CA-CB	-5.60	1.44	1.53
3	F	78	GLN	N-CA	5.60	1.53	1.46
1	A	247	MET	SD-CE	-5.58	1.65	1.79
1	A	461	ASP	C-O	-5.58	1.17	1.24
2	B	418	GLU	CD-OE2	5.55	1.35	1.25
2	B	175	ASP	CG-OD2	5.53	1.35	1.25
2	B	17	SER	CA-CB	-5.51	1.46	1.54
1	A	389	GLU	N-CA	5.51	1.53	1.46
2	E	449	GLU	CD-OE2	5.50	1.35	1.25
1	A	210	ASP	N-CA	5.49	1.52	1.46
2	E	307	ARG	CB-CG	-5.49	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	139	PHE	C-O	-5.46	1.18	1.24
2	E	180	GLY	N-CA	5.46	1.53	1.45
2	B	103	TYR	CA-C	5.46	1.58	1.52
2	B	466	ARG	CZ-NH2	5.45	1.40	1.33
3	F	95	LEU	C-O	5.44	1.30	1.24
3	F	84	ILE	CA-C	-5.43	1.45	1.52
3	F	57	LEU	CG-CD2	-5.42	1.34	1.52
2	B	309	ARG	N-CA	-5.40	1.40	1.46
3	C	57	LEU	CG-CD2	-5.40	1.34	1.52
1	D	7	GLU	CD-OE2	5.40	1.35	1.25
1	A	14	GLU	CD-OE1	5.39	1.35	1.25
1	D	11	ASP	CG-OD2	-5.39	1.15	1.25
1	A	107	VAL	CA-C	-5.38	1.46	1.52
1	D	36	ASN	CG-OD1	5.38	1.33	1.23
2	E	469	GLU	CD-OE2	5.37	1.35	1.25
1	D	155	MET	SD-CE	-5.36	1.66	1.79
2	E	422	PRO	CA-CB	-5.36	1.46	1.53
3	F	82	GLU	CA-CB	5.35	1.63	1.53
2	E	14	VAL	CA-C	-5.34	1.47	1.52
1	D	276	ARG	C-O	5.33	1.30	1.24
1	A	423	HIS	CE1-NE2	5.32	1.37	1.32
1	A	35	ALA	CA-C	-5.30	1.46	1.52
2	B	423	MET	SD-CE	-5.29	1.66	1.79
1	D	441	ARG	CD-NE	-5.25	1.38	1.46
1	D	154	VAL	N-CA	-5.24	1.40	1.46
3	C	89	ASP	CG-OD1	5.24	1.35	1.25
1	A	145	ASP	N-CA	5.22	1.52	1.46
2	E	284	LYS	CE-NZ	-5.22	1.33	1.49
3	F	78	GLN	CD-NE2	5.20	1.44	1.33
1	A	130	LYS	CA-C	-5.20	1.46	1.52
3	C	57	LEU	CB-CG	5.20	1.63	1.53
1	D	457	VAL	CA-C	-5.19	1.46	1.52
1	D	72	PRO	CA-C	5.18	1.58	1.52
1	D	226	ARG	CZ-NH1	5.18	1.40	1.32
2	E	466	ARG	CZ-NH2	5.17	1.40	1.33
1	D	80	TRP	CZ2-CH2	-5.16	1.27	1.37
1	A	198	GLU	CD-OE1	5.16	1.35	1.25
2	B	307	ARG	CB-CG	-5.15	1.36	1.52
1	A	30	GLU	CD-OE1	5.12	1.35	1.25
1	A	275	PRO	CA-C	5.11	1.59	1.52
1	D	397	VAL	C-N	-5.11	1.27	1.33
2	E	343	GLN	CD-OE1	5.10	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	43	LEU	N-CA	-5.09	1.39	1.46
3	C	67	ASN	C-O	5.09	1.30	1.24
1	D	441	ARG	NE-CZ	-5.09	1.27	1.33
2	B	82	GLU	N-CA	-5.09	1.40	1.46
2	B	280	PRO	CA-CB	-5.08	1.48	1.53
2	E	230	SER	CB-OG	-5.08	1.32	1.42
1	A	34	ILE	CA-C	5.07	1.58	1.52
1	A	366	GLU	CB-CG	-5.07	1.37	1.52
2	B	231	ILE	N-CA	-5.06	1.40	1.46
1	A	300	ILE	CA-CB	-5.06	1.47	1.54
3	C	41	ARG	NE-CZ	5.06	1.38	1.33
2	E	54	GLN	CD-OE1	5.06	1.33	1.23
2	E	414	TYR	CZ-OH	5.05	1.48	1.38
2	E	374	LEU	CA-C	5.02	1.59	1.52
1	D	195	MET	CG-SD	5.01	1.93	1.80
1	D	461	ASP	CA-CB	5.01	1.60	1.53
1	D	253	ASN	CA-C	-5.01	1.46	1.52
1	A	452	ARG	N-CA	-5.00	1.40	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	466	ARG	NE-CZ-NH2	-11.96	108.43	119.20
3	F	83	GLU	N-CA-C	-11.57	97.46	111.69
1	A	148	LYS	CD-CE-NZ	-9.34	82.01	111.90
2	B	449	GLU	CB-CG-CD	8.85	127.64	112.60
2	B	307	ARG	NE-CZ-NH2	8.11	126.50	119.20
3	F	56	ARG	NE-CZ-NH2	-7.99	112.01	119.20
3	F	78	GLN	CA-C-O	7.90	131.81	120.51
2	B	418	GLU	OE1-CD-OE2	7.84	141.71	122.90
2	B	239	VAL	O-C-N	7.54	129.49	121.94
3	F	77	SER	O-C-N	7.26	130.53	122.11
1	D	172	SER	N-CA-CB	7.26	120.62	110.17
3	F	78	GLN	CG-CD-NE2	-7.16	105.66	116.40
2	B	418	GLU	CG-CD-OE1	-6.94	102.44	118.40
1	D	195	MET	CG-SD-CE	-6.89	85.74	100.90
3	F	77	SER	CA-C-N	6.86	134.65	121.54
3	F	77	SER	C-N-CA	6.86	134.65	121.54
3	F	56	ARG	NE-CZ-NH1	6.83	128.32	121.50
2	B	466	ARG	NE-CZ-NH1	6.78	128.28	121.50
2	E	13	GLU	N-CA-C	-6.65	98.36	109.07
1	A	14	GLU	CB-CG-CD	6.47	123.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	133	ARG	CD-NE-CZ	-6.44	115.39	124.40
1	D	325	ARG	NE-CZ-NH1	6.42	127.92	121.50
2	B	158	HIS	CA-CB-CG	6.40	120.20	113.80
2	E	421	ILE	CA-C-O	-6.31	115.60	119.51
1	D	310	GLU	CG-CD-OE1	-6.22	104.10	118.40
2	E	80	HIS	CA-CB-CG	6.17	119.97	113.80
3	F	83	GLU	CA-C-O	-6.15	113.41	120.24
2	E	396	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	172	SER	CB-CA-C	6.14	120.75	109.46
3	F	78	GLN	CB-CG-CD	6.11	122.98	112.60
1	A	196	GLU	CA-CB-CG	-6.11	101.89	114.10
2	B	307	ARG	NE-CZ-NH1	-6.05	115.45	121.50
3	F	80	ASN	O-C-N	6.05	130.46	122.36
1	A	73	LEU	CB-CG-CD1	6.03	128.78	110.70
2	B	80	HIS	CA-CB-CG	6.02	119.82	113.80
2	E	439	LYS	CG-CD-CE	6.00	125.11	111.30
2	B	307	ARG	CB-CG-CD	-6.00	97.50	111.30
2	E	133	ARG	NE-CZ-NH2	-6.00	113.80	119.20
2	E	466	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	D	184	ASN	CA-CB-CG	5.87	118.47	112.60
2	B	160	THR	OG1-CB-CG2	-5.84	97.62	109.30
3	F	82	GLU	N-CA-C	-5.75	105.97	112.87
2	E	211	GLU	CB-CG-CD	-5.74	102.84	112.60
2	E	69	LYS	CG-CD-CE	5.74	124.49	111.30
2	E	16	LEU	CD1-CG-CD2	5.72	123.38	110.80
3	C	57	LEU	CA-CB-CG	-5.69	96.39	116.30
2	B	249	LEU	CA-C-O	5.66	126.47	119.97
1	D	310	GLU	OE1-CD-OE2	5.49	136.07	122.90
2	B	208	MET	CG-SD-CE	-5.48	88.84	100.90
1	A	216	ASP	CA-CB-CG	5.47	118.08	112.60
3	F	82	GLU	CA-CB-CG	5.42	124.95	114.10
1	A	184	ASN	CA-CB-CG	5.38	117.98	112.60
3	F	84	ILE	CA-C-N	5.36	127.41	120.44
3	F	84	ILE	C-N-CA	5.36	127.41	120.44
2	E	208	MET	CG-SD-CE	-5.35	89.13	100.90
2	E	241	ASP	CA-CB-CG	5.35	117.95	112.60
3	C	70	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	E	307	ARG	CG-CD-NE	-5.34	100.25	112.00
1	D	316	LYS	CA-C-O	5.31	123.49	118.34
3	F	69	VAL	CA-CB-CG1	5.29	119.39	110.40
2	B	203	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	A	34	ILE	CB-CA-C	-5.28	103.24	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	D	441	ARG	CD-NE-CZ	5.25	131.75	124.40
1	A	440	ALA	O-C-N	5.22	127.65	122.12
2	E	181	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	D	156	LYS	CD-CE-NZ	5.20	128.53	111.90
2	E	449	GLU	CB-CG-CD	5.20	121.44	112.60
1	D	14	GLU	CB-CG-CD	5.18	121.41	112.60
3	C	71	GLU	CB-CG-CD	-5.17	103.82	112.60
2	E	92	VAL	CB-CA-C	-5.15	105.38	111.97
2	B	19	ARG	CD-NE-CZ	5.09	131.52	124.40
1	A	149	ALA	N-CA-C	5.09	116.91	111.36
1	A	211	PHE	CA-CB-CG	-5.07	108.73	113.80
2	B	179	LYS	CD-CE-NZ	-5.05	95.73	111.90
2	E	203	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	A	95	LYS	CD-CE-NZ	5.02	127.96	111.90
1	D	10	LYS	CA-CB-CG	5.01	124.13	114.10

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
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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3764	0	3673	31	0
1	D	3764	0	3673	23	0
2	B	3644	0	3616	8	0
2	E	3659	0	3625	14	0
3	C	953	0	916	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	947	0	909	8	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	5	1
11	F	155	0	0	2	1
All	All	19493	0	16424	95	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 (95) 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:CD1	1:A:73:LEU:CG	1.76	1.55
2:E:13:GLU:CA	2:E:13:GLU:C	1.83	1.52
1:A:195:MET:CG	1:A:195:MET:SD	2.02	1.48
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:CD1	1:A:73:LEU:CD2	2.53	0.87
2:B:327:LYS:NZ	11:B:601:HOH:O	1.95	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:13:GLU:C	2:E:13:GLU:N	2.45	0.74
1:A:195:MET:CG	1:A:195:MET:CE	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:SD	1:A:195:MET:CB	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:C	2:E:13:GLU:CB	2.70	0.64
1:D:120:HIS:HE1	11:D:685:HOH:O	1.81	0.63
3:C:80:ASN:C	3:C:80:ASN:HD22	2.07	0.63
1:A:120:HIS:HE1	11:A:662:HOH:O	1.83	0.62
1:D:307[B]:LEU:HD23	1:D:307[B]:LEU:C	2.25	0.61
2:E:383:GLU:CD	2:E:396:ARG:HH12	2.09	0.61
1:D:120:HIS:CD2	1:D:158:ARG:HH11	2.14	0.60
1:A:73:LEU:C	1:A:73:LEU:HD22	2.27	0.60
3:F:81:LYS:HD2	3:F:81:LYS:C	2.25	0.59
2:E:177:HIS:HE1	11:E:1012:HOH:O	1.86	0.58
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
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
1:A:307[B]:LEU:C	1:A:307[B]:LEU:HD23	2.33	0.53
1:D:73:LEU:HD22	1:D:73:LEU:C	2.34	0.52
3:F:78:GLN:O	3:F:78:GLN:HG3	2.09	0.52
3:F:94[A]:ARG:HH21	3:F:94[A]:ARG:HG3	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
3:C:80:ASN:HD21	3:C:83:GLU:HG3	1.77	0.49
1:D:452:ARG:HD3	11:D:670:HOH:O	2.12	0.48
1:A:395[B]:ASP:OD1	11:A:602:HOH:O	2.20	0.48
1:A:95:LYS:NZ	2:B:418:GLU:OE1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:115:CYS:HB3	2:B:153:SER:OG	2.16	0.46
1:D:282:TRP:CG	1:D:343:TRP:HE1	2.34	0.46
1:D:219:LEU:C	1:D:219:LEU:HD23	2.42	0.45
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:137:THR:O	1:A:138:CYS:C	2.60	0.43
1:A:176:GLN:OE1	5:A:502:D6N:N2B	2.51	0.43
3:F:81:LYS:C	3:F:81:LYS:CD	2.90	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:117:LYS:NZ	11:D:611:HOH:O	2.46	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
2:B:307:ARG:CG	2:B:307:ARG:NH1	2.83	0.41
3:C:80:ASN:ND2	3:C:83:GLU:HG3	2.34	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:66:ILE:HG21	1:D:132:MET:HE2	2.04	0.40
1:A:183:LEU:HD23	1:A:183:LEU:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:THR:O	1:D:138:CYS:C	2.63	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 [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	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 [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	402/404 (100%)	399 (99%)	3 (1%)	76	47
1	D	402/404 (100%)	396 (98%)	6 (2%)	57	21
2	B	389/398 (98%)	387 (100%)	2 (0%)	81	59
2	E	391/398 (98%)	387 (99%)	4 (1%)	68	36
3	C	103/102 (101%)	101 (98%)	2 (2%)	50	13
3	F	102/102 (100%)	97 (95%)	5 (5%)	22	2
All	All	1789/1808 (99%)	1767 (99%)	22 (1%)	63	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	85	TYR
1	A	188	ILE
2	B	16	LEU
2	B	364	LYS
3	C	1	MET
3	C	80	ASN
1	D	17	LYS
1	D	73	LEU
1	D	85	TYR
1	D	156	LYS
1	D	178	LYS
1	D	462	LYS
2	E	16	LEU
2	E	208	MET
2	E	307	ARG
2	E	364	LYS
3	F	69	VAL
3	F	71	GLU
3	F	81	LYS
3	F	94[A]	ARG
3	F	94[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	218	GLN
2	B	32	GLN
2	B	260	ASN
2	B	274	ASN
2	B	278	ASN
2	B	285	ASN
3	C	54	GLN
3	C	80	ASN
3	C	110	HIS
3	C	111	HIS
1	D	120	HIS
1	D	218	GLN
2	E	32	GLN
2	E	278	ASN
2	E	285	ASN
2	E	376	ASN
3	F	46	GLN
3	F	54	GLN
3	F	109	ASN
3	F	111	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
9	CLF	A	506[B]	2	0,24,24	-	-	-		
9	CLF	A	506[A]	2	0,24,24	-	-	-		
4	HCA	D	502	5	13,13,13	1.34	2 (15%)	14,18,18	1.45	2 (14%)
5	D6N	D	501	1,6,4	6,28,28	1.46	1 (16%)	-		
5	D6N	A	502	1,6,4	6,28,28	1.56	1 (16%)	-		
6	CO3	D	503	5	2,3,3	0.60	0	2,3,3	0.82	0
9	CLF	D	505[A]	2	0,24,24	-	-	-		
9	CLF	D	505[B]	2	0,24,24	-	-	-		
4	HCA	A	501	5	13,13,13	1.93	3 (23%)	14,18,18	1.52	3 (21%)
6	CO3	A	503	5	2,3,3	0.63	0	2,3,3	1.30	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
9	CLF	A	506[B]	2	-	-	0/12/10/10
9	CLF	A	506[A]	2	-	-	0/12/10/10
4	HCA	D	502	5	-	2/17/17/17	-
9	CLF	D	505[B]	2	-	-	0/12/10/10
9	CLF	D	505[A]	2	-	-	0/12/10/10
4	HCA	A	501	5	-	2/17/17/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	HCA	C3-C7	-4.98	1.48	1.53
4	D	502	HCA	C2-C3	-2.98	1.50	1.53
4	A	501	HCA	O1-C1	2.79	1.31	1.22
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	O2-C1	-2.32	1.22	1.30
4	D	502	HCA	O4-C6	-2.23	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	502	HCA	O5-C7-C3	-3.52	117.26	122.25
4	D	502	HCA	O6-C7-C3	3.39	118.94	113.05
4	A	501	HCA	O2-C1-C2	2.79	123.30	114.35
4	A	501	HCA	O6-C7-C3	2.78	117.87	113.05
4	A	501	HCA	O1-C1-C2	-2.77	114.83	122.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

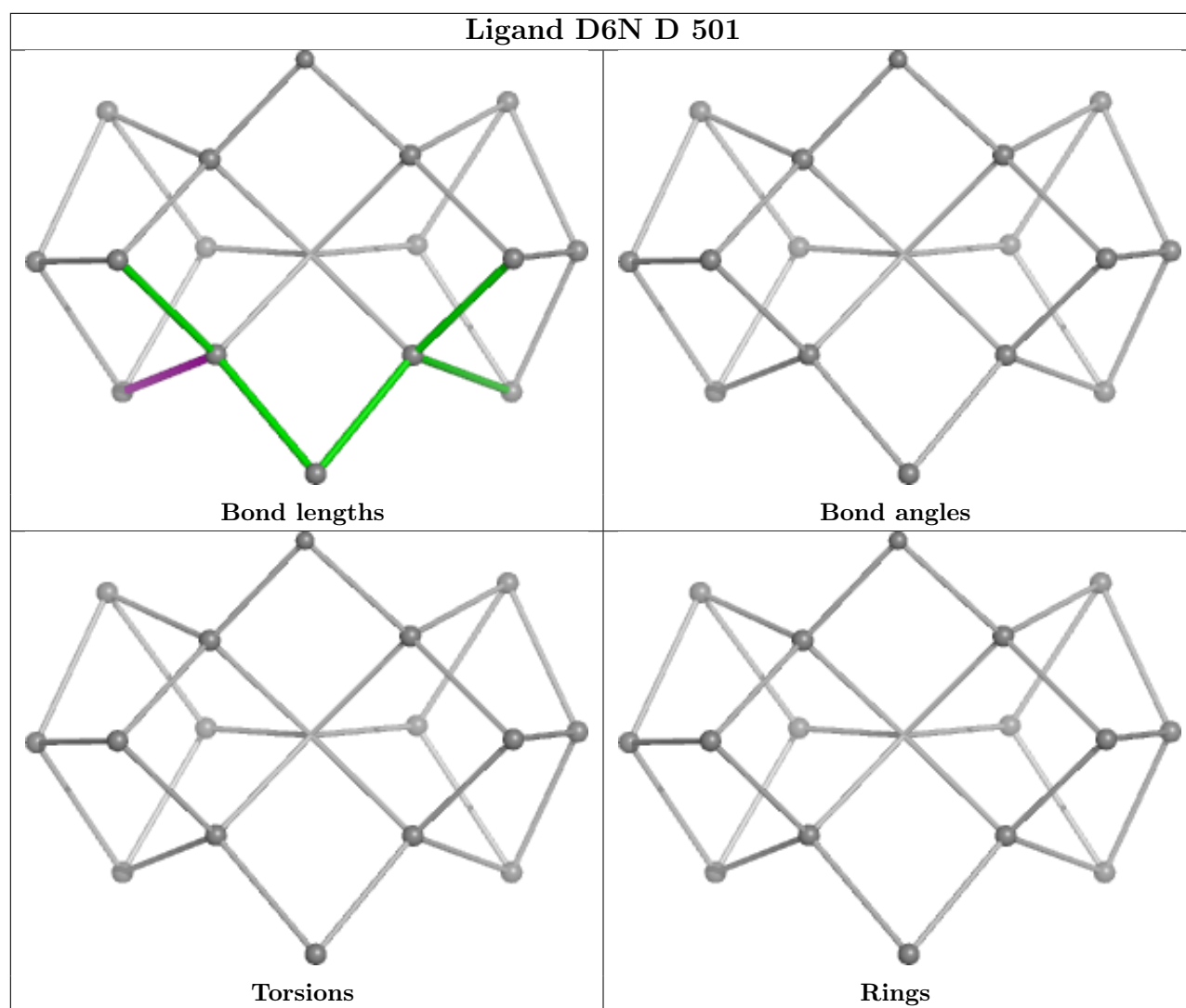
Mol	Chain	Res	Type	Atoms
4	D	502	HCA	C4-C5-C6-O4
4	D	502	HCA	C4-C5-C6-O3
4	A	501	HCA	C4-C5-C6-O3
4	A	501	HCA	C4-C5-C6-O4

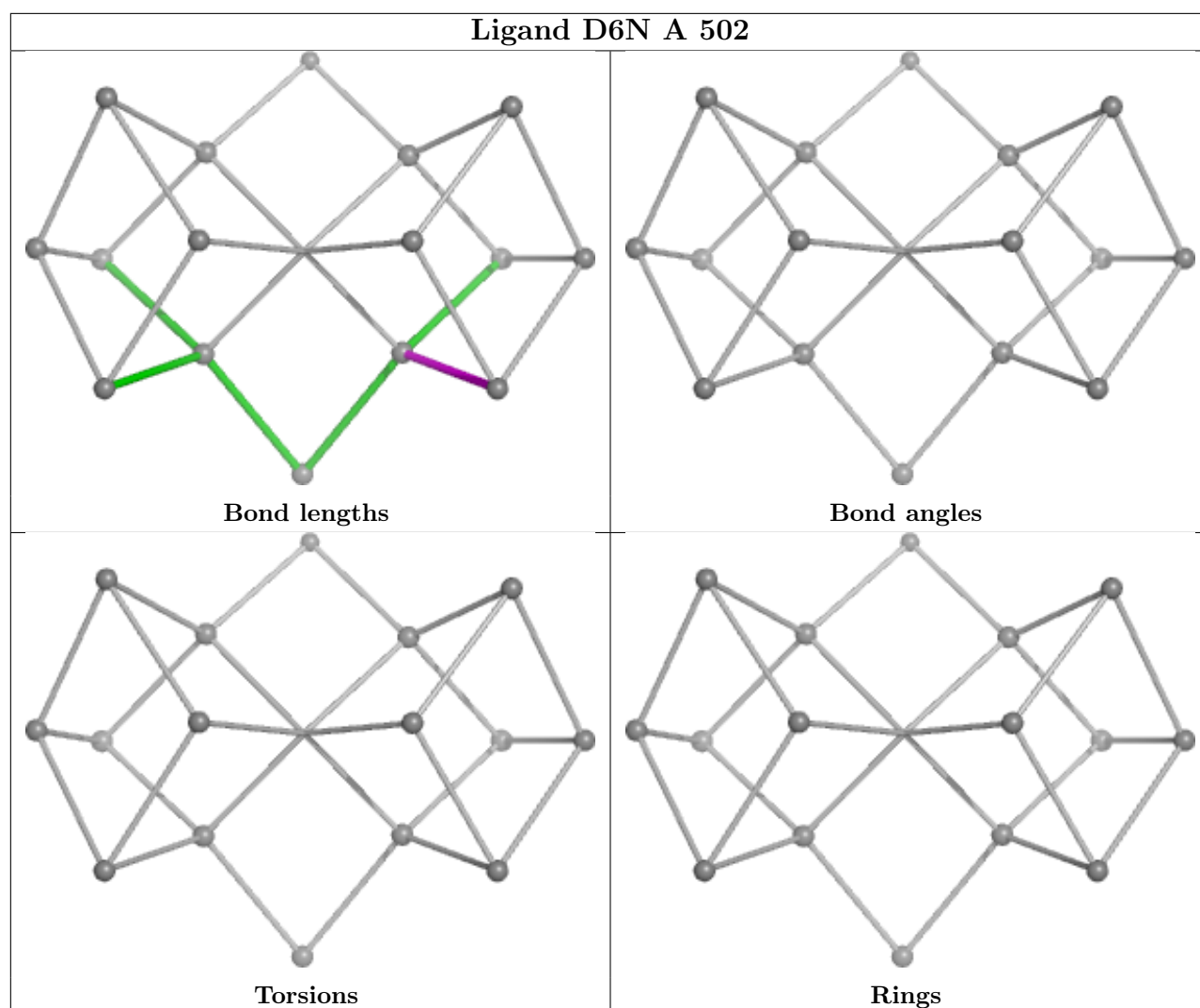
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	502	HCA	1	0
5	D	501	D6N	1	0
5	A	502	D6N	1	0
4	A	501	HCA	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

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	461/474 (97%)	-0.63	1 (0%)	91 92	6, 12, 24, 60	8 (1%)
1	D	461/474 (97%)	-0.70	2 (0%)	88 91	5, 11, 24, 67	8 (1%)
2	B	464/475 (97%)	-0.59	3 (0%)	85 89	8, 13, 27, 56	2 (0%)
2	E	464/475 (97%)	-0.71	2 (0%)	88 91	6, 11, 24, 48	4 (0%)
3	C	113/113 (100%)	-0.34	1 (0%)	81 84	8, 17, 36, 74	1 (0%)
3	F	111/113 (98%)	-0.07	6 (5%)	31 34	9, 17, 52, 82	2 (1%)
All	All	2074/2124 (97%)	-0.61	15 (0%)	84 87	5, 12, 28, 82	25 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	79	VAL	6.1
3	F	84	ILE	5.2
2	E	12	ALA	3.9
2	B	376	ASN	3.3
2	B	12	ALA	3.3
3	F	80	ASN	3.0
3	F	78	GLN	2.9
1	A	462	LYS	2.8
3	F	77	SER	2.7
3	C	1	MET	2.5
3	F	81	LYS	2.4
2	E	379[A]	HIS	2.4
2	B	379[A]	HIS	2.1
1	D	462	LYS	2.1
1	D	395[A]	ASP	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

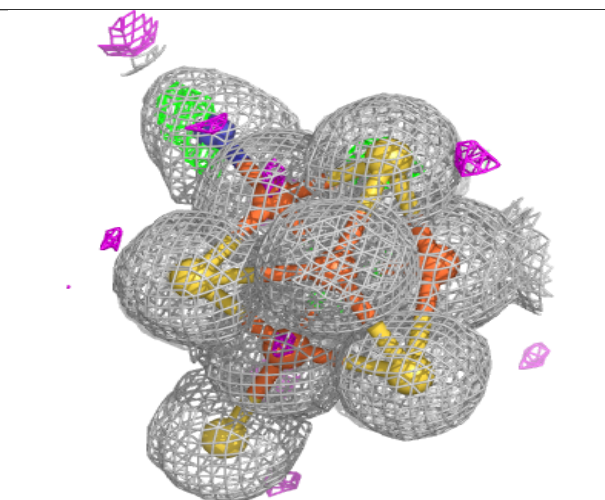
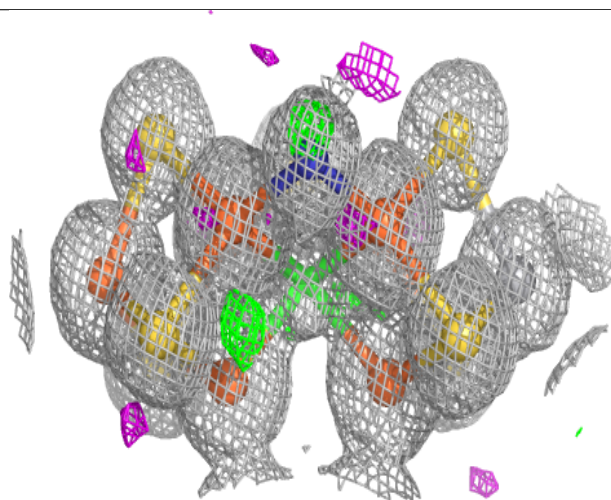
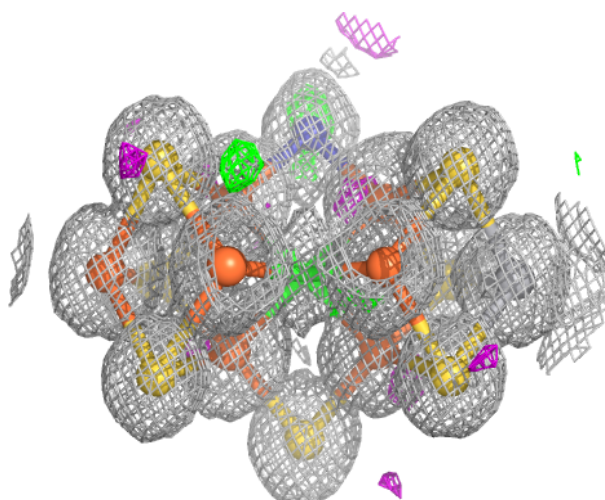
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

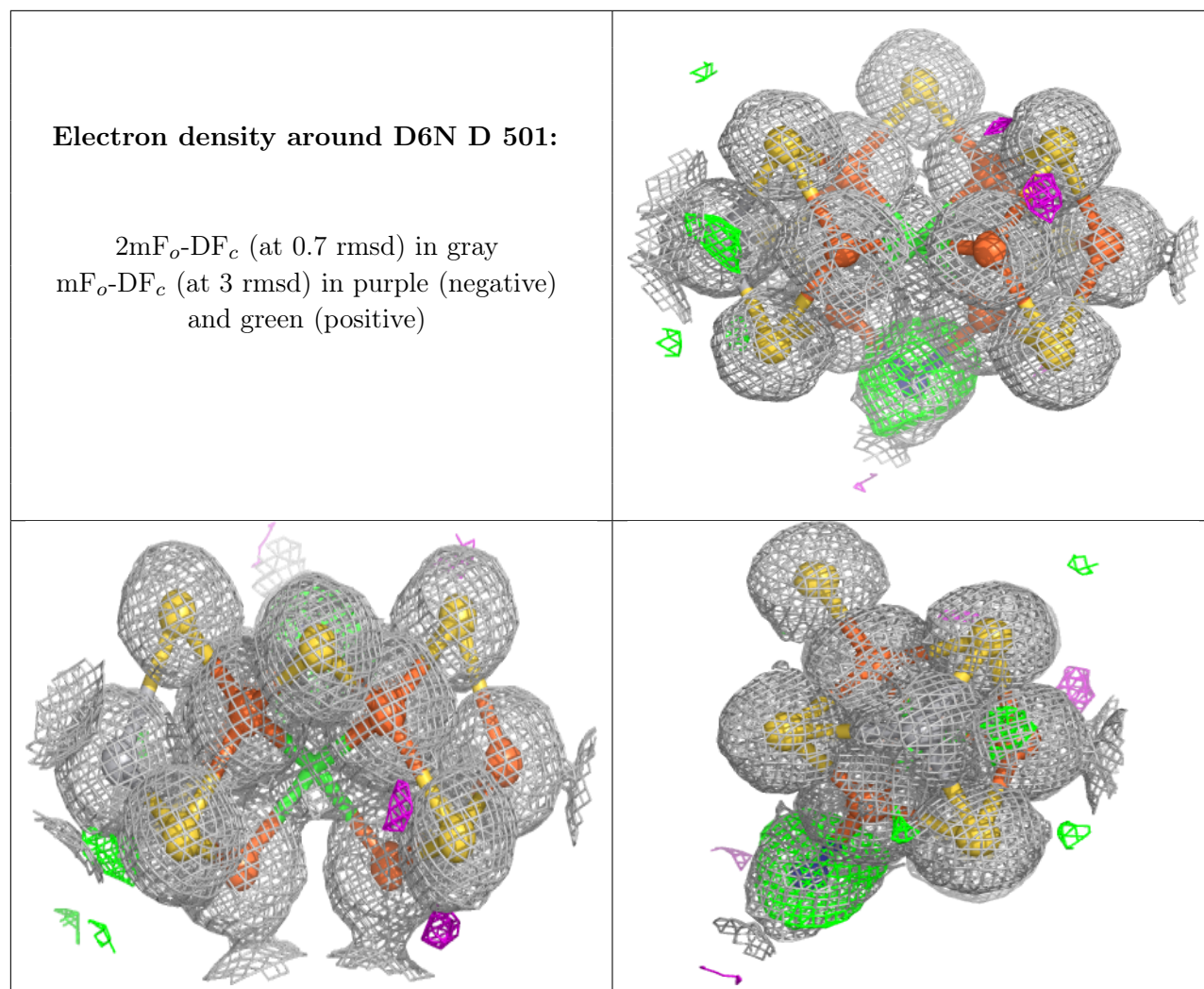
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HCA	A	501	14/14	0.99	0.03	7,9,13,14	0
4	HCA	D	502	14/14	0.99	0.03	6,7,12,13	0
5	D6N	A	502	17/17	1.00	0.01	6,9,9,9	0
5	D6N	D	501	17/17	1.00	0.01	5,7,8,8	0
6	CO3	A	503	4/4	1.00	0.02	9,9,9,9	0
6	CO3	D	503	4/4	1.00	0.01	7,7,8,8	0
7	H2S	A	504	1/1	1.00	0.04	17,17,17,17	0
7	H2S	D	504	1/1	1.00	0.03	16,16,16,16	0
8	ZN	A	505	1/1	1.00	0.04	16,16,16,16	1
8	ZN	B	503	1/1	1.00	0.04	22,22,22,22	1
9	CLF	A	506[A]	15/15	1.00	0.01	7,9,10,10	1
9	CLF	A	506[B]	15/15	1.00	0.01	9,9,10,18	1
9	CLF	D	505[A]	15/15	1.00	0.01	5,7,8,8	1
9	CLF	D	505[B]	15/15	1.00	0.01	7,7,8,13	1
10	MG	B	501	1/1	1.00	0.03	10,10,10,10	0
10	MG	B	502	1/1	1.00	0.02	9,9,9,9	0
10	MG	C	201	1/1	1.00	0.06	17,17,17,17	0
10	MG	F	201	1/1	1.00	0.06	15,15,15,15	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 A 502:

$2mF_o-DF_c$ (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.