



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 11:05 am BST

PDB ID : 5N6Y
Title : Azotobacter vinelandii vanadium nitrogenase
Authors : Sippel, D.; Einsle, O.
Deposited on : 2017-02-16
Resolution : 1.35 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

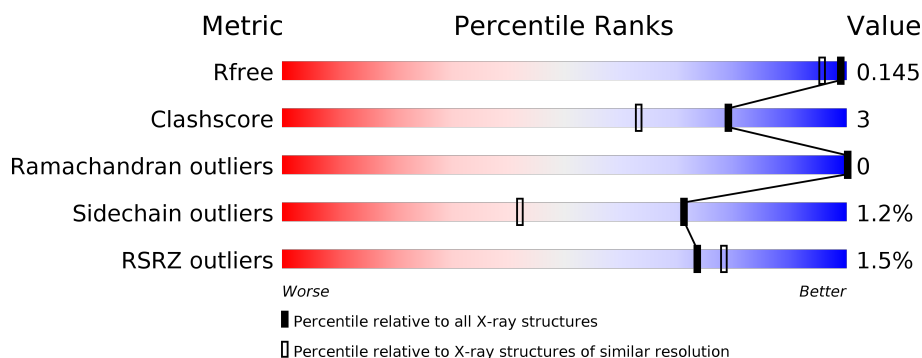
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	474	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
1	D	474	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
2	B	475	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
2	E	475	<div> <div></div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
3	C	113	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>..</div> </div> </div>
3	F	113	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19130 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 vanadium-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	3	0
			3804	2427	650	701	26			
1	D	473	Total	C	N	O	S	0	3	0
			3807	2428	651	702	26			

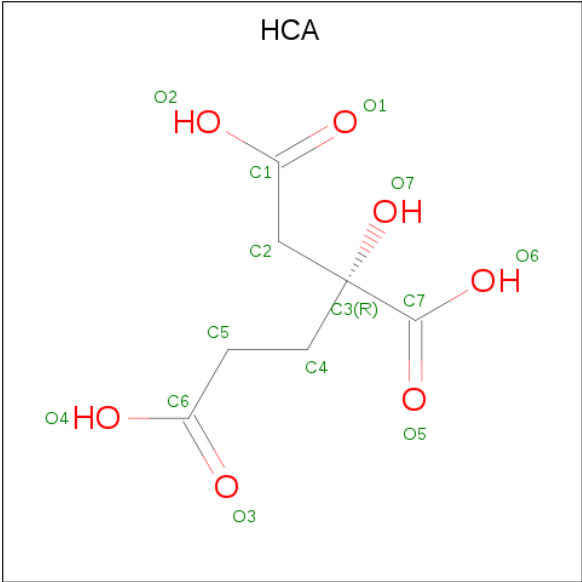
- Molecule 2 is a protein called Nitrogenase vanadium-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	464	Total	C	N	O	S	0	2	0
			3643	2315	625	682	21			
2	B	464	Total	C	N	O	S	0	2	0
			3643	2315	625	682	21			

- Molecule 3 is a protein called Nitrogenase vanadium-iron protein delta chain.

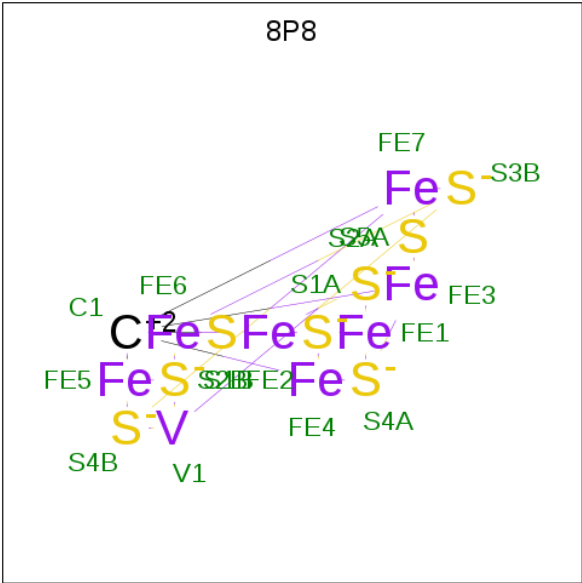
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	112	Total	C	N	O	S	0	0	0
			936	588	168	178	2			
3	F	111	Total	C	N	O	S	0	2	0
			944	592	169	181	2			

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



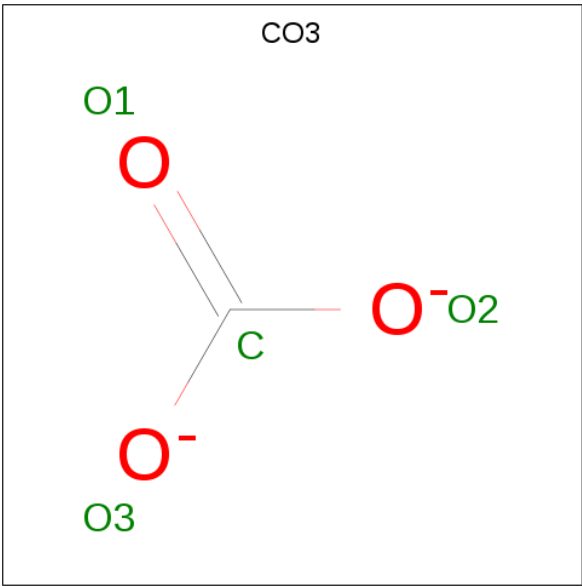
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			14	7	7			
4	D	1	Total	C	O		0	0
			14	7	7			

- Molecule 5 is C Fe7 S8 V (three-letter code: 8P8) (formula: CFe₇S₈V).



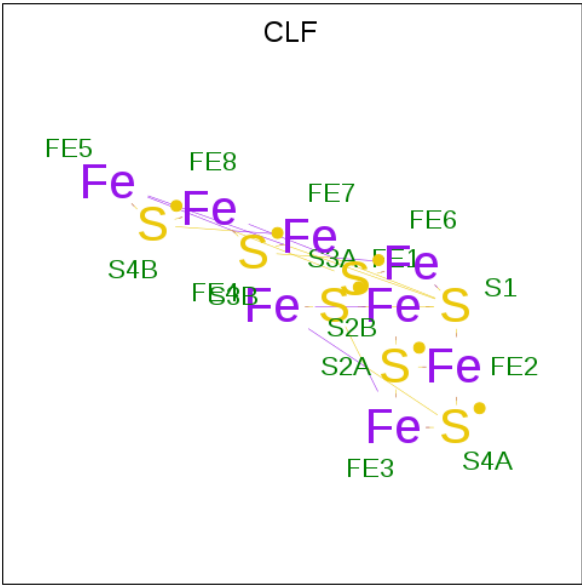
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	S	V	0	0
			17	1	7	8	1		
5	D	1	Total	C	Fe	S	V	0	0
			17	1	7	8	1		

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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 FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇).



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

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	E	2	Total	Mg	0	0
			2	2		

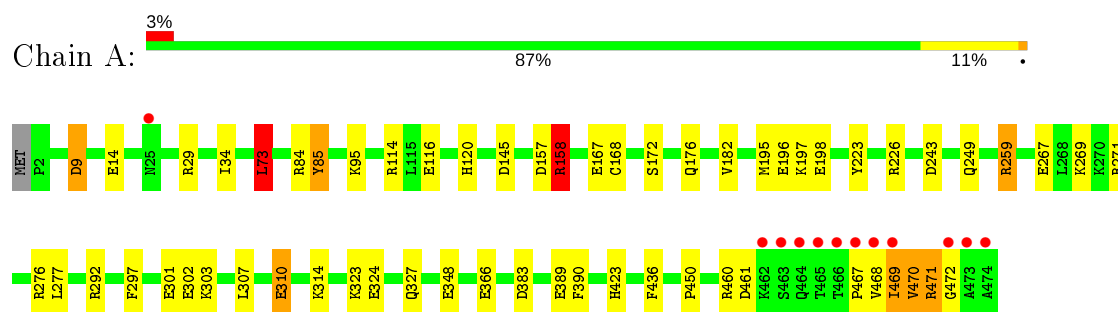
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	479	Total	O	0	0
			479	479		
9	E	521	Total	O	0	0
			521	521		
9	C	125	Total	O	0	0
			125	125		
9	D	494	Total	O	0	0
			494	494		
9	B	503	Total	O	0	0
			503	503		
9	F	127	Total	O	0	0
			127	127		

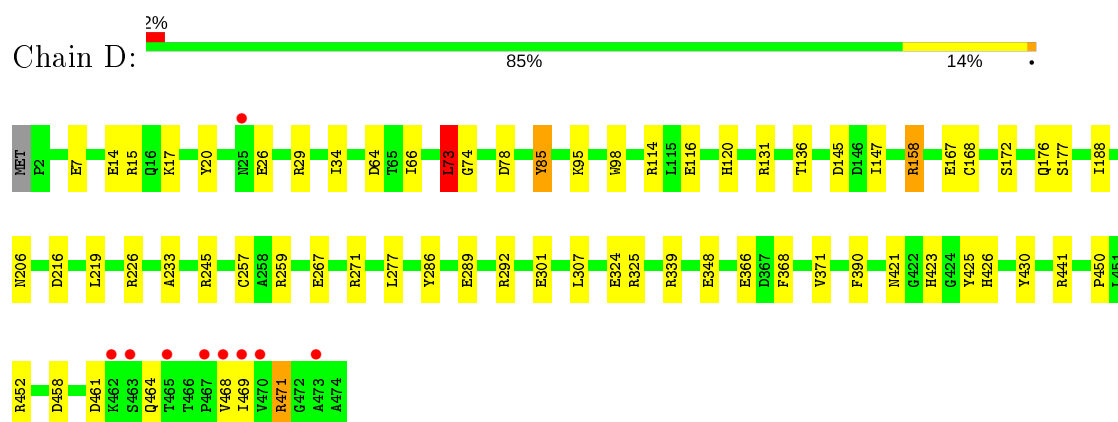
3 Residue-property plots [i](#)

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.

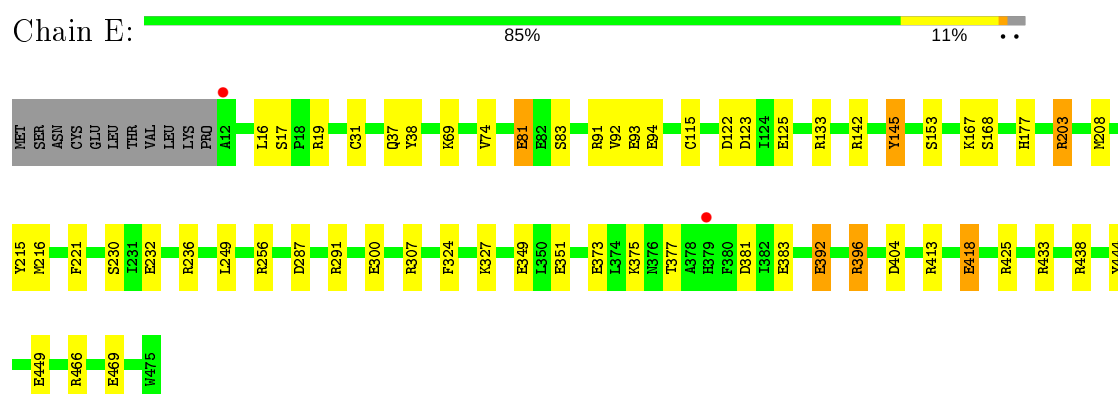
- Molecule 1: Nitrogenase vanadium-iron protein alpha chain



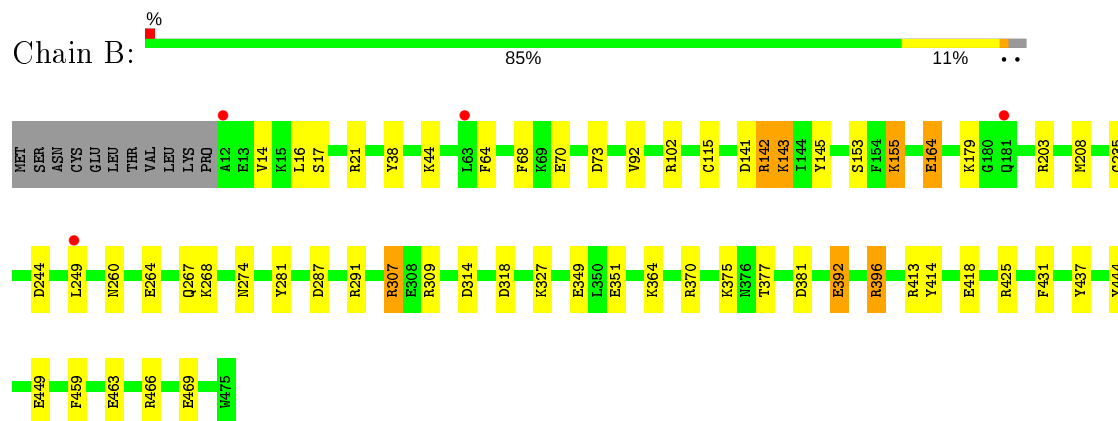
- Molecule 1: Nitrogenase vanadium-iron protein alpha chain



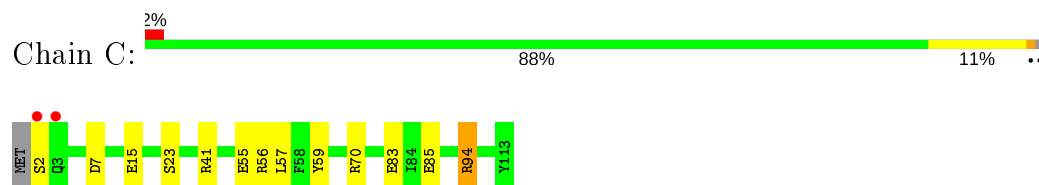
- Molecule 2: Nitrogenase vanadium-iron protein beta chain



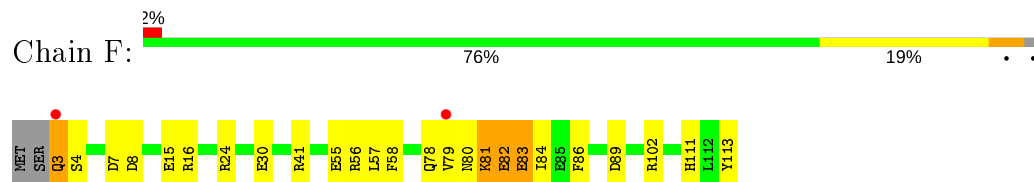
- Molecule 2: Nitrogenase vanadium-iron protein beta chain



- Molecule 3: Nitrogenase vanadium-iron protein delta chain



- Molecule 3: Nitrogenase vanadium-iron protein delta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.25Å 79.79Å 106.97Å 84.06° 72.62° 75.15°	Depositor
Resolution (Å)	102.04 – 1.35 46.52 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.1 (102.04-1.35) 96.1 (46.52-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.109 , 0.146 0.109 , 0.145	Depositor DCC
R_{free} test set	23846 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19130	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: MG, HCA, CLF, 8P8, 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	1.37	25/3902 (0.6%)	1.26	33/5272 (0.6%)
1	D	1.33	24/3902 (0.6%)	1.25	38/5272 (0.7%)
2	B	1.36	20/3720 (0.5%)	1.35	38/5035 (0.8%)
2	E	1.35	29/3720 (0.8%)	1.32	35/5035 (0.7%)
3	C	1.52	13/956 (1.4%)	1.59	5/1293 (0.4%)
3	F	1.58	12/964 (1.2%)	1.76	10/1304 (0.8%)
All	All	1.37	123/17164 (0.7%)	1.34	159/23211 (0.7%)

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	SER	CB-OG	-15.74	1.21	1.42
3	F	56	ARG	CZ-NH1	13.92	1.51	1.33
1	A	324	GLU	CG-CD	12.38	1.70	1.51
1	D	324	GLU	CD-OE2	-11.98	1.12	1.25
1	A	172	SER	CB-OG	-11.73	1.27	1.42
1	A	302	GLU	CD-OE2	-10.69	1.13	1.25
3	F	15	GLU	CD-OE1	10.29	1.36	1.25
1	A	324	GLU	CD-OE2	10.12	1.36	1.25
3	C	55	GLU	CD-OE1	9.99	1.36	1.25
3	C	15	GLU	CD-OE1	9.74	1.36	1.25
2	E	133	ARG	CD-NE	9.09	1.61	1.46
1	A	324	GLU	CD-OE1	8.91	1.35	1.25
1	D	168	CYS	CB-SG	8.78	1.97	1.82
3	C	56	ARG	CZ-NH1	8.58	1.44	1.33
3	F	15	GLU	CD-OE2	8.46	1.34	1.25
1	A	348	GLU	CD-OE2	-8.26	1.16	1.25
1	A	176	GLN	CD-OE1	8.19	1.42	1.24
2	E	469	GLU	CD-OE2	8.05	1.34	1.25
2	B	396	ARG	NE-CZ	-8.05	1.22	1.33
3	C	85	GLU	CD-OE1	7.86	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	GLU	CD-OE2	7.79	1.34	1.25
2	E	383	GLU	CD-OE1	7.72	1.34	1.25
2	E	236	ARG	CG-CD	7.70	1.71	1.51
1	D	292	ARG	CZ-NH2	7.61	1.43	1.33
1	A	14	GLU	CG-CD	7.56	1.63	1.51
2	E	392	GLU	CD-OE2	-7.45	1.17	1.25
2	E	392	GLU	CG-CD	7.43	1.63	1.51
3	F	4	SER	CA-CB	-7.32	1.42	1.52
3	F	82	GLU	CD-OE2	7.28	1.33	1.25
1	D	366	GLU	CB-CG	-7.28	1.38	1.52
2	E	133	ARG	CZ-NH1	7.26	1.42	1.33
1	D	441	ARG	CD-NE	-7.25	1.34	1.46
1	D	177	SER	CB-OG	-7.18	1.32	1.42
2	E	375	LYS	C-O	-7.16	1.09	1.23
3	C	56	ARG	CD-NE	-7.15	1.34	1.46
1	D	176	GLN	CD-OE1	7.10	1.39	1.24
2	E	466	ARG	CZ-NH1	7.01	1.42	1.33
3	F	78	GLN	CD-NE2	7.00	1.50	1.32
2	B	392	GLU	CB-CG	-6.95	1.39	1.52
2	B	351	GLU	CD-OE2	6.92	1.33	1.25
2	B	449	GLU	CG-CD	-6.91	1.41	1.51
2	B	469	GLU	CD-OE2	6.90	1.33	1.25
2	E	351	GLU	CD-OE2	6.88	1.33	1.25
1	A	310	GLU	CD-OE2	6.78	1.33	1.25
1	A	158	ARG	CB-CG	-6.75	1.34	1.52
2	B	466	ARG	CZ-NH2	6.73	1.41	1.33
1	D	14	GLU	CG-CD	6.66	1.61	1.51
2	E	230	SER	CB-OG	-6.65	1.33	1.42
2	B	444	TYR	CE2-CZ	-6.60	1.29	1.38
2	E	83	SER	CB-OG	-6.49	1.33	1.42
2	B	14	VAL	C-O	-6.49	1.11	1.23
3	C	83	GLU	CD-OE1	6.40	1.32	1.25
2	B	349	GLU	CD-OE1	-6.35	1.18	1.25
1	D	176	GLN	CG-CD	6.34	1.65	1.51
2	B	164	GLU	CD-OE2	-6.32	1.18	1.25
1	D	441	ARG	NE-CZ	-6.27	1.24	1.33
3	F	55	GLU	CD-OE1	6.27	1.32	1.25
1	A	267	GLU	CD-OE1	-6.25	1.18	1.25
1	D	301	GLU	CD-OE2	6.25	1.32	1.25
3	C	56	ARG	NE-CZ	6.18	1.41	1.33
1	A	198	GLU	CD-OE1	6.16	1.32	1.25
2	E	449	GLU	CG-CD	-6.16	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	167	GLU	CD-OE1	-6.16	1.18	1.25
1	D	34	ILE	C-O	6.16	1.35	1.23
3	F	30	GLU	CD-OE2	6.12	1.32	1.25
2	E	349	GLU	CD-OE1	-6.11	1.19	1.25
2	E	38	TYR	CE2-CZ	-6.10	1.30	1.38
1	A	14	GLU	CD-OE2	6.08	1.32	1.25
2	B	463	GLU	CD-OE2	6.05	1.32	1.25
3	C	15	GLU	CG-CD	6.03	1.60	1.51
2	B	155	LYS	CB-CG	-6.00	1.36	1.52
3	F	3	GLN	N-CA	5.97	1.58	1.46
2	E	396	ARG	NE-CZ	-5.95	1.25	1.33
2	B	38	TYR	CE2-CZ	-5.88	1.30	1.38
2	E	168	SER	CB-OG	5.83	1.49	1.42
1	A	469	ILE	C-O	5.83	1.34	1.23
3	C	59	TYR	CE1-CZ	-5.78	1.31	1.38
1	D	7	GLU	CD-OE2	5.70	1.31	1.25
1	A	467	PRO	C-O	5.69	1.34	1.23
1	A	267	GLU	CG-CD	5.67	1.60	1.51
1	D	425	TYR	CE1-CZ	-5.64	1.31	1.38
2	B	17	SER	CB-OG	-5.63	1.34	1.42
1	A	14	GLU	CD-OE1	5.60	1.31	1.25
2	E	373	GLU	CD-OE1	-5.60	1.19	1.25
2	B	142	ARG	CB-CG	-5.60	1.37	1.52
1	D	267	GLU	CD-OE1	-5.59	1.19	1.25
1	A	366	GLU	CB-CG	-5.57	1.41	1.52
3	C	23	SER	CB-OG	5.53	1.49	1.42
1	A	196	GLU	CD-OE2	5.50	1.31	1.25
1	A	366	GLU	CD-OE2	5.49	1.31	1.25
2	B	235	GLY	N-CA	-5.48	1.37	1.46
1	A	470	VAL	C-O	-5.47	1.12	1.23
2	E	145	TYR	CG-CD2	-5.46	1.32	1.39
2	B	281	TYR	CE2-CZ	-5.44	1.31	1.38
2	E	93	GLU	CD-OE1	5.42	1.31	1.25
2	E	396	ARG	CD-NE	5.41	1.55	1.46
2	B	145	TYR	CD1-CE1	5.37	1.47	1.39
3	C	83	GLU	CG-CD	5.36	1.59	1.51
1	A	116	GLU	CD-OE1	-5.36	1.19	1.25
2	E	203	ARG	CD-NE	5.33	1.55	1.46
2	E	92	VAL	CB-CG2	-5.28	1.41	1.52
1	A	472	GLY	C-O	5.28	1.32	1.23
3	C	2	SER	CA-CB	5.27	1.60	1.52
1	A	172	SER	CA-CB	-5.26	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	289	GLU	CD-OE2	5.23	1.31	1.25
2	B	92	VAL	CB-CG2	-5.23	1.41	1.52
1	D	301	GLU	CD-OE1	5.20	1.31	1.25
1	A	34	ILE	C-O	5.19	1.33	1.23
1	D	34	ILE	C-N	-5.19	1.22	1.34
1	D	464	GLN	CG-CD	5.18	1.62	1.51
2	E	69	LYS	CG-CD	-5.16	1.34	1.52
2	E	94	GLU	CD-OE2	5.16	1.31	1.25
2	E	17	SER	CB-OG	-5.15	1.35	1.42
1	D	348	GLU	CD-OE2	-5.14	1.20	1.25
3	C	70	ARG	CZ-NH2	5.12	1.39	1.33
1	D	26	GLU	CD-OE1	5.10	1.31	1.25
2	E	300	GLU	CD-OE1	5.05	1.31	1.25
3	F	56	ARG	CD-NE	-5.05	1.37	1.46
3	F	83	GLU	CD-OE2	5.05	1.31	1.25
2	E	19	ARG	CB-CG	-5.04	1.39	1.52
3	F	113	TYR	CE1-CZ	-5.01	1.32	1.38
2	B	375	LYS	C-O	-5.01	1.13	1.23
2	E	125	GLU	CD-OE1	5.01	1.31	1.25

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	56	ARG	NE-CZ-NH2	-30.61	105.00	120.30
3	F	56	ARG	NE-CZ-NH1	28.48	134.54	120.30
3	C	56	ARG	NE-CZ-NH1	28.01	134.31	120.30
3	C	56	ARG	NE-CZ-NH2	-22.39	109.11	120.30
2	B	466	ARG	NE-CZ-NH1	-19.03	110.78	120.30
2	E	208	MET	CG-SD-CE	18.60	129.96	100.20
2	B	396	ARG	NE-CZ-NH2	-13.43	113.59	120.30
2	E	291	ARG	NE-CZ-NH2	12.41	126.50	120.30
2	B	466	ARG	NE-CZ-NH2	12.30	126.45	120.30
2	E	291	ARG	NE-CZ-NH1	-11.84	114.38	120.30
2	E	466	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	D	471	ARG	NE-CZ-NH1	-10.31	115.15	120.30
1	D	471	ARG	NE-CZ-NH2	10.30	125.45	120.30
3	F	41	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	A	259	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	A	271	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	D	15	ARG	NE-CZ-NH2	-9.74	115.43	120.30
2	E	381	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	D	15	ARG	NE-CZ-NH1	9.38	124.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	ARG	NE-CZ-NH1	-9.12	115.74	120.30
2	B	141	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	D	325	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	B	309	ARG	NE-CZ-NH2	8.44	124.52	120.30
2	B	309	ARG	NE-CZ-NH1	-8.43	116.08	120.30
2	B	459	PHE	CB-CG-CD1	8.28	126.60	120.80
3	F	41	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	259	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	D	131	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	145	ASP	CB-CG-OD1	8.11	125.60	118.30
3	C	56	ARG	CD-NE-CZ	7.91	134.68	123.60
1	A	73	LEU	CB-CG-CD1	7.88	124.40	111.00
2	E	404	ASP	CB-CG-OD2	7.86	125.37	118.30
2	B	102	ARG	NE-CZ-NH2	-7.77	116.42	120.30
3	C	41	ARG	NE-CZ-NH2	-7.75	116.42	120.30
2	B	327	LYS	CD-CE-NZ	-7.71	93.97	111.70
1	D	461	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	471	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	E	122	ASP	CB-CG-OD1	7.64	125.18	118.30
3	F	16	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	D	286	TYR	CB-CG-CD1	7.59	125.55	121.00
1	D	441	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	B	396	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	292	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	172	SER	CB-CA-C	7.46	124.26	110.10
2	B	370	ARG	NE-CZ-NH2	-7.44	116.58	120.30
3	F	58	PHE	CB-CG-CD2	-7.34	115.66	120.80
1	D	78	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	D	131	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	E	203	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	158	ARG	CG-CD-NE	-7.17	96.75	111.80
1	D	78	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	114	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	B	70	GLU	OE1-CD-OE2	-7.07	114.82	123.30
1	A	470	VAL	O-C-N	-7.02	111.47	122.70
2	B	21	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	E	466	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	D	366	GLU	CA-CB-CG	6.83	128.44	113.40
2	B	307	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	390	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	A	470	VAL	CA-C-O	6.72	134.22	120.10
1	D	325	ARG	NE-CZ-NH2	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	D	441	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	D	158	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	E	167	LYS	CD-CE-NZ	-6.67	96.36	111.70
2	E	203	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	B	244	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	D	34	ILE	CG1-CB-CG2	6.55	125.82	111.40
1	D	271	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	E	425	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	157	ASP	CB-CG-OD1	6.43	124.08	118.30
1	D	339	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	D	85	TYR	CB-CG-CD1	6.39	124.84	121.00
2	B	381	ASP	CB-CG-OD2	-6.38	112.56	118.30
2	E	324	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	D	292	ARG	CD-NE-CZ	6.34	132.47	123.60
2	B	68	PHE	CB-CG-CD2	6.31	125.22	120.80
1	A	84	ARG	NE-CZ-NH1	6.29	123.44	120.30
3	F	24	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	E	307	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	318	ASP	CB-CG-OD2	6.24	123.92	118.30
1	D	64	ASP	CB-CG-OD1	6.22	123.90	118.30
2	E	256	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	E	249	LEU	CB-CG-CD2	-6.18	100.49	111.00
2	E	123	ASP	CB-CG-OD1	6.18	123.86	118.30
2	E	133	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	B	21	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	E	19	ARG	CD-NE-CZ	6.16	132.22	123.60
2	B	291	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	461	ASP	CB-CG-OD1	6.14	123.83	118.30
2	E	287	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	85	TYR	CB-CG-CD1	6.05	124.63	121.00
2	E	413	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	D	34	ILE	CA-CB-CG2	-6.03	98.84	110.90
2	B	314	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	20	TYR	CB-CG-CD2	5.97	124.58	121.00
2	E	221	PHE	CB-CG-CD1	5.97	124.98	120.80
1	D	339	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	E	418[A]	GLU	OE1-CD-OE2	5.94	130.43	123.30
2	E	418[B]	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	A	182	VAL	CG1-CB-CG2	-5.94	101.40	110.90
2	E	444	TYR	CB-CG-CD2	-5.93	117.44	121.00
2	E	469	GLU	OE1-CD-OE2	-5.93	116.19	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	91	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	245	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	458	ASP	CB-CG-OD1	5.90	123.61	118.30
2	B	425	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	B	431	PHE	CB-CG-CD2	-5.88	116.68	120.80
1	D	114	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	D	167	GLU	OE1-CD-OE2	-5.82	116.31	123.30
1	D	430	TYR	CB-CG-CD1	5.80	124.48	121.00
2	E	433	ARG	NE-CZ-NH2	-5.80	117.40	120.30
3	F	8	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	D	461	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	E	438	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	B	413	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	B	64	PHE	CB-CG-CD1	5.75	124.82	120.80
2	B	287	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	158	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	276	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	B	437	TYR	CB-CG-CD1	5.64	124.38	121.00
1	A	324	GLU	CA-CB-CG	5.63	125.79	113.40
2	B	208	MET	CG-SD-CE	-5.62	91.21	100.20
2	E	392	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	A	383	ASP	CB-CG-OD1	-5.58	113.28	118.30
2	B	179	LYS	CD-CE-NZ	-5.57	98.88	111.70
2	B	370	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	B	73	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	216	ASP	CB-CG-OD2	-5.45	113.40	118.30
3	F	7	ASP	CB-CG-OD2	-5.45	113.40	118.30
2	E	375	LYS	O-C-N	5.35	131.26	122.70
3	F	102	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	73	LEU	CB-CG-CD1	5.33	120.06	111.00
1	A	9	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	E	433	ARG	NE-CZ-NH1	5.29	122.94	120.30
3	C	7	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	116	GLU	OE1-CD-OE2	-5.28	116.96	123.30
2	E	373	GLU	OE1-CD-OE2	-5.26	116.98	123.30
1	A	195	MET	CB-CG-SD	-5.25	96.66	112.40
1	A	470	VAL	C-N-CA	-5.24	108.61	121.70
2	B	203	ARG	CD-NE-CZ	-5.23	116.27	123.60
1	A	243	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	257	CYS	CA-CB-SG	-5.22	104.61	114.00
2	B	249	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	167	GLU	OE1-CD-OE2	-5.20	117.07	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	E	142	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	271	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	A	366	GLU	CG-CD-OE2	5.16	128.63	118.30
2	B	16	LEU	CB-CG-CD1	-5.16	102.24	111.00
1	D	390	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	D	145	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	414	TYR	CG-CD2-CE2	5.07	125.36	121.30
1	A	297	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	A	145	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	B	102	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	E	81	GLU	OE1-CD-OE2	5.03	129.34	123.30
2	B	459	PHE	CB-CG-CD2	-5.02	117.29	120.80
1	A	223	TYR	CB-CG-CD1	5.01	124.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3804	0	3725	24	0
1	D	3807	0	3724	27	0
2	B	3643	0	3622	25	0
2	E	3643	0	3622	19	0
3	C	936	0	897	2	0
3	F	944	0	899	9	0
4	A	14	0	6	1	0
4	D	14	0	6	1	0
5	A	17	0	0	0	0
5	D	17	0	0	0	0
6	A	4	0	0	0	0
6	D	4	0	0	0	0
7	A	15	0	0	0	0
7	E	15	0	0	0	0
8	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	2	0	0	0	0
8	F	1	0	0	0	0
9	A	479	0	0	8	1
9	B	503	0	0	8	0
9	C	125	0	0	1	0
9	D	494	0	0	4	6
9	E	521	0	0	5	7
9	F	127	0	0	4	0
All	All	19130	0	16501	93	7

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 (93) 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:81:GLU:HB3	9:E:882:HOH:O	1.35	1.25
2:E:327:LYS:HE3	9:E:634:HOH:O	1.35	1.19
3:F:3:GLN:HB2	9:F:357:HOH:O	1.64	0.97
1:D:17:LYS:HG3	9:D:887:HOH:O	1.66	0.93
1:D:226:ARG:HD3	1:D:307[A]:LEU:HD13	1.52	0.91
2:B:392:GLU:OE1	2:B:396:ARG:NH2	2.04	0.91
3:F:80:ASN:HB3	9:F:303:HOH:O	1.72	0.88
2:E:81:GLU:CB	9:E:882:HOH:O	2.02	0.86
2:B:392:GLU:HG3	2:B:396:ARG:NH2	1.93	0.83
1:A:197:LYS:H	1:A:249:GLN:HE22	1.24	0.82
1:A:226:ARG:HD3	1:A:307[A]:LEU:HD13	1.62	0.80
1:A:120:HIS:HD2	1:A:158:ARG:HH11	1.27	0.79
1:A:323:LYS:O	1:A:327[B]:GLN:HG3	1.84	0.78
1:D:468:VAL:HG11	2:B:377:THR:HG21	1.69	0.75
2:B:164:GLU:OE1	9:B:601:HOH:O	2.05	0.73
2:B:418[A]:GLU:HG3	9:B:953:HOH:O	1.88	0.72
1:A:468:VAL:HG13	2:E:377:THR:HG22	1.70	0.71
2:B:264:GLU:HG2	9:B:926:HOH:O	1.91	0.71
2:B:392:GLU:CG	2:B:396:ARG:HH22	2.05	0.70
2:B:267:GLN:HE21	2:B:274:ASN:H	1.40	0.69
1:D:120:HIS:HD2	1:D:158:ARG:HH11	1.41	0.67
1:D:421:ASN:H	1:D:426:HIS:CD2	2.13	0.67
1:D:421:ASN:H	1:D:426:HIS:HD2	1.42	0.67
2:B:264:GLU:OE1	9:B:602:HOH:O	2.13	0.66
1:A:468:VAL:HG13	2:E:377:THR:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:HIS:HE1	9:D:644:HOH:O	1.80	0.64
1:D:468:VAL:HG11	2:B:377:THR:CG2	2.26	0.64
2:E:81:GLU:CG	9:E:882:HOH:O	2.38	0.64
2:B:392:GLU:HG3	2:B:396:ARG:HH22	1.62	0.63
1:A:95:LYS:NZ	2:B:418[A]:GLU:OE2	2.30	0.63
2:B:268:LYS:HE3	9:B:988:HOH:O	1.98	0.62
2:B:392:GLU:CD	2:B:396:ARG:HH22	2.03	0.60
2:B:392:GLU:CG	2:B:396:ARG:NH2	2.64	0.60
3:C:94:ARG:HD3	9:C:364:HOH:O	2.01	0.60
1:D:120:HIS:CD2	1:D:158:ARG:HH11	2.19	0.60
1:A:307[B]:LEU:HD23	1:A:307[B]:LEU:C	2.23	0.59
2:E:392:GLU:OE1	2:E:396:ARG:NH1	2.27	0.59
2:E:232:GLU:OE1	2:B:307:ARG:NH2	2.36	0.59
1:D:452:ARG:HD3	9:D:632:HOH:O	2.02	0.59
3:F:89[B]:ASP:OD1	9:F:301:HOH:O	2.17	0.59
1:A:120:HIS:HE1	9:A:666:HOH:O	1.85	0.58
1:A:277:LEU:HD13	3:C:57:LEU:HD11	1.85	0.57
3:F:79:VAL:HG11	3:F:84:ILE:HD11	1.86	0.57
3:F:79:VAL:HG22	3:F:83:GLU:HB3	1.86	0.57
1:A:310:GLU:HG3	9:A:769:HOH:O	2.04	0.56
1:A:301:GLU:OE2	9:A:601:HOH:O	2.16	0.56
2:B:44[B]:LYS:HE2	9:B:772:HOH:O	2.05	0.56
1:A:450:PRO:HD3	1:A:471:ARG:HD2	1.89	0.54
3:F:81:LYS:HG2	3:F:82:GLU:N	2.23	0.53
1:D:426:HIS:HE1	9:D:1024:HOH:O	1.92	0.52
1:D:468:VAL:CG1	2:B:377:THR:HG21	2.37	0.52
1:A:468:VAL:CG1	2:E:377:THR:HG22	2.38	0.52
2:E:81:GLU:HG2	9:E:882:HOH:O	2.06	0.51
1:D:73:LEU:HD22	1:D:73:LEU:C	2.32	0.50
1:D:277:LEU:HD13	3:F:57:LEU:HD11	1.94	0.50
1:A:468:VAL:CG1	2:E:377:THR:CG2	2.89	0.49
1:A:303:LYS:HD3	9:A:649:HOH:O	2.11	0.49
1:A:423:HIS:HB3	4:A:501:HCA:O5	2.13	0.49
2:B:268:LYS:CE	9:B:988:HOH:O	2.58	0.48
1:A:73:LEU:C	1:A:73:LEU:HD22	2.35	0.48
2:B:260:ASN:ND2	2:B:274:ASN:HD21	2.12	0.48
3:F:111:HIS:HD2	9:F:404:HOH:O	1.96	0.48
2:B:267:GLN:NE2	2:B:274:ASN:H	2.07	0.47
1:D:73:LEU:HD22	1:D:74:GLY:N	2.30	0.46
1:D:136:THR:HG23	1:D:147:ILE:HD13	1.97	0.46
2:B:115:CYS:HB3	2:B:153:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:HD3	9:A:987:HOH:O	2.16	0.45
1:D:468:VAL:CG1	2:B:377:THR:CG2	2.91	0.45
1:D:219:LEU:HD23	1:D:219:LEU:C	2.37	0.45
1:D:368:PHE:HA	1:D:371:VAL:HG12	1.99	0.45
1:D:226:ARG:CD	1:D:307[A]:LEU:HD13	2.34	0.44
2:B:143:LYS:HE3	9:B:654:HOH:O	2.16	0.44
1:A:168:CYS:HA	9:A:989:HOH:O	2.18	0.44
2:B:392:GLU:HG3	2:B:396:ARG:HH21	1.81	0.43
1:D:307[B]:LEU:HD23	1:D:307[B]:LEU:C	2.37	0.43
1:D:423:HIS:HB3	4:D:501:HCA:O6	2.18	0.43
1:A:120:HIS:CD2	1:A:158:ARG:HD2	2.53	0.43
2:E:37:GLN:NE2	2:E:74:VAL:HG11	2.34	0.43
1:D:450:PRO:HD3	1:D:471:ARG:HD2	2.01	0.43
1:A:168:CYS:CB	9:A:989:HOH:O	2.67	0.42
1:D:471:ARG:HD3	1:D:471:ARG:HH11	1.64	0.42
2:E:115:CYS:HB3	2:E:153:SER:OG	2.18	0.42
1:D:206:ASN:HD22	1:D:233:ALA:H	1.68	0.42
1:A:470:VAL:O	9:A:602:HOH:O	2.22	0.42
1:A:9:ASP:OD2	1:A:389:GLU:OE2	2.38	0.41
2:E:215:TYR:HA	2:E:216:MET:HA	1.84	0.41
2:E:203:ARG:HH11	2:E:203:ARG:HD3	1.61	0.41
3:F:3:GLN:OE1	3:F:86:PHE:CE2	2.74	0.41
2:E:37:GLN:HE21	2:E:74:VAL:HG11	1.86	0.41
2:E:31:CYS:HB2	2:E:153:SER:HB2	2.01	0.41
2:E:145:TYR:OH	2:E:177:HIS:HE1	2.04	0.40
2:E:418[A]:GLU:CD	1:D:95:LYS:NZ	2.75	0.40
1:D:66:ILE:HG23	1:D:98:TRP:CD2	2.56	0.40

All (7) 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)
9:E:1110:HOH:O	9:D:985:HOH:O[1_455]	0.70	1.50
9:E:1120:HOH:O	9:D:971:HOH:O[1_455]	0.77	1.43
9:E:1116:HOH:O	9:D:994:HOH:O[1_455]	0.78	1.42
9:E:1053:HOH:O	9:D:1069:HOH:O[1_455]	0.81	1.39
9:E:1093:HOH:O	9:D:982:HOH:O[1_455]	1.07	1.13
9:E:1117:HOH:O	9:D:1093:HOH:O[1_455]	1.10	1.10
9:A:874:HOH:O	9:E:1119:HOH:O[1_654]	2.19	0.01

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	474/474 (100%)	463 (98%)	11 (2%)	0	100	100
1	D	474/474 (100%)	459 (97%)	15 (3%)	0	100	100
2	B	464/475 (98%)	457 (98%)	7 (2%)	0	100	100
2	E	464/475 (98%)	456 (98%)	8 (2%)	0	100	100
3	C	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
3	F	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
All	All	2097/2124 (99%)	2047 (98%)	50 (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	406/404 (100%)	398 (98%)	8 (2%)	55	21
1	D	406/404 (100%)	400 (98%)	6 (2%)	65	33
2	B	389/398 (98%)	385 (99%)	4 (1%)	76	49
2	E	389/398 (98%)	388 (100%)	1 (0%)	92	83
3	C	101/102 (99%)	100 (99%)	1 (1%)	76	49
3	F	102/102 (100%)	101 (99%)	1 (1%)	76	49
All	All	1793/1808 (99%)	1772 (99%)	21 (1%)	71	42

All (21) 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	158	ARG
1	A	259	ARG
1	A	314	LYS
1	A	436	PHE
1	A	469	ILE
2	E	16	LEU
3	C	94	ARG
1	D	29	ARG
1	D	73	LEU
1	D	85	TYR
1	D	188	ILE
1	D	259	ARG
1	D	469	ILE
2	B	142	ARG
2	B	143	LYS
2	B	155	LYS
2	B	364	LYS
3	F	81	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	249	GLN
1	A	448	HIS
2	E	37	GLN
2	E	105	ASN
2	E	177	HIS
2	E	361	GLN
3	C	3	GLN
3	C	46	GLN
3	C	109	ASN
1	D	120	HIS
1	D	206	ASN
1	D	253	ASN
1	D	426	HIS
2	B	260	ASN
2	B	267	GLN

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Mol	Chain	Res	Type
2	B	361	GLN
3	F	109	ASN
3	F	111	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	A	503	5	0,3,3	0.00	-	0,3,3	0.00	-
7	CLF	E	501	1,2	0,24,24	0.00	-	-		
6	CO3	D	503	5	0,3,3	0.00	-	0,3,3	0.00	-
7	CLF	A	504	1,2	0,24,24	0.00	-	-		
4	HCA	D	501	5	4,13,13	0.59	0	4,18,18	1.69	1 (25%)
5	8P8	A	502	1,4,6	12,28,28	2.20	7 (58%)	-		
4	HCA	A	501	5	4,13,13	0.56	0	4,18,18	2.53	1 (25%)
5	8P8	D	502	1,4,6	12,28,28	2.17	5 (41%)	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLF	E	501	1,2	-	-	0/12/10/10
4	HCA	A	501	5	-	0/7/17/17	-
7	CLF	A	504	1,2	-	-	0/12/10/10
4	HCA	D	501	5	-	0/7/17/17	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	8P8	S1A-FE2	-4.32	2.21	2.32
5	A	502	8P8	S1A-FE2	-3.21	2.24	2.32
5	D	502	8P8	S3B-FE6	-3.12	2.21	2.31
5	A	502	8P8	S2B-FE6	-3.00	2.17	2.24
5	A	502	8P8	S3B-FE6	-2.90	2.21	2.31
5	D	502	8P8	S1B-FE6	-2.77	2.22	2.31
5	A	502	8P8	S4B-FE7	-2.54	2.23	2.31
5	D	502	8P8	S4A-FE3	-2.40	2.26	2.32
5	A	502	8P8	S2A-FE3	-2.31	2.26	2.32
5	D	502	8P8	S4B-FE7	-2.09	2.24	2.31
5	A	502	8P8	S3B-FE7	-2.08	2.24	2.31
5	A	502	8P8	S1B-FE6	-2.05	2.24	2.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	HCA	C3-C2-C1	-4.95	107.05	114.98
4	D	501	HCA	C3-C2-C1	-2.74	110.60	114.98

There are no chirality outliers.

There are no torsion outliers.

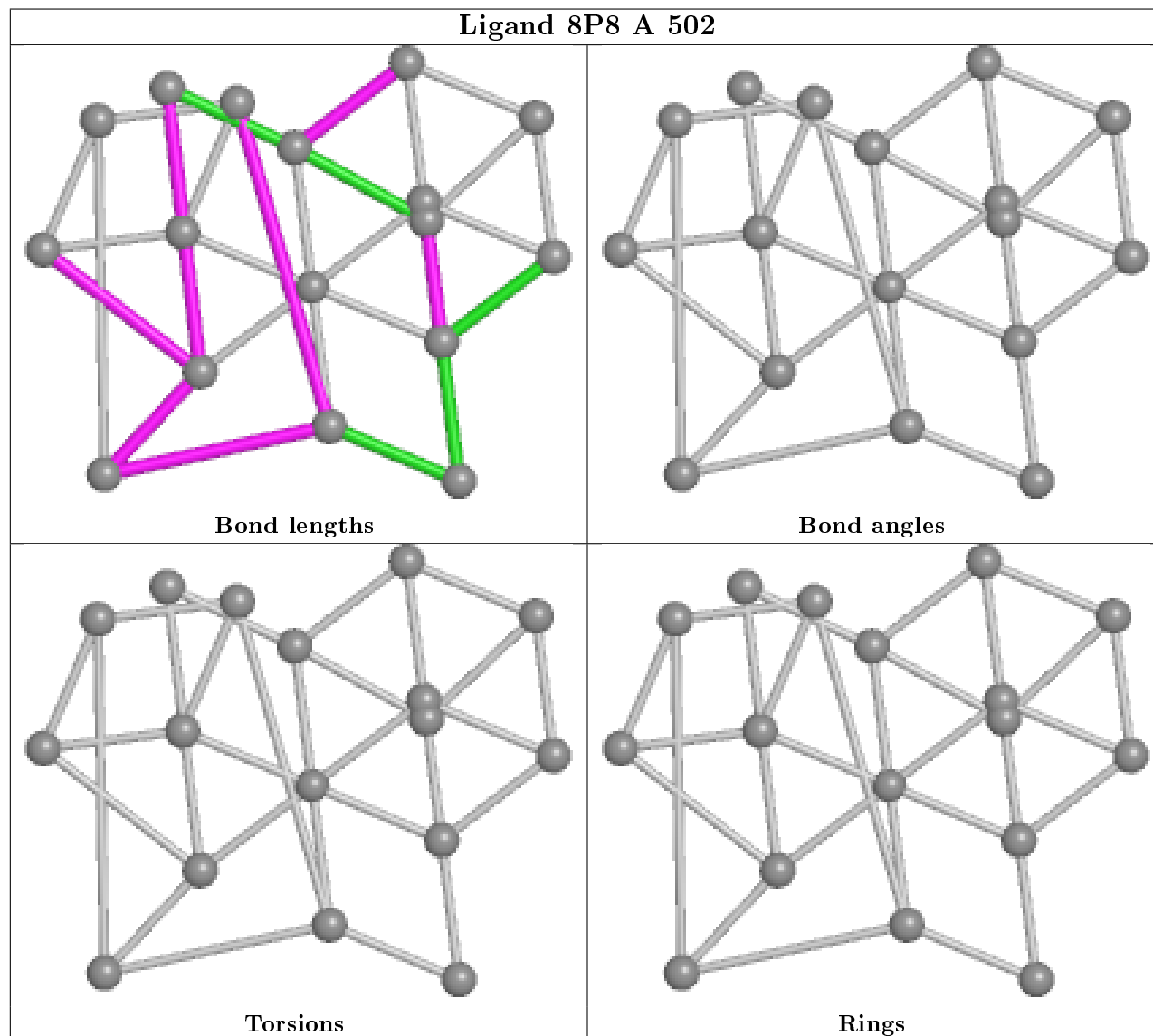
There are no ring outliers.

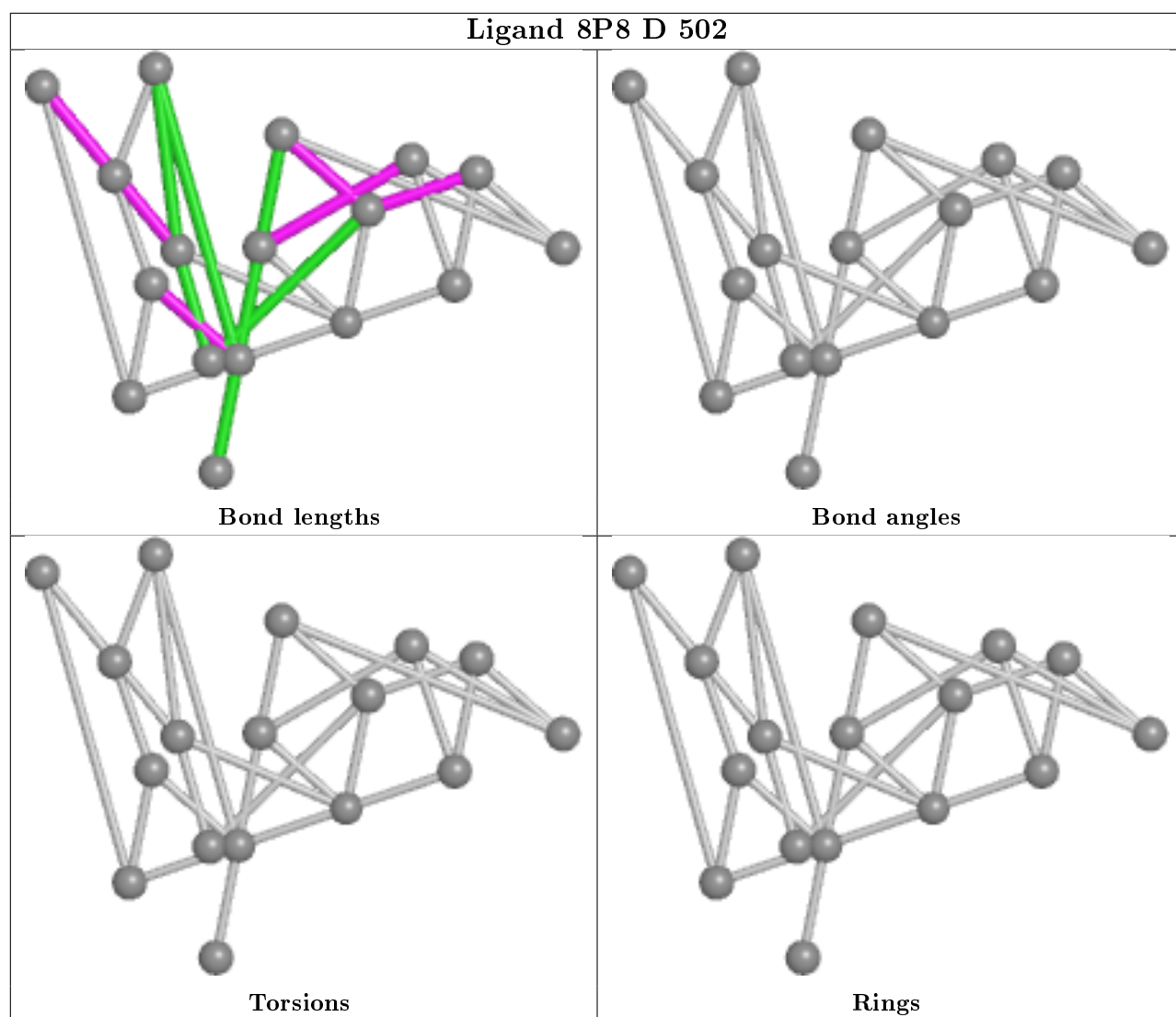
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	HCA	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	473/474 (99%)	-0.16	12 (2%) 57 63	10, 15, 32, 55	0
1	D	473/474 (99%)	-0.25	9 (1%) 66 71	8, 14, 30, 52	0
2	B	464/475 (97%)	-0.25	4 (0%) 84 87	10, 15, 30, 57	0
2	E	464/475 (97%)	-0.27	2 (0%) 92 93	9, 14, 26, 52	0
3	C	112/113 (99%)	-0.19	2 (1%) 68 73	14, 21, 37, 48	0
3	F	111/113 (98%)	-0.12	2 (1%) 68 73	13, 20, 50, 70	0
All	All	2097/2124 (98%)	-0.22	31 (1%) 73 78	8, 15, 32, 70	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	VAL	6.5
2	E	12	ALA	5.5
1	A	469	ILE	5.1
1	A	465	THR	4.8
3	F	3	GLN	4.7
1	D	468	VAL	4.5
1	A	473	ALA	4.3
1	A	467	PRO	4.1
1	A	463	SER	3.9
1	D	469	ILE	3.8
1	A	25	ASN	3.8
1	A	474	ALA	3.7
2	B	12	ALA	3.6
1	D	465	THR	3.2
3	C	2	SER	3.0
2	B	181	GLN	2.8
1	A	464	GLN	2.8
1	D	467	PRO	2.7
1	D	462	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	3	GLN	2.7
1	D	470	VAL	2.6
1	D	25	ASN	2.6
1	A	466	THR	2.5
1	D	473	ALA	2.5
3	F	79	VAL	2.5
1	A	472	GLY	2.4
1	D	463	SER	2.4
2	B	63	LEU	2.2
1	A	462	LYS	2.2
2	B	249	LEU	2.2
2	E	379	HIS	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 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(Å ²)	Q<0.9
6	CO3	A	503	4/4	0.99	0.09	10,10,10,11	0
6	CO3	D	503	4/4	0.99	0.09	8,10,10,10	0
4	HCA	D	501	14/14	0.99	0.08	7,9,15,16	0
4	HCA	A	501	14/14	0.99	0.09	8,11,17,18	0
8	MG	C	201	1/1	1.00	0.10	22,22,22,22	0
7	CLF	A	504	15/15	1.00	0.06	10,11,12,14	0
8	MG	F	201	1/1	1.00	0.11	22,22,22,22	0
5	8P8	A	502	17/17	1.00	0.07	10,10,11,14	0
7	CLF	E	501	15/15	1.00	0.06	8,9,10,13	0
8	MG	E	502	1/1	1.00	0.06	14,14,14,14	0
5	8P8	D	502	17/17	1.00	0.07	8,9,10,12	0

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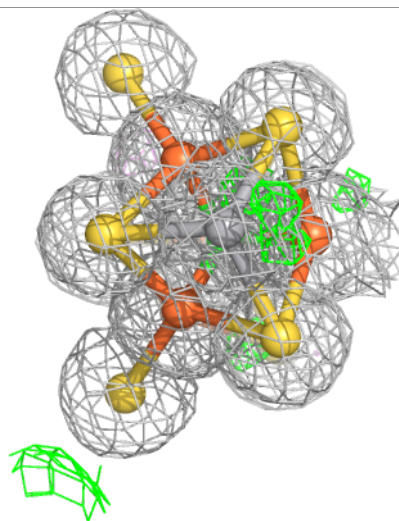
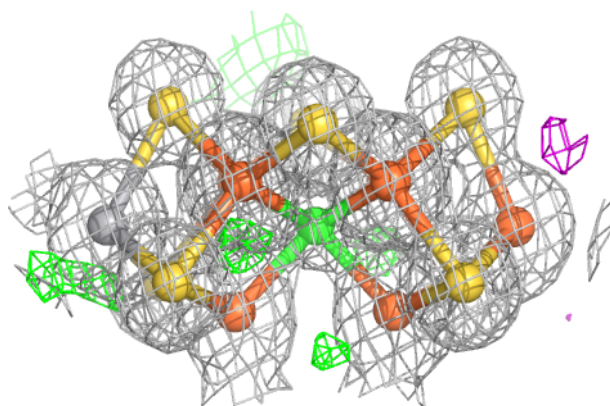
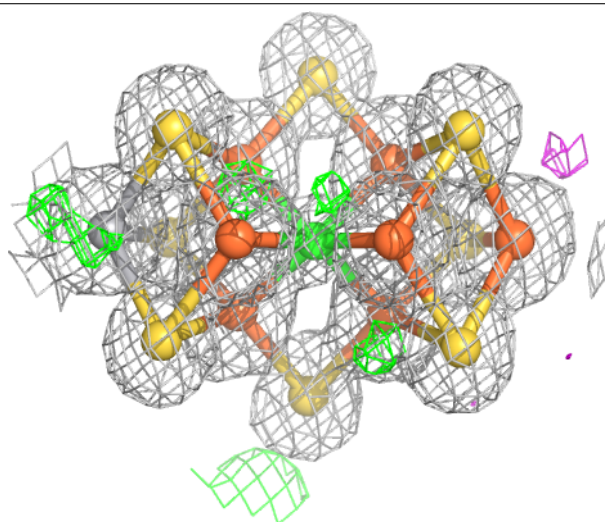
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	E	503	1/1	1.00	0.05	13,13,13,13	0

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.

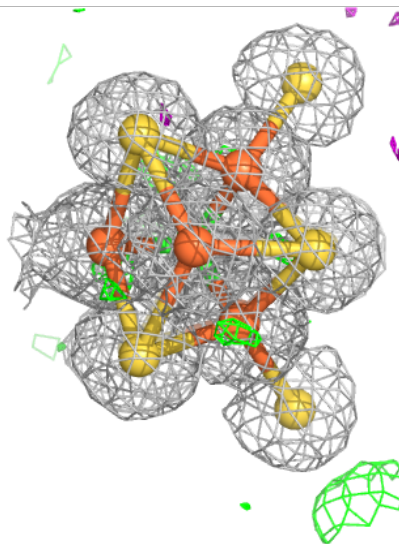
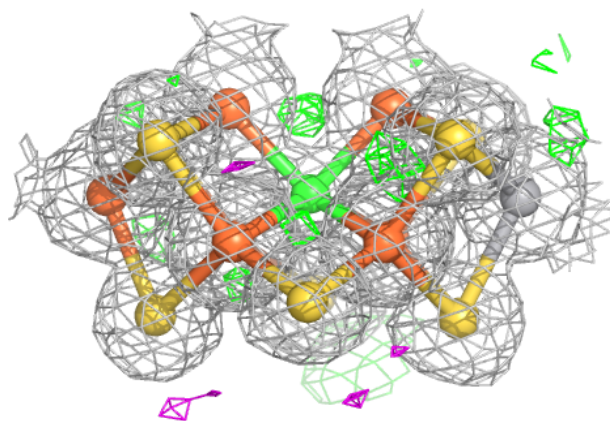
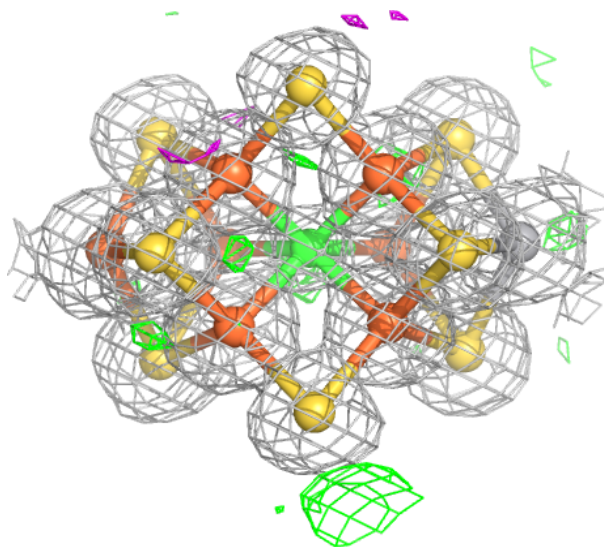
Electron density around 8P8 A 502:

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



Electron density around 8P8 D 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 [i](#)

There are no such residues in this entry.