



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:58 PM UTC

PDB ID : 7AIZ / pdb_00007aiz
Title : Vanadium nitrogenase VFe protein, high CO state
Authors : Rohde, M.; Einsle, O.
Deposited on : 2020-09-28
Resolution : 1.05 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

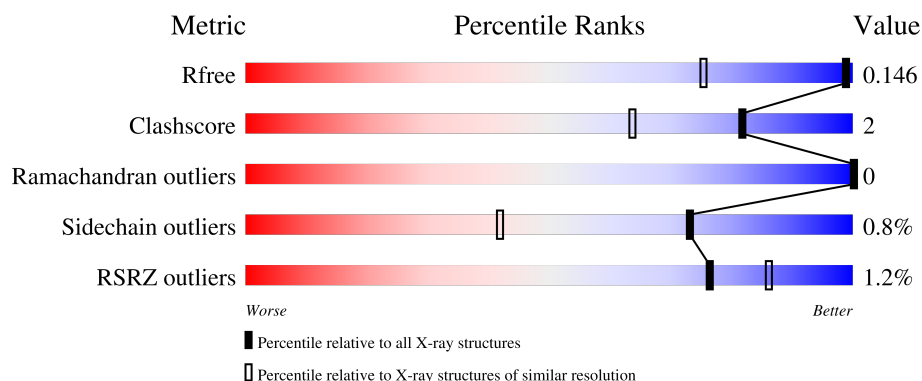
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1182 (1.08-1.04)
Clashscore	190562	1204 (1.08-1.04)
Ramachandran outliers	187476	1175 (1.08-1.04)
Sidechain outliers	187428	1176 (1.08-1.04)
RSRZ outliers	180081	1181 (1.08-1.04)

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	% 92% 7% .
1	D	474	% 91% 7% .
2	B	475	93% 5% .
2	E	475	% 92% 5% ..
3	C	113	95% . ..

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Mol	Chain	Length	Quality of chain
3	F	113	9% 90%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19918 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	11	0
			3871	2466	664	713	28			
1	D	473	Total	C	N	O	S	0	11	0
			3865	2464	658	715	28			

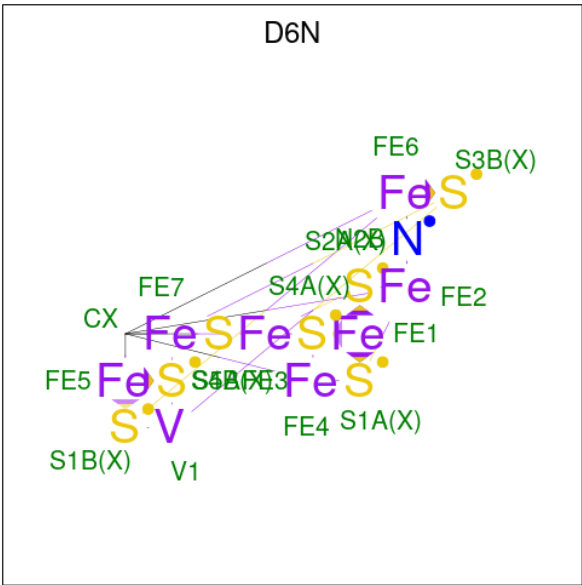
- Molecule 2 is a protein called Nitrogenase vanadium-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	0	12	0
			3721	2367	637	694	23			
2	E	465	Total	C	N	O	S	0	16	0
			3756	2388	645	700	23			

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

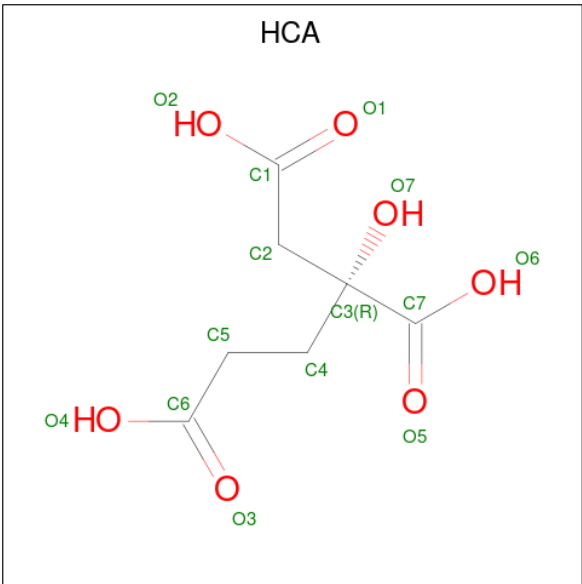
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	112	Total	C	N	O	S	0	2	0
			956	599	173	182	2			
3	F	111	Total	C	N	O	S	0	4	0
			967	605	177	183	2			

- Molecule 4 is FeV (CCD ID: D6N) (formula: CFe₇NS₇V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	S	V	0	0
			16	1	7	7	1		
4	D	1	Total	C	Fe	S	V	0	0
			16	1	7	7	1		

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



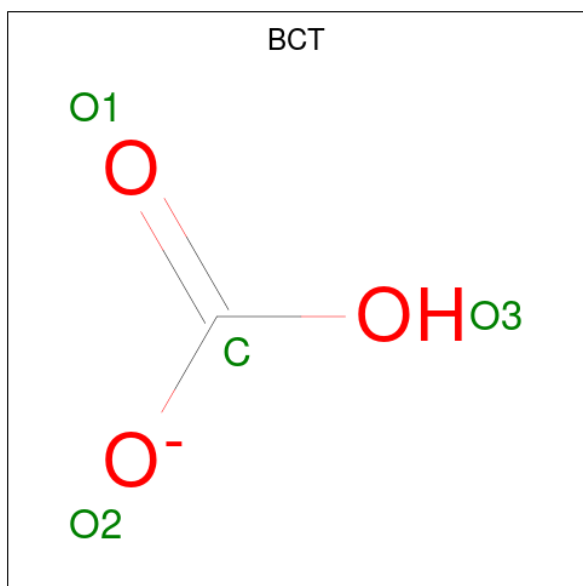
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	7	7		

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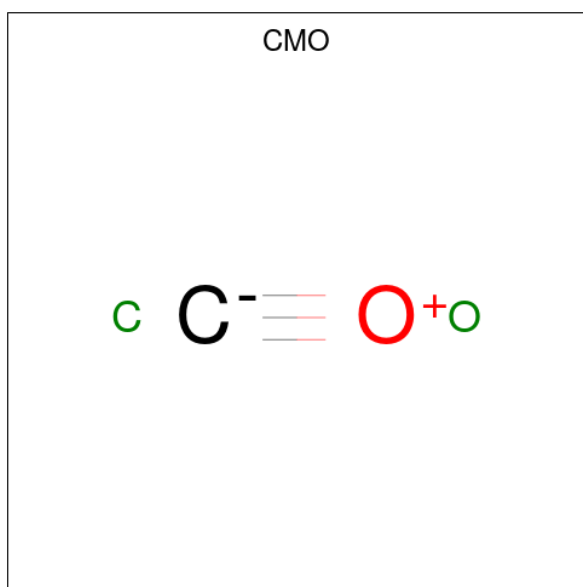
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



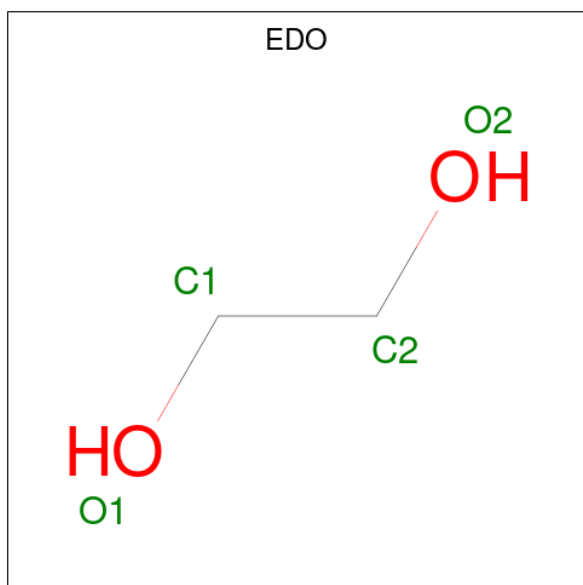
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



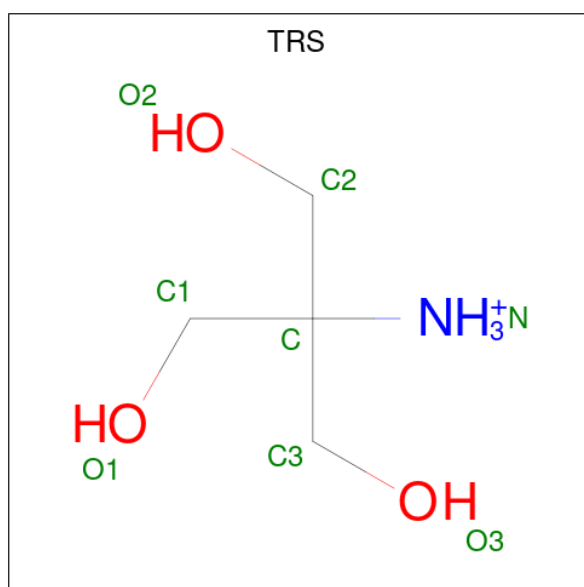
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			2	1	1		
7	A	1	Total	C	O	0	0
			2	1	1		
7	D	1	Total	C	O	0	0
			2	1	1		
7	D	1	Total	C	O	0	0
			2	1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



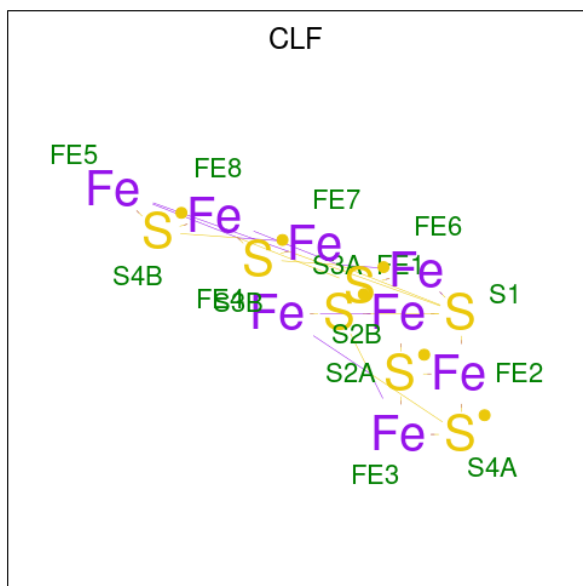
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			8	4	1	3		
9	A	1	Total	C	N	O	0	0
			8	4	1	3		
9	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	1
			16	9	7		
10	E	1	Total	Fe	S	0	1
			16	9	7		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

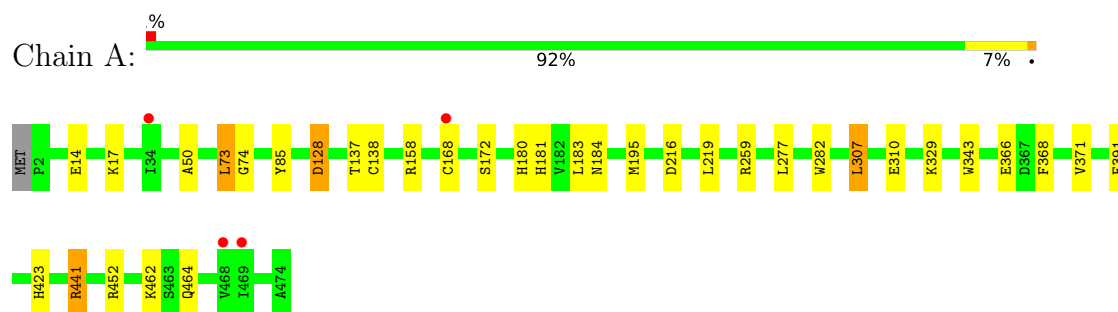
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	529	Total 547	O 547	0	17
12	B	529	Total 549	O 549	0	18
12	C	169	Total 172	O 172	0	4
12	D	550	Total 570	O 570	0	18
12	E	585	Total 623	O 623	0	35
12	F	137	Total 141	O 141	0	4

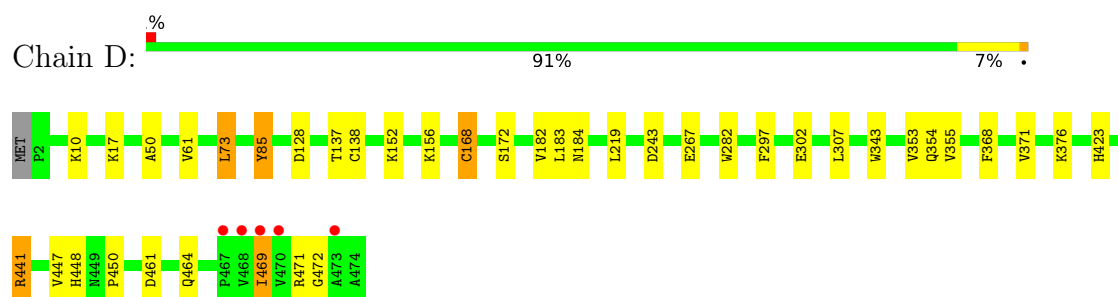
3 Residue-property plots [i](#)

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

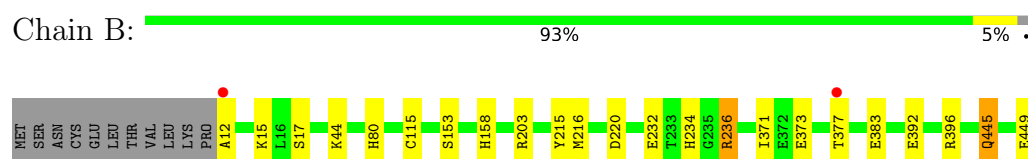
- Molecule 1: Nitrogenase vanadium-iron protein alpha chain



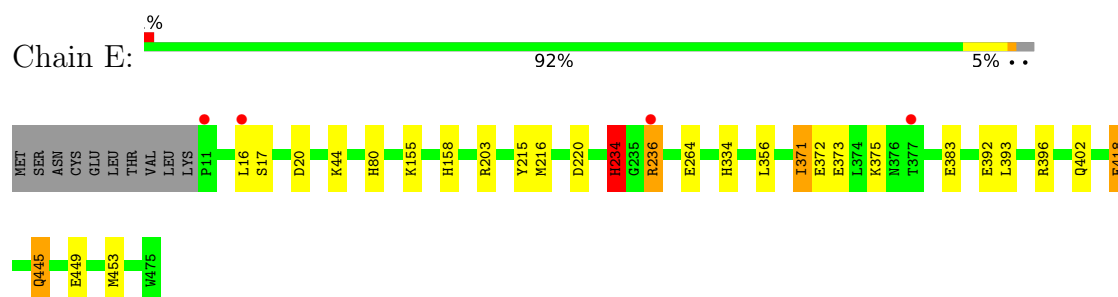
- Molecule 1: Nitrogenase vanadium-iron protein alpha chain



- Molecule 2: Nitrogenase vanadium-iron protein beta chain

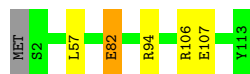


- Molecule 2: Nitrogenase vanadium-iron protein beta chain



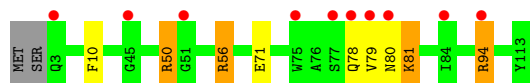
- Molecule 3: Nitrogenase vanadium-iron protein delta chain

Chain C:  95% . ..



- Molecule 3: Nitrogenase vanadium-iron protein delta chain

Chain F:  9% 90% . . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.52Å 80.04Å 107.21Å 84.00° 72.48° 75.03°	Depositor
Resolution (Å)	48.39 – 1.05 48.39 – 1.05	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.39-1.05) 93.2 (48.39-1.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.124 , 0.146 (Not available) , 0.146	Depositor DCC
R_{free} test set	49975 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19918	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 4.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, HCA, MG, TRS, EDO, D6N, CMO, 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	1.09	7/3970 (0.2%)	1.12	10/5363 (0.2%)
1	D	1.04	5/3972 (0.1%)	1.11	5/5366 (0.1%)
2	B	1.04	1/3818 (0.0%)	1.13	11/5165 (0.2%)
2	E	1.08	8/3848 (0.2%)	1.08	10/5206 (0.2%)
3	C	1.09	1/976 (0.1%)	1.15	0/1319
3	F	1.11	1/987 (0.1%)	1.24	2/1333 (0.2%)
All	All	1.07	23/17571 (0.1%)	1.12	38/23752 (0.2%)

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	3
3	F	0	1
All	All	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	ASP	CG-OD1	12.16	1.48	1.25
2	E	375	LYS	C-O	-10.13	1.11	1.24
2	E	396	ARG	NE-CZ	-9.12	1.23	1.33
1	A	441	ARG	CD-NE	-9.06	1.33	1.46
1	A	462	LYS	C-N	8.71	1.46	1.33
2	E	17	SER	CA-CB	-6.96	1.43	1.54
1	D	441	ARG	NE-CZ	-6.93	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	HIS	ND1-CE1	-6.71	1.25	1.32
1	A	172	SER	CB-OG	-6.61	1.28	1.42
1	D	441	ARG	CD-NE	-6.46	1.37	1.46
1	A	181	HIS	CE1-NE2	6.45	1.39	1.32
2	E	373	GLU	CD-OE1	-6.33	1.13	1.25
2	E	234[A]	HIS	CE1-NE2	5.73	1.38	1.32
2	E	234[B]	HIS	CE1-NE2	5.73	1.38	1.32
1	D	172	SER	CB-OG	-5.69	1.30	1.42
3	F	50	ARG	C-O	5.57	1.31	1.24
1	A	172	SER	CA-CB	-5.51	1.44	1.53
2	E	383	GLU	CD-OE1	5.48	1.35	1.25
2	E	392	GLU	CD-OE1	-5.39	1.15	1.25
3	C	82	GLU	CD-OE2	5.25	1.35	1.25
1	D	267	GLU	CD-OE2	-5.24	1.15	1.25
2	B	17	SER	CA-CB	-5.06	1.47	1.54
1	D	472	GLY	C-O	5.05	1.29	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	377	THR	CA-CB-OG1	9.35	123.63	109.60
2	B	449	GLU	CB-CG-CD	8.30	126.71	112.60
1	A	181	HIS	CE1-NE2-CD2	-7.54	101.46	109.00
1	D	184	ASN	CA-CB-CG	7.02	119.62	112.60
1	D	168[A]	CYS	CA-C-N	-6.63	113.46	120.03
1	D	168[A]	CYS	C-N-CA	-6.63	113.46	120.03
1	D	168[B]	CYS	CA-C-N	-6.63	113.46	120.03
1	D	168[B]	CYS	C-N-CA	-6.63	113.46	120.03
1	A	184	ASN	CA-CB-CG	6.57	119.17	112.60
2	E	373	GLU	CB-CG-CD	6.50	123.65	112.60
1	A	172	SER	CB-CA-C	6.37	121.25	109.54
2	B	373	GLU	CB-CG-CD	6.31	123.32	112.60
2	B	158	HIS	CA-CB-CG	5.94	119.74	113.80
1	A	181	HIS	CG-CD2-NE2	5.93	113.14	107.20
2	E	236	ARG	NE-CZ-NH2	-5.79	113.99	119.20
2	B	236	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	180	HIS	CA-CB-CG	5.45	119.25	113.80
2	E	334	HIS	CG-CD2-NE2	5.41	112.61	107.20
1	A	216	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	371[A]	ILE	CB-CA-C	5.37	119.64	112.22
2	B	371[B]	ILE	CB-CA-C	5.37	119.64	112.22
2	B	12	ALA	CA-C-O	-5.36	111.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	373	GLU	O-C-N	-5.36	116.44	122.12
2	E	80	HIS	CA-CB-CG	5.32	119.12	113.80
1	A	14	GLU	CB-CG-CD	5.31	121.63	112.60
2	E	449	GLU	CB-CG-CD	5.27	121.56	112.60
2	E	158	HIS	CA-CB-CG	5.21	119.00	113.80
1	A	391	PHE	CA-CB-CG	5.20	119.00	113.80
2	E	402	GLN	CB-CG-CD	-5.16	103.83	112.60
2	E	371[A]	ILE	CB-CA-C	5.13	119.31	112.22
2	E	371[B]	ILE	CB-CA-C	5.13	119.31	112.22
2	E	20	ASP	CA-CB-CG	5.13	117.73	112.60
3	F	56[A]	ARG	CG-CD-NE	5.08	123.17	112.00
3	F	56[B]	ARG	CG-CD-NE	5.08	123.17	112.00
2	B	236	ARG	NH1-CZ-NH2	5.08	125.90	119.30
2	B	80	HIS	CA-CB-CG	5.03	118.83	113.80
1	A	366[A]	GLU	N-CA-CB	-5.02	102.47	109.94
1	A	366[B]	GLU	N-CA-CB	-5.02	102.47	109.94

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	ARG	Sidechain
2	B	445	GLN	Sidechain
1	D	441	ARG	Sidechain
2	E	234[A]	HIS	Sidechain
2	E	234[B]	HIS	Peptide
2	E	445	GLN	Sidechain
3	F	50	ARG	Mainchain

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	3871	0	3783	17	0
1	D	3865	0	3781	28	0
2	B	3721	0	3706	17	0
2	E	3756	0	3740	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	956	0	915	5	0
3	F	967	0	926	9	0
4	A	16	0	0	0	0
4	D	16	0	0	0	0
5	A	14	0	6	1	0
5	D	14	0	6	1	0
6	A	4	0	0	0	0
6	D	4	0	0	0	0
7	A	4	0	0	0	0
7	D	4	0	0	0	0
8	A	8	0	12	0	0
8	B	12	0	18	0	0
8	C	4	0	6	0	0
8	E	16	0	23	0	0
8	F	4	0	6	0	0
9	A	16	0	24	1	0
9	D	8	0	12	2	0
10	B	16	0	0	0	0
10	E	16	0	0	0	0
11	B	2	0	0	0	0
11	C	1	0	0	0	0
11	F	1	0	0	0	0
12	A	547	0	0	2	0
12	B	549	0	0	2	0
12	C	172	0	0	3	0
12	D	570	0	0	6	0
12	E	623	0	0	5	0
12	F	141	0	0	3	0
All	All	19918	0	16964	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (86) 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:B:392[B]:GLU:OE2	2:B:396[B]:ARG:NH2	1.68	1.26
2:B:392[B]:GLU:CD	2:B:396[B]:ARG:HH22	1.58	1.11
2:B:392[B]:GLU:HG3	2:B:396[B]:ARG:NH2	1.70	1.06
2:B:392[B]:GLU:CG	2:B:396[B]:ARG:NH2	2.19	1.05
1:D:17:LYS:HG3	12:D:901:HOH:O	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:VAL:C	1:D:354[B]:GLN:CA	2.36	0.99
2:B:392[B]:GLU:CG	2:B:396[B]:ARG:HH22	1.72	0.99
2:B:392[B]:GLU:HG3	2:B:396[B]:ARG:HH21	1.38	0.89
2:B:392[B]:GLU:CD	2:B:396[B]:ARG:NH2	2.24	0.88
1:D:168[B]:CYS:HB2	1:D:182[B]:VAL:HG11	1.55	0.88
1:D:354[B]:GLN:CA	1:D:355:VAL:N	2.47	0.77
3:F:78:GLN:HG2	12:F:347:HOH:O	1.86	0.75
2:E:44[B]:LYS:HZ2	2:E:234[B]:HIS:CG	2.05	0.74
1:D:354[C]:GLN:HG3	1:D:376:LYS:HE2	1.78	0.65
1:A:73:LEU:C	1:A:73:LEU:HD22	2.22	0.65
3:F:94[A]:ARG:CG	3:F:94[A]:ARG:HH21	2.10	0.65
1:D:168[B]:CYS:CB	1:D:182[B]:VAL:HG11	2.27	0.65
3:C:107[A]:GLU:OE2	12:C:302:HOH:O	2.15	0.64
3:F:94[A]:ARG:HH21	3:F:94[A]:ARG:HG3	1.63	0.61
1:A:307:LEU:C	1:A:307:LEU:HD23	2.26	0.61
1:D:152[B]:LYS:HG3	12:D:1010:HOH:O	2.00	0.60
1:A:452:ARG:HD2	12:A:787:HOH:O	2.01	0.60
1:D:307:LEU:C	1:D:307:LEU:HD23	2.28	0.59
2:B:44[B]:LYS:HZ2	2:B:234[B]:HIS:CG	2.20	0.58
2:E:372:GLU:HB2	12:E:699[B]:HOH:O	2.04	0.57
1:A:310:GLU:HG3	12:A:921:HOH:O	2.04	0.57
2:E:418[A]:GLU:HG2	12:E:993[A]:HOH:O	2.04	0.56
2:B:392[B]:GLU:OE2	2:B:396[B]:ARG:CZ	2.50	0.56
2:B:15:LYS:HE2	2:B:383[B]:GLU:OE1	2.05	0.56
3:F:79:VAL:O	12:F:302:HOH:O	2.18	0.55
1:A:50:ALA:HB1	1:A:168[B]:CYS:SG	2.48	0.54
1:D:73:LEU:HD22	1:D:73:LEU:C	2.33	0.54
2:B:220:ASP:OD2	2:B:236:ARG:NE	2.27	0.53
3:C:94:ARG:HD3	12:C:400:HOH:O	2.09	0.52
12:B:724:HOH:O	1:D:464:GLN:HB2	2.09	0.52
3:F:81:LYS:CD	3:F:81:LYS:C	2.82	0.52
1:D:243:ASP:OD2	12:D:601:HOH:O	2.19	0.52
1:D:128[B]:ASP:OD1	9:D:506:TRS:O3	2.24	0.52
12:D:805:HOH:O	2:E:155:LYS:HE3	2.09	0.51
1:A:128:ASP:OD2	9:A:509:TRS:O1	2.27	0.51
1:A:464:GLN:HB2	12:E:801:HOH:O	2.11	0.50
3:F:10:PHE:CD1	3:F:94[A]:ARG:HG2	2.47	0.50
3:C:106[B]:ARG:NH1	12:C:304:HOH:O	2.44	0.49
2:E:264:GLU:HG2	12:E:968:HOH:O	2.12	0.49
1:D:128[B]:ASP:OD2	9:D:506:TRS:O2	2.22	0.49
1:D:302:GLU:HG3	12:D:979:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447[A]:VAL:HG23	1:D:448:HIS:ND1	2.28	0.47
2:E:453[B]:MET:HE2	2:E:453[B]:MET:HB2	1.70	0.47
1:D:219:LEU:C	1:D:219:LEU:HD23	2.40	0.47
1:D:423:HIS:HB3	5:D:502:HCA:O6	2.16	0.46
2:E:234[A]:HIS:CD2	12:E:639:HOH:O	2.67	0.46
2:E:16:LEU:HD21	2:E:371[B]:ILE:HD13	1.98	0.46
1:D:282:TRP:CG	1:D:343:TRP:HE1	2.35	0.45
1:D:461:ASP:C	1:D:461:ASP:OD1	2.60	0.45
1:D:450:PRO:HD3	1:D:471:ARG:HD2	1.99	0.45
1:A:183:LEU:C	1:A:183:LEU:HD23	2.42	0.45
3:F:80:ASN:C	12:F:302:HOH:O	2.60	0.45
1:D:183:LEU:C	1:D:183:LEU:HD23	2.42	0.45
1:A:368:PHE:HA	1:A:371:VAL:HG12	1.98	0.44
1:D:368:PHE:HA	1:D:371:VAL:HG12	2.00	0.44
1:A:423:HIS:HB3	5:A:502:HCA:O5	2.18	0.44
2:B:453[B]:MET:HE2	2:B:453[B]:MET:HB2	1.59	0.44
1:A:17[A]:LYS:HD3	1:A:17[A]:LYS:HA	1.83	0.44
1:A:73:LEU:HD22	1:A:74:GLY:N	2.33	0.43
2:B:234[B]:HIS:HB2	2:B:236:ARG:NH1	2.33	0.43
1:D:50:ALA:HB1	1:D:168[B]:CYS:SG	2.58	0.43
2:E:356[B]:LEU:HD11	2:E:393:LEU:HB2	1.99	0.43
1:D:137:THR:O	1:D:138:CYS:C	2.61	0.43
3:F:94[A]:ARG:CG	3:F:94[A]:ARG:NH2	2.73	0.43
1:D:61:VAL:HG22	1:D:85:TYR:CE2	2.54	0.43
1:A:282:TRP:CG	1:A:343:TRP:HE1	2.37	0.42
2:B:203:ARG:HH22	2:B:445:GLN:HE21	1.68	0.42
2:E:203:ARG:HH22	2:E:445:GLN:HE21	1.67	0.42
2:B:115:CYS:HB3	2:B:153:SER:OG	2.20	0.42
1:A:137:THR:O	1:A:138:CYS:C	2.62	0.42
1:A:219:LEU:C	1:A:219:LEU:HD23	2.44	0.42
1:D:469:ILE:HG23	12:D:977:HOH:O	2.18	0.42
2:E:220:ASP:OD2	2:E:236:ARG:NE	2.51	0.41
1:D:297:PHE:O	3:F:56[B]:ARG:HD2	2.21	0.41
3:C:82:GLU:CD	3:C:82:GLU:H	2.29	0.41
1:A:277:LEU:HD13	3:C:57:LEU:HD11	2.03	0.41
2:B:232:GLU:HG2	12:B:908:HOH:O	2.21	0.41
2:E:215:TYR:HA	2:E:216:MET:HA	1.88	0.41
1:A:259:ARG:CZ	1:A:259:ARG:HA	2.51	0.40
2:B:215:TYR:HA	2:B:216:MET:HA	1.87	0.40

There are no symmetry-related clashes.

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	482/474 (102%)	465 (96%)	17 (4%)	0	100	100
1	D	483/474 (102%)	469 (97%)	14 (3%)	0	100	100
2	B	475/475 (100%)	467 (98%)	8 (2%)	0	100	100
2	E	479/475 (101%)	470 (98%)	9 (2%)	0	100	100
3	C	112/113 (99%)	107 (96%)	5 (4%)	0	100	100
3	F	113/113 (100%)	111 (98%)	2 (2%)	0	100	100
All	All	2144/2124 (101%)	2089 (97%)	55 (3%)	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	414/404 (102%)	407 (98%)	7 (2%)	53	16
1	D	415/404 (103%)	410 (99%)	5 (1%)	63	26
2	B	400/398 (100%)	400 (100%)	0	100	100
2	E	404/398 (102%)	402 (100%)	2 (0%)	81	58
3	C	103/102 (101%)	103 (100%)	0	100	100
3	F	104/102 (102%)	100 (96%)	4 (4%)	29	2
All	All	1840/1808 (102%)	1822 (99%)	18 (1%)	73	36

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	85	TYR
1	A	158	ARG
1	A	195[A]	MET
1	A	195[B]	MET
1	A	307	LEU
1	A	329	LYS
1	D	10	LYS
1	D	73	LEU
1	D	85	TYR
1	D	156	LYS
1	D	469	ILE
2	E	418[A]	GLU
2	E	418[B]	GLU
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	54	GLN
2	B	278	ASN
2	B	285	ASN
2	B	445	GLN
3	C	54	GLN
3	C	110	HIS
3	C	111	HIS
1	D	25	ASN
2	E	54	GLN
2	E	278	ASN
2	E	285	ASN
2	E	445	GLN
3	F	80	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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
7	CMO	A	505	-	0,1,1	-	-	-		
5	HCA	A	502	4	13,13,13	1.32	2 (15%)	15,18,18	1.53	3 (20%)
9	TRS	A	508	-	7,7,7	0.25	0	9,9,9	0.60	0
4	D6N	A	501	5,1,6,7	4,26,28	0.96	0	-		
7	CMO	D	504	4	0,1,1	-	-	-		
7	CMO	A	504	4	0,1,1	-	-	-		
8	EDO	E	504	-	3,3,3	0.52	0	2,2,2	0.19	0
8	EDO	F	202	-	3,3,3	0.71	0	2,2,2	0.32	0
5	HCA	D	502	4	13,13,13	0.96	1 (7%)	15,18,18	1.49	3 (20%)
8	EDO	B	504	-	3,3,3	0.67	0	2,2,2	0.34	0
6	BCT	A	503	4	3,3,3	0.31	0	2,3,3	1.02	0
7	CMO	D	505	-	0,1,1	-	-	-		
6	BCT	D	503	4	3,3,3	1.43	1 (33%)	2,3,3	1.39	0
8	EDO	B	506	-	3,3,3	0.69	0	2,2,2	0.17	0
8	EDO	A	506	-	3,3,3	0.37	0	2,2,2	0.50	0
9	TRS	D	506	-	7,7,7	0.31	0	9,9,9	0.57	0
10	CLF	B	501[A]	2	0,24,24	-	-	-		
10	CLF	B	501[B]	2	0,24,24	-	-	-		
4	D6N	D	501	5,1,6,7	4,26,28	1.03	0	-		
8	EDO	E	505	-	3,3,3	0.76	0	2,2,2	0.51	0
8	EDO	B	505	-	3,3,3	0.35	0	2,2,2	0.37	0
10	CLF	E	501[A]	2	0,24,24	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	E	503	-	3,3,3	0.18	0	2,2,2	0.32	0
8	EDO	C	202	-	3,3,3	0.88	0	2,2,2	0.20	0
8	EDO	E	502	-	3,3,3	0.87	0	2,2,2	0.10	0
9	TRS	A	509	-	7,7,7	0.27	0	9,9,9	0.33	0
10	CLF	E	501[B]	2	0,24,24	-	-	-	-	-
8	EDO	A	507	-	3,3,3	0.41	0	2,2,2	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HCA	A	502	4	-	2/17/17/17	-
9	TRS	A	508	-	-	0/9/9/9	-
8	EDO	E	504	-	-	0/1/1/1	-
8	EDO	F	202	-	-	0/1/1/1	-
5	HCA	D	502	4	-	2/17/17/17	-
8	EDO	B	504	-	-	0/1/1/1	-
8	EDO	B	506	-	-	0/1/1/1	-
8	EDO	A	506	-	-	0/1/1/1	-
9	TRS	D	506	-	-	2/9/9/9	-
10	CLF	B	501[A]	2	-	-	0/12/10/10
10	CLF	B	501[B]	2	-	-	0/12/10/10
8	EDO	E	505	-	-	0/1/1/1	-
8	EDO	B	505	-	-	0/1/1/1	-
10	CLF	E	501[A]	2	-	-	0/12/10/10
8	EDO	E	503	-	-	0/1/1/1	-
8	EDO	C	202	-	-	0/1/1/1	-
8	EDO	E	502	-	-	0/1/1/1	-
9	TRS	A	509	-	-	3/9/9/9	-
10	CLF	E	501[B]	2	-	-	0/12/10/10
8	EDO	A	507	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	HCA	O1-C1	2.53	1.30	1.22
6	D	503	BCT	O1-C	2.20	1.33	1.25
5	D	502	HCA	O4-C6	-2.16	1.23	1.30
5	A	502	HCA	O2-C1	-2.08	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	HCA	O5-C7-C3	-3.29	115.71	122.09
5	D	502	HCA	O6-C7-C3	3.23	119.34	113.14
5	A	502	HCA	O1-C1-C2	-3.18	113.94	122.95
5	A	502	HCA	O6-C7-C3	2.63	118.19	113.14
5	D	502	HCA	O7-C3-C7	-2.16	105.90	108.96
5	A	502	HCA	O2-C1-C2	2.09	120.98	114.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	509	TRS	N-C-C3-O3
9	A	509	TRS	C2-C-C3-O3
9	A	509	TRS	C1-C-C3-O3
9	D	506	TRS	C3-C-C1-O1
5	A	502	HCA	C4-C5-C6-O4
5	D	502	HCA	C4-C5-C6-O3
5	A	502	HCA	C4-C5-C6-O3
5	D	502	HCA	C4-C5-C6-O4
9	D	506	TRS	N-C-C1-O1

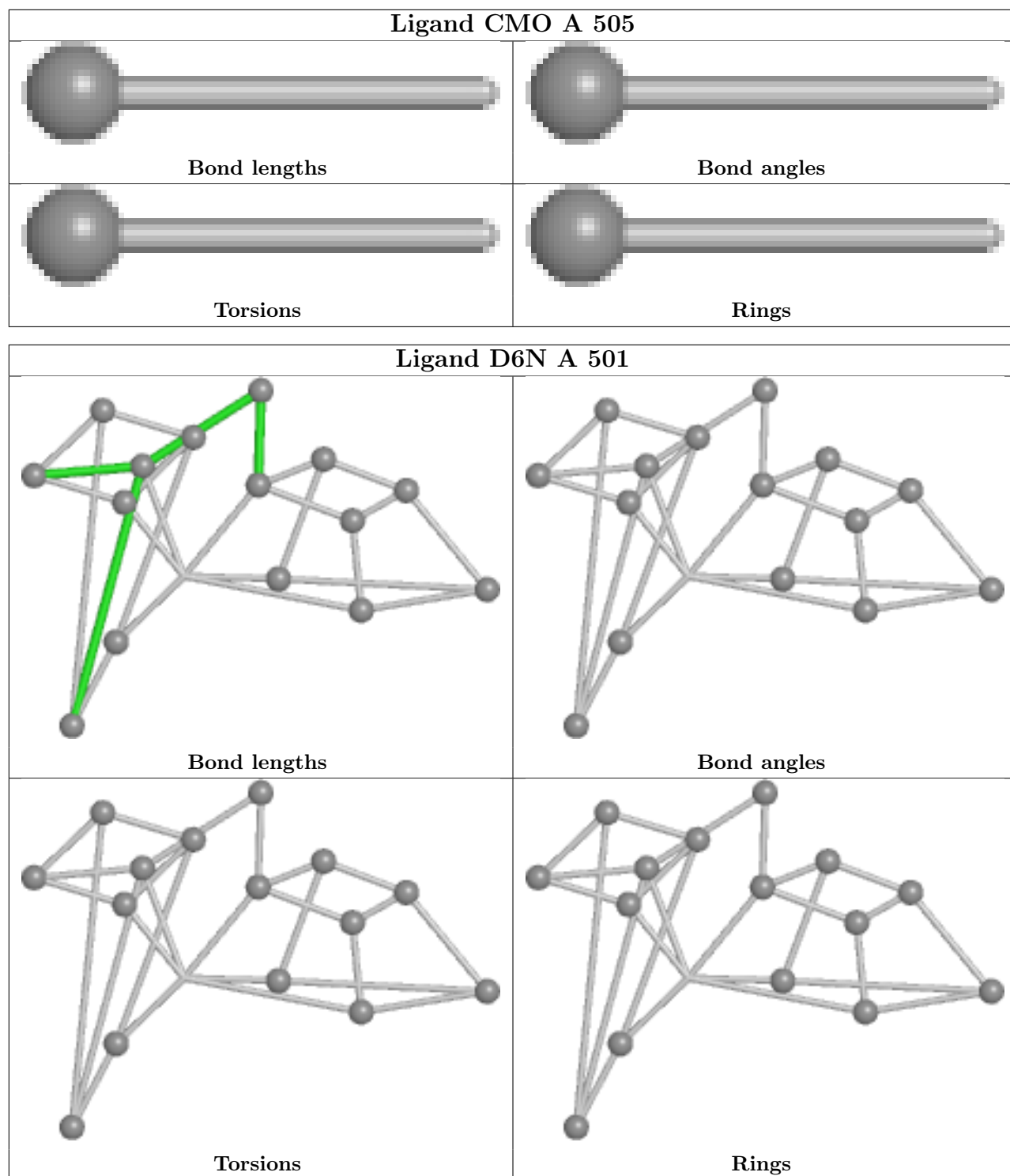
There are no ring outliers.

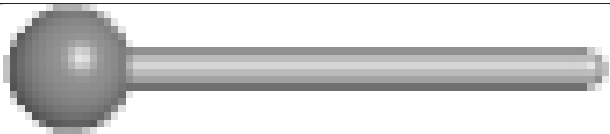
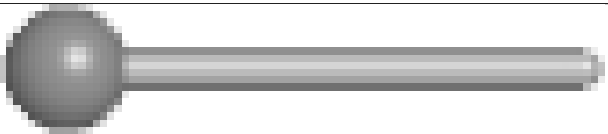
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	HCA	1	0
5	D	502	HCA	1	0
9	D	506	TRS	2	0
9	A	509	TRS	1	0

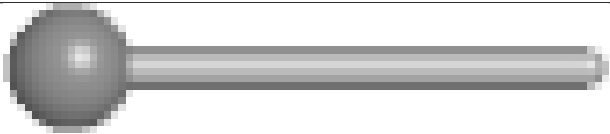
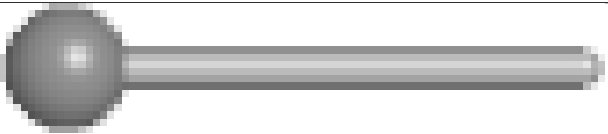
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

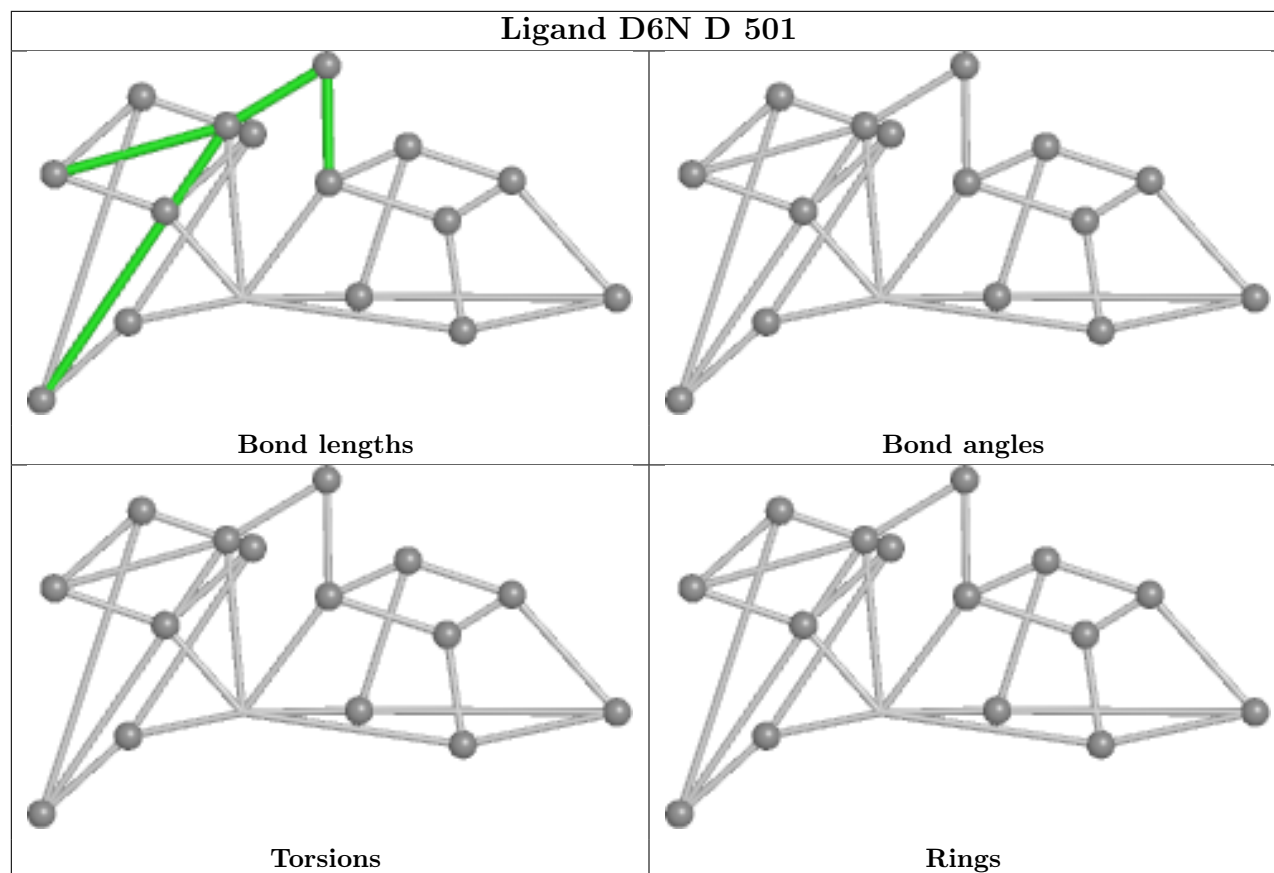
equivalents in the CSD to analyse the geometry.



Ligand CMO D 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CMO A 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CMO D 505	
 Bond lengths	 Bond angles
 Torsions	 Rings



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%)	-0.25	4 (0%) 82 91	6, 13, 23, 41	11 (2%)
1	D	473/474 (99%)	-0.30	5 (1%) 78 88	5, 12, 24, 41	11 (2%)
2	B	464/475 (97%)	-0.26	2 (0%) 88 94	5, 13, 24, 66	12 (2%)
2	E	465/475 (97%)	-0.38	4 (0%) 81 90	5, 11, 21, 39	16 (3%)
3	C	112/113 (99%)	-0.02	0 100 100	8, 16, 26, 38	2 (1%)
3	F	111/113 (98%)	0.46	10 (9%) 15 18	7, 18, 40, 54	4 (3%)
All	All	2098/2124 (98%)	-0.24	25 (1%) 76 86	5, 12, 25, 66	56 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	12	ALA	7.3
2	B	377	THR	6.3
1	A	168[A]	CYS	5.6
3	F	84	ILE	4.9
3	F	79	VAL	4.8
1	D	468	VAL	4.2
3	F	78	GLN	3.7
3	F	80	ASN	3.6
1	A	468	VAL	3.3
1	D	470	VAL	3.3
1	D	469	ILE	3.2
3	F	75	TRP	2.8
2	E	11	PRO	2.7
2	E	377	THR	2.7
2	E	236	ARG	2.5
2	E	16	LEU	2.5
1	D	473	ALA	2.5
3	F	51	GLY	2.4
1	D	467	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	3	GLN	2.3
1	A	469	ILE	2.3
3	F	45	GLY	2.2
1	A	34	ILE	2.1
3	F	94[A]	ARG	2.1
3	F	77	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	EDO	E	505	4/4	0.84	0.13	22,25,27,28	0
8	EDO	C	202	4/4	0.86	0.19	13,13,14,14	4
9	TRS	A	509	8/8	0.90	0.11	29,38,43,47	0
9	TRS	D	506	8/8	0.90	0.09	25,30,33,38	0
8	EDO	A	506	4/4	0.91	0.13	17,18,19,22	4
8	EDO	F	202	4/4	0.91	0.12	17,18,18,20	4
9	TRS	A	508	8/8	0.94	0.08	18,22,26,27	0
8	EDO	A	507	4/4	0.95	0.10	12,15,17,18	4
8	EDO	B	504	4/4	0.95	0.07	16,18,18,18	0
8	EDO	B	506	4/4	0.95	0.07	21,22,23,26	0
8	EDO	E	503	4/4	0.96	0.07	14,15,15,16	0
7	CMO	A	505	2/2	0.96	0.08	11,11,11,12	2
8	EDO	B	505	4/4	0.96	0.07	16,21,23,23	0
7	CMO	A	504	2/2	0.97	0.08	9,9,9,20	0
7	CMO	D	504	2/2	0.97	0.07	7,7,7,14	0
8	EDO	E	504	4/4	0.98	0.05	13,16,17,18	4
8	EDO	E	502	4/4	0.98	0.06	17,18,18,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CMO	D	505	2/2	0.99	0.08	8,8,8,11	2
5	HCA	D	502	14/14	0.99	0.03	7,8,12,13	0
5	HCA	A	502	14/14	0.99	0.03	8,9,12,14	0
11	MG	F	201	1/1	0.99	0.08	16,16,16,16	0
6	BCT	D	503	4/4	1.00	0.04	8,8,8,9	0
4	D6N	A	501	16/17	1.00	0.01	8,9,10,10	0
4	D6N	D	501	16/17	1.00	0.01	7,8,9,9	0
10	CLF	B	501[A]	15/15	1.00	0.01	8,9,10,10	1
10	CLF	B	501[B]	15/15	1.00	0.01	9,10,10,14	1
10	CLF	E	501[A]	15/15	1.00	0.01	7,8,8,8	1
10	CLF	E	501[B]	15/15	1.00	0.01	7,8,8,8	1
11	MG	B	502	1/1	1.00	0.02	10,10,10,10	0
11	MG	B	503	1/1	1.00	0.03	9,9,9,9	0
11	MG	C	201	1/1	1.00	0.05	15,15,15,15	0
6	BCT	A	503	4/4	1.00	0.02	9,9,9,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.