



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 1M1N / pdb_00001m1n
Title : Nitrogenase MoFe protein from Azotobacter vinelandii
Authors : Einsle, O.; Tezcan, F.A.; Andrade, S.L.A.; Schmid, B.; Yoshida, M.; Howard, J.B.; Rees, D.C.
Deposited on : 2002-06-19
Resolution : 1.16 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

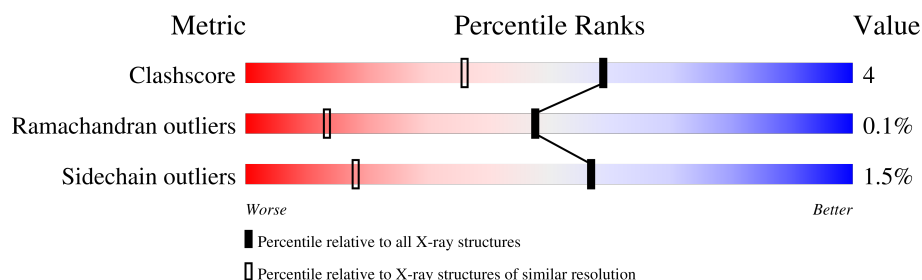
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.16 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))
Clashscore	190562	1272 (1.18-1.14)
Ramachandran outliers	187476	1246 (1.18-1.14)
Sidechain outliers	187428	1246 (1.18-1.14)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	88% 8% . .
1	C	491	84% 11% . .
1	E	491	88% 8% .
1	G	491	85% 10% . .
2	B	522	89% 9% .
2	D	522	89% 9% .
2	F	522	89% 10% .
2	H	522	88% 11% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 37384 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

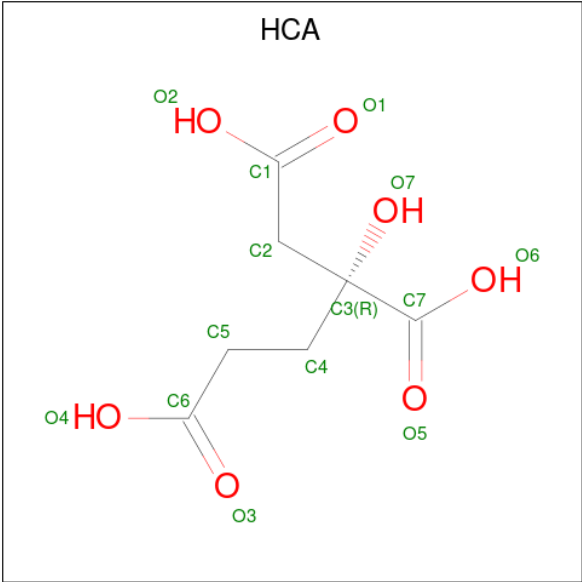
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	6	0
			3810	2423	647	713	27			
1	C	477	Total	C	N	O	S	0	6	0
			3814	2424	652	710	28			
1	E	477	Total	C	N	O	S	0	7	0
			3815	2426	647	715	27			
1	G	477	Total	C	N	O	S	0	7	0
			3819	2428	653	710	28			

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

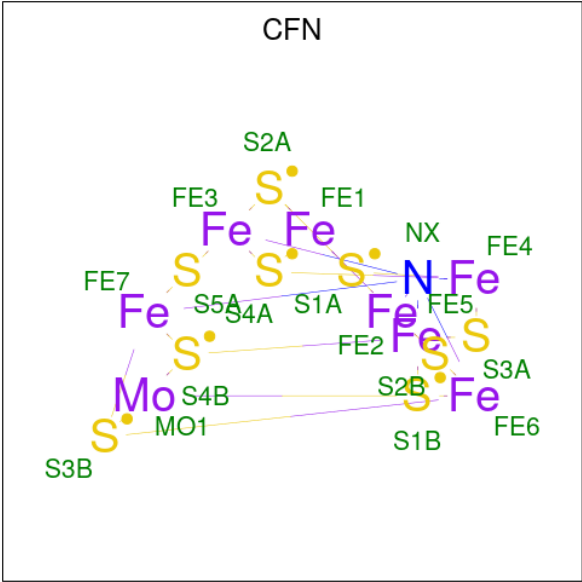
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	18	0
			4236	2710	707	784	35			
2	D	522	Total	C	N	O	S	0	15	0
			4225	2701	707	782	35			
2	F	522	Total	C	N	O	S	0	17	0
			4234	2709	707	783	35			
2	H	522	Total	C	N	O	S	0	13	0
			4218	2696	707	780	35			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		
3	E	1	Total	C	O	0	0
			14	7	7		
3	G	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is FE(7)-MO-S(9)-N CLUSTER (CCD ID: CFN) (formula: Fe₇MoNS₉).

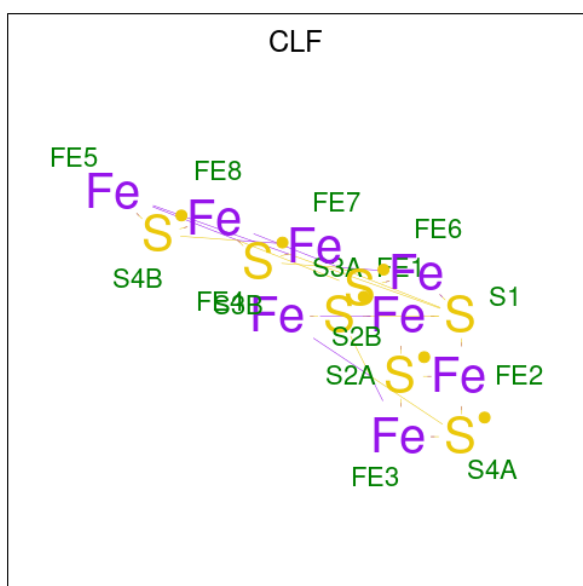


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		
4	C	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		
4	E	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		
4	G	1	Total	Fe	Mo	N	S	0	0
			18	7	1	1	9		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	Fe	S	0	0
			15	8	7		
6	H	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	553	Total	O	0	0
			553	553		
7	B	723	Total	O	0	0
			723	723		
7	C	570	Total	O	0	0
			570	570		
7	D	704	Total	O	0	0
			704	704		
7	E	536	Total	O	0	0
			536	536		
7	F	708	Total	O	0	0
			708	708		
7	G	533	Total	O	0	0
			533	533		
7	H	694	Total	O	0	0
			694	694		

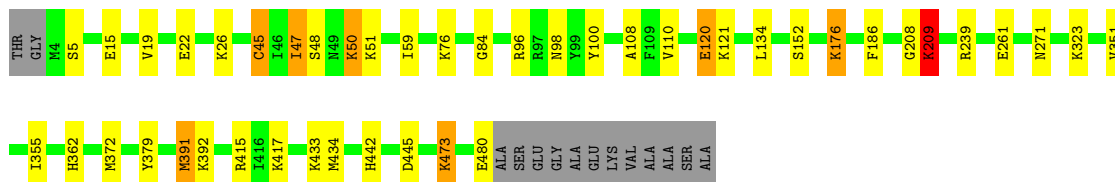
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

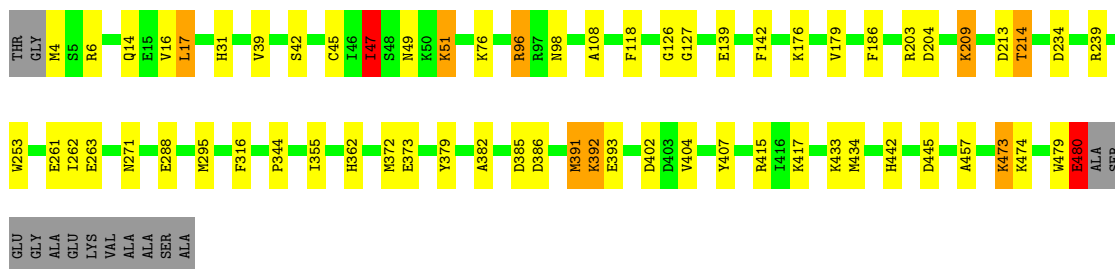
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain A: 



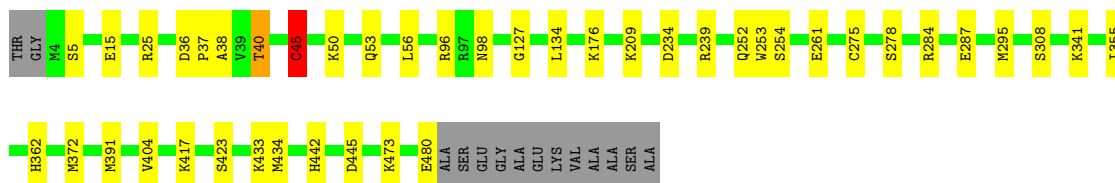
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain C: 



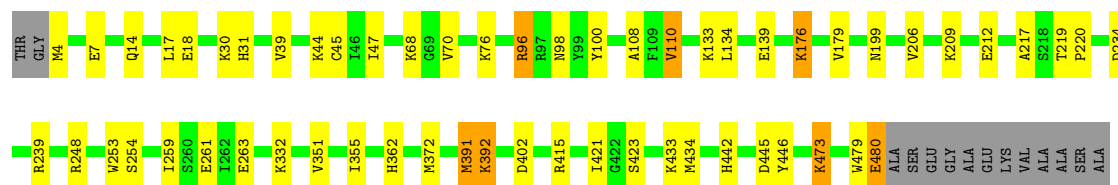
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain E: 



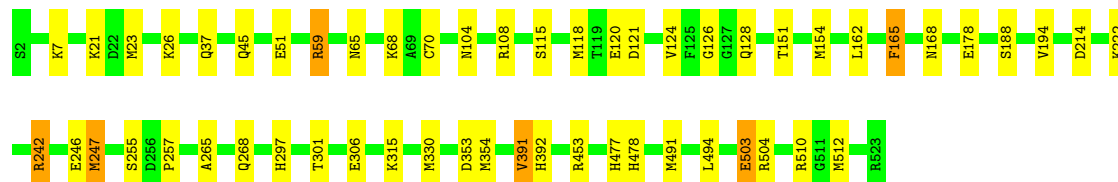
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain G: 



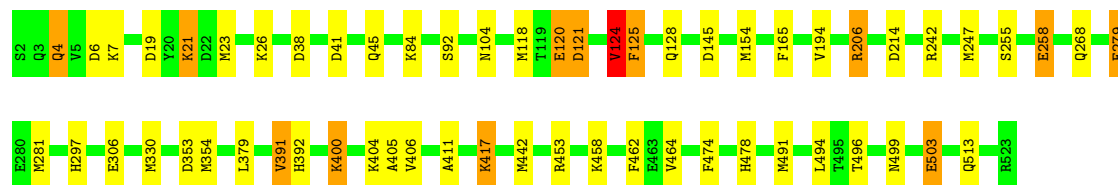
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B: 89% 9% .



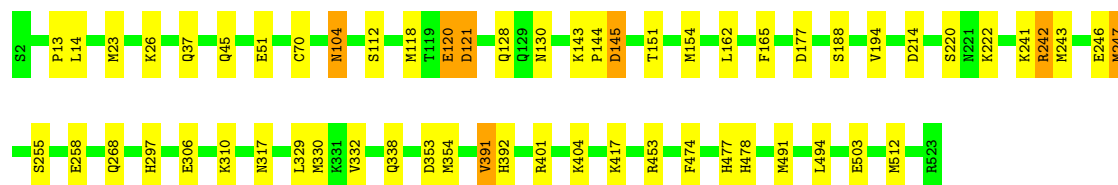
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D: 89% 9% .



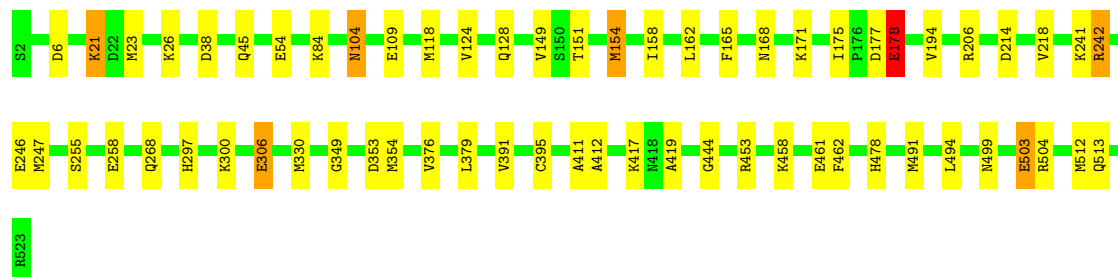
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain F: 89% 10% .



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain H: 88% 11% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.31Å 131.63Å 159.16Å 90.00° 108.37° 90.00°	Depositor
Resolution (Å)	50.00 – 1.16	Depositor
% Data completeness (in resolution range)	95.6 (50.00-1.16)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.123 , 0.149	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	37384	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CLF, CFN, HCA

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	1.48	15/3922 (0.4%)	1.27	10/5286 (0.2%)
1	C	1.52	26/3926 (0.7%)	1.29	18/5291 (0.3%)
1	E	1.48	12/3931 (0.3%)	1.28	10/5298 (0.2%)
1	G	1.43	16/3935 (0.4%)	1.23	7/5302 (0.1%)
2	B	1.53	24/4414 (0.5%)	1.25	15/5960 (0.3%)
2	D	1.52	29/4391 (0.7%)	1.29	11/5930 (0.2%)
2	F	1.44	15/4408 (0.3%)	1.19	9/5952 (0.2%)
2	H	1.46	22/4376 (0.5%)	1.23	16/5909 (0.3%)
All	All	1.48	159/33303 (0.5%)	1.25	96/44928 (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	2
1	C	0	2
1	E	0	1
1	G	0	2
2	B	0	3
2	H	0	1
All	All	0	11

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	MET	SD-CE	-21.04	1.26	1.79
2	F	330	MET	SD-CE	-17.33	1.36	1.79
2	H	330	MET	SD-CE	-16.75	1.37	1.79
1	E	434	MET	SD-CE	-16.54	1.38	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	330	MET	SD-CE	-16.35	1.38	1.79
1	C	434	MET	SD-CE	-15.95	1.39	1.79
2	D	491	MET	SD-CE	-15.24	1.41	1.79
2	B	491	MET	SD-CE	-14.52	1.43	1.79
1	A	434	MET	SD-CE	-12.68	1.47	1.79
2	B	65	ASN	C-O	-12.46	1.18	1.23
2	B	247[A]	MET	SD-CE	-11.91	1.49	1.79
2	B	247[B]	MET	SD-CE	-11.91	1.49	1.79
1	C	391	MET	CG-SD	-11.81	1.51	1.80
1	G	391	MET	CG-SD	-10.29	1.55	1.80
2	D	453	ARG	NE-CZ	9.49	1.43	1.33
1	A	417	LYS	C-O	-9.43	1.19	1.23
2	F	247[A]	MET	SD-CE	8.90	2.01	1.79
2	F	247[B]	MET	SD-CE	8.90	2.01	1.79
1	G	434	MET	SD-CE	-8.87	1.57	1.79
2	F	491	MET	SD-CE	-8.84	1.57	1.79
1	E	372	MET	SD-CE	-8.50	1.58	1.79
2	D	247	MET	SD-CE	-8.37	1.58	1.79
2	H	491	MET	SD-CE	-8.30	1.58	1.79
1	C	372	MET	SD-CE	-8.19	1.59	1.79
2	B	121	ASP	C-O	8.16	1.33	1.24
1	C	391	MET	CB-CG	7.88	1.76	1.52
1	A	391	MET	CG-SD	-7.75	1.61	1.80
2	F	453	ARG	NE-CZ	7.61	1.41	1.33
1	C	17	LEU	CG-CD2	-7.28	1.28	1.52
1	C	186	PHE	CA-CB	7.28	1.66	1.53
1	A	51	LYS	CB-CG	-7.11	1.31	1.52
1	G	217	ALA	CA-CB	7.08	1.62	1.52
2	B	222	LYS	CD-CE	7.06	1.73	1.52
1	G	17	LEU	CG-CD2	-6.96	1.29	1.52
1	C	209	LYS	CE-NZ	6.71	1.69	1.49
2	B	268	GLN	CB-CG	-6.64	1.32	1.52
2	B	121	ASP	CA-C	6.62	1.61	1.52
2	B	453	ARG	NE-CZ	6.57	1.40	1.33
2	D	92	SER	CB-OG	-6.42	1.29	1.42
2	H	453	ARG	NE-CZ	6.41	1.40	1.33
1	A	261	GLU	CB-CG	-6.39	1.33	1.52
1	A	19	VAL	CA-CB	6.37	1.63	1.54
2	H	268	GLN	CB-CG	-6.37	1.33	1.52
1	C	261	GLU	CA-C	-6.35	1.44	1.52
1	E	261	GLU	CB-CG	-6.33	1.33	1.52
1	E	423	SER	CA-CB	-6.32	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	404	VAL	CA-CB	6.30	1.60	1.54
2	H	412	ALA	CA-CB	-6.27	1.42	1.53
2	D	411	ALA	CA-C	-6.26	1.44	1.52
1	E	295	MET	SD-CE	-6.25	1.64	1.79
2	D	391[A]	VAL	CA-CB	-6.15	1.46	1.54
2	D	391[B]	VAL	CA-CB	-6.15	1.46	1.54
2	D	491	MET	CG-SD	6.14	1.96	1.80
2	D	145	ASP	CB-CG	6.13	1.67	1.52
1	A	59	ILE	CA-CB	6.13	1.62	1.54
1	C	214	THR	CA-CB	6.09	1.61	1.53
2	F	242	ARG	CG-CD	-6.09	1.34	1.52
2	D	503	GLU	CD-OE1	6.08	1.36	1.25
2	D	281[A]	MET	SD-CE	6.07	1.94	1.79
2	D	281[B]	MET	SD-CE	6.07	1.94	1.79
2	F	391[A]	VAL	CA-CB	-6.03	1.46	1.54
2	F	391[B]	VAL	CA-CB	-6.03	1.46	1.54
2	H	247	MET	CB-CG	-6.03	1.34	1.52
2	D	7	LYS	CA-CB	-6.00	1.47	1.53
1	G	433	LYS	CG-CD	-6.00	1.34	1.52
2	D	6	ASP	CG-OD1	5.99	1.36	1.25
1	E	308	SER	N-CA	-5.97	1.39	1.46
2	D	268	GLN	CB-CG	-5.94	1.34	1.52
2	B	242	ARG	CG-CD	-5.94	1.34	1.52
2	B	391[A]	VAL	CA-CB	-5.93	1.46	1.54
2	B	391[B]	VAL	CA-CB	-5.93	1.46	1.54
2	H	158	ILE	CA-CB	-5.91	1.47	1.54
1	C	433	LYS	CG-CD	-5.85	1.34	1.52
1	C	393	GLU	CD-OE1	5.82	1.36	1.25
1	A	209	LYS	CG-CD	5.81	1.69	1.52
1	G	332	LYS	CD-CE	5.80	1.69	1.52
2	B	491	MET	CG-SD	5.80	1.95	1.80
1	C	407	TYR	CZ-OH	5.79	1.50	1.38
1	A	433	LYS	CG-CD	-5.78	1.35	1.52
1	A	271	ASN	CG-OD1	5.77	1.34	1.23
2	B	126	GLY	CA-C	-5.75	1.46	1.52
1	G	179	VAL	CA-CB	5.72	1.59	1.53
2	H	349	GLY	CA-C	5.70	1.59	1.51
1	E	127	GLY	C-O	-5.68	1.20	1.24
2	D	279	GLU	CG-CD	5.67	1.66	1.52
2	H	242	ARG	CD-NE	5.66	1.54	1.46
2	D	400	LYS	CA-C	-5.62	1.45	1.52
2	F	306	GLU	CD-OE1	5.60	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	6	ASP	CG-OD1	5.58	1.35	1.25
1	G	391	MET	CB-CG	5.56	1.69	1.52
2	D	41	ASP	CA-C	5.55	1.59	1.52
1	C	142	PHE	N-CA	5.54	1.52	1.46
2	D	379	LEU	CA-CB	-5.54	1.44	1.53
2	F	268	GLN	CB-CG	-5.50	1.35	1.52
2	H	149	VAL	CA-CB	5.50	1.60	1.54
2	B	124	VAL	C-O	5.50	1.29	1.23
2	F	121	ASP	CB-CG	5.50	1.65	1.52
2	B	306	GLU	CD-OE1	5.50	1.35	1.25
2	H	175	ILE	C-O	-5.50	1.20	1.24
2	H	444	GLY	C-O	-5.49	1.17	1.23
2	D	258	GLU	C-O	-5.49	1.17	1.24
1	C	51	LYS	CB-CG	-5.48	1.36	1.52
2	B	257	PRO	CA-C	5.47	1.58	1.52
2	H	419	ALA	CA-CB	-5.47	1.45	1.53
1	A	50	LYS	C-O	-5.46	1.16	1.23
1	C	49	ASN	CG-OD1	5.46	1.33	1.23
1	G	96	ARG	NE-CZ	-5.46	1.27	1.33
2	D	120	GLU	CD-OE1	5.43	1.35	1.25
2	H	218	VAL	C-O	5.43	1.29	1.24
1	C	271	ASN	CG-OD1	5.42	1.33	1.23
1	C	407	TYR	CE1-CZ	-5.42	1.25	1.38
1	G	248	ARG	NE-CZ	-5.40	1.27	1.33
1	G	423	SER	CA-C	5.39	1.58	1.53
2	B	165	PHE	N-CA	-5.38	1.39	1.46
2	D	406	VAL	CA-CB	-5.36	1.47	1.54
1	G	70	VAL	C-O	-5.34	1.17	1.24
2	H	391	VAL	CB-CG2	-5.34	1.34	1.52
1	E	252	GLN	CB-CG	-5.33	1.36	1.52
2	F	338	GLN	CD-NE2	-5.32	1.22	1.33
1	A	176	LYS	CE-NZ	-5.31	1.33	1.49
1	G	212	GLU	N-CA	5.30	1.52	1.46
2	D	121	ASP	CB-CG	5.30	1.65	1.52
2	D	405	ALA	CA-C	5.29	1.59	1.52
2	D	464	VAL	CA-C	5.29	1.57	1.53
2	B	265	ALA	CA-CB	-5.28	1.46	1.52
2	H	6	ASP	CB-CG	5.27	1.65	1.52
2	B	68	LYS	CA-C	5.27	1.58	1.52
1	G	392	LYS	CB-CG	5.27	1.68	1.52
1	C	118	PHE	CA-C	-5.24	1.46	1.52
2	D	442	MET	CA-CB	5.24	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	PHE	C-N	-5.22	1.25	1.33
1	A	186	PHE	CA-CB	5.21	1.62	1.53
2	H	503	GLU	CD-OE1	5.21	1.35	1.25
1	C	404	VAL	CA-CB	5.20	1.59	1.54
1	C	16	VAL	CA-CB	-5.20	1.47	1.54
1	C	127	GLY	C-O	-5.20	1.20	1.24
1	A	84	GLY	CA-C	5.19	1.59	1.51
1	C	344	PRO	C-O	-5.18	1.17	1.24
1	C	295	MET	SD-CE	-5.17	1.66	1.79
2	H	491	MET	CG-SD	5.17	1.93	1.80
2	B	178	GLU	CD-OE1	5.17	1.35	1.25
1	C	457	ALA	CA-CB	-5.17	1.45	1.53
1	E	433	LYS	CG-CD	-5.15	1.36	1.52
2	F	51	GLU	CD-OE2	5.14	1.35	1.25
2	H	300	LYS	CD-CE	-5.13	1.37	1.52
2	H	241	LYS	CD-CE	-5.13	1.37	1.52
1	G	421	ILE	CA-CB	-5.11	1.48	1.54
2	H	379	LEU	CA-CB	-5.09	1.45	1.53
1	G	30	LYS	C-O	-5.08	1.17	1.24
1	E	209	LYS	CE-NZ	5.08	1.64	1.49
2	F	241	LYS	CD-CE	-5.08	1.37	1.52
2	F	145	ASP	CG-OD2	-5.08	1.15	1.25
2	D	242	ARG	CG-CD	-5.07	1.37	1.52
2	B	503	GLU	CD-OE1	5.04	1.34	1.25
1	E	45	CYS	C-O	-5.04	1.17	1.24
1	C	47	ILE	CB-CG2	-5.02	1.35	1.52
1	A	152	SER	N-CA	-5.01	1.40	1.46
2	B	301	THR	CA-CB	5.01	1.61	1.53
2	D	496	THR	N-CA	-5.01	1.40	1.46

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	GLU	CA-C-O	10.00	137.80	120.80
2	H	247	MET	CG-SD-CE	9.92	122.72	100.90
2	B	491	MET	CG-SD-CE	-9.75	79.44	100.90
1	C	480	GLU	CA-C-O	9.69	137.28	120.80
2	D	491	MET	CG-SD-CE	-9.30	80.44	100.90
1	A	209	LYS	CB-CG-CD	7.94	129.57	111.30
2	D	104	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	209	LYS	CG-CD-CE	7.72	129.06	111.30
1	E	480	GLU	CA-C-O	7.27	133.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	45	CYS	N-CA-CB	-7.08	98.53	110.49
1	C	391	MET	CB-CA-C	6.99	122.39	110.79
2	H	178	GLU	CB-CG-CD	-6.83	100.99	112.60
1	C	42	SER	N-CA-C	6.68	120.53	112.38
2	D	121	ASP	CB-CA-C	6.65	122.16	110.85
2	F	104	ASN	CA-CB-CG	6.65	119.25	112.60
1	A	261	GLU	CB-CA-C	6.64	122.13	110.85
2	D	124	VAL	CB-CA-C	-6.55	103.74	110.88
2	B	121	ASP	N-CA-CB	-6.52	100.55	110.01
2	D	474	PHE	CA-CB-CG	6.44	120.24	113.80
1	C	253	TRP	CA-C-N	6.36	133.15	121.70
1	C	253	TRP	C-N-CA	6.36	133.15	121.70
1	G	47	ILE	CA-CB-CG2	6.28	121.18	110.50
1	C	179	VAL	N-CA-C	6.13	114.16	107.60
1	E	5	SER	N-CA-C	6.13	117.95	110.41
2	B	121	ASP	CB-CA-C	6.11	120.47	110.88
1	C	17	LEU	CA-CB-CG	-6.10	94.95	116.30
2	B	51	GLU	CB-CG-CD	6.10	122.97	112.60
1	G	234	ASP	CA-CB-CG	6.08	118.68	112.60
1	C	96	ARG	NE-CZ-NH2	6.07	124.66	119.20
2	H	104	ASN	CA-CB-CG	6.01	118.61	112.60
2	D	19	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	104	ASN	CA-CB-CG	5.94	118.54	112.60
2	H	491	MET	CG-SD-CE	-5.93	87.85	100.90
2	D	121	ASP	N-CA-CB	-5.92	101.40	110.16
1	C	126	GLY	CA-C-O	-5.91	118.15	122.23
2	B	121	ASP	CA-C-O	5.90	127.02	120.82
1	G	261	GLU	CB-CG-CD	-5.88	102.60	112.60
2	D	206	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	C	47	ILE	CB-CG1-CD1	-5.79	101.65	113.80
2	B	503	GLU	CB-CG-CD	5.77	122.41	112.60
1	E	37	PRO	N-CA-C	-5.74	106.97	114.03
2	H	206	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	A	391	MET	CB-CA-C	5.72	120.29	110.79
1	G	391	MET	CB-CA-C	5.71	120.27	110.79
1	G	110	VAL	N-CA-C	5.70	116.44	110.62
2	B	65	ASN	CA-C-O	5.65	124.83	120.48
1	E	287	GLU	CB-CG-CD	5.61	122.13	112.60
1	E	234	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	5	SER	N-CA-C	5.43	118.47	110.59
2	B	512[A]	MET	N-CA-CB	-5.42	101.39	109.69
2	B	512[B]	MET	N-CA-CB	-5.42	101.39	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	LYS	CD-CE-NZ	-5.41	94.58	111.90
2	B	59	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	C	392	LYS	CB-CG-CD	5.35	123.61	111.30
2	D	417	LYS	N-CA-C	5.35	118.03	111.82
1	C	316	PHE	O-C-N	-5.34	115.48	122.59
1	A	417	LYS	CA-C-O	5.34	124.59	120.48
2	F	220	SER	N-CA-C	5.34	117.85	111.71
1	E	278	SER	N-CA-C	5.33	118.94	112.23
1	C	261	GLU	CB-CG-CD	-5.32	103.55	112.60
1	C	393	GLU	CG-CD-OE2	-5.31	106.19	118.40
2	H	512[A]	MET	N-CA-CB	5.30	117.80	109.69
2	H	512[B]	MET	N-CA-CB	5.30	117.80	109.69
2	F	474	PHE	CA-CB-CG	5.29	119.08	113.80
2	H	504	ARG	NE-CZ-NH1	-5.28	116.22	121.50
2	F	120	GLU	CB-CG-CD	5.27	121.55	112.60
1	C	234	ASP	CA-CB-CG	5.26	117.86	112.60
2	F	112	SER	CB-CA-C	5.25	118.42	109.80
2	B	510	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	E	40	THR	OG1-CB-CG2	-5.24	98.82	109.30
2	H	444	GLY	CA-C-O	5.24	126.39	121.41
1	E	275	CYS	CA-C-O	5.21	126.61	120.98
2	H	149	VAL	N-CA-C	5.21	115.81	108.36
1	A	120	GLU	N-CA-C	5.21	117.63	111.33
2	H	26	LYS	CA-CB-CG	5.19	124.48	114.10
1	C	393	GLU	CG-CD-OE1	5.19	130.34	118.40
1	A	45	CYS	CA-CB-SG	5.19	126.33	114.40
2	H	38	ASP	CB-CG-OD2	5.14	130.23	118.40
2	H	206	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	G	199	ASN	CA-CB-CG	5.13	117.73	112.60
1	E	284	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	H	306	GLU	CB-CG-CD	5.10	121.27	112.60
2	F	241	LYS	CB-CG-CD	5.09	123.00	111.30
1	C	385	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	242	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	H	154[A]	MET	CB-CA-C	-5.07	102.91	110.88
2	H	154[B]	MET	CB-CA-C	-5.07	102.91	110.88
2	B	391[A]	VAL	CB-CA-C	-5.07	105.23	112.22
2	B	391[B]	VAL	CB-CA-C	-5.07	105.23	112.22
1	C	118	PHE	CA-C-O	5.06	126.76	121.19
2	F	14	LEU	N-CA-C	5.06	117.19	111.11
2	D	206	ARG	CD-NE-CZ	-5.04	117.34	124.40
2	F	512[A]	MET	N-CA-CB	-5.04	101.99	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	512[B]	MET	N-CA-CB	-5.04	101.99	109.69
2	B	306	GLU	CB-CG-CD	-5.03	104.04	112.60
1	G	248	ARG	NE-CZ-NH2	-5.00	114.70	119.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	TYR	Sidechain
1	A	96	ARG	Sidechain
2	B	108	ARG	Sidechain
2	B	315	LYS	Mainchain
2	B	59	ARG	Sidechain
1	C	379	TYR	Sidechain
1	C	96	ARG	Sidechain
1	E	96	ARG	Sidechain
1	G	446	TYR	Sidechain
1	G	96	ARG	Sidechain
2	H	109	GLU	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3810	0	3748	31	0
1	C	3814	0	3755	42	2
1	E	3815	0	3750	16	0
1	G	3819	0	3764	36	0
2	B	4236	0	4156	33	0
2	D	4225	0	4141	49	0
2	F	4234	0	4155	41	0
2	H	4218	0	4136	48	0
3	A	14	0	6	2	0
3	C	14	0	6	2	0
3	E	14	0	6	1	0
3	G	14	0	6	2	0
4	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	18	0	0	0	0
4	E	18	0	0	0	0
4	G	18	0	0	0	0
5	B	1	0	0	1	0
5	D	1	0	0	1	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	15	0	0	0	0
6	D	15	0	0	0	0
6	F	15	0	0	0	0
6	H	15	0	0	0	0
7	A	553	0	0	11	5
7	B	723	0	0	15	2
7	C	570	0	0	11	12
7	D	704	0	0	25	6
7	E	536	0	0	6	0
7	F	708	0	0	14	4
7	G	533	0	0	7	4
7	H	694	0	0	18	5
All	All	37384	0	31629	279	20

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 4.

All (279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LYS:NZ	1:C:209:LYS:CE	1.69	1.56
1:C:391:MET:CB	1:C:391:MET:CG	1.76	1.55
2:F:247[A]:MET:SD	2:F:247[A]:MET:CE	2.01	1.48
2:B:247[A]:MET:SD	2:B:247[A]:MET:CE	2.10	1.38
2:D:124:VAL:HG13	7:D:8044:HOH:O	1.35	1.20
7:B:7790:HOH:O	1:C:474:LYS:HE2	1.02	1.17
2:H:461:GLU:HG3	7:H:4510:HOH:O	1.45	1.14
1:C:373:GLU:HG3	7:C:8065:HOH:O	1.42	1.13
2:D:124:VAL:HG23	7:D:7966:HOH:O	1.48	1.11
2:B:214:ASP:OD1	7:B:8171:HOH:O	1.66	1.10
2:D:214:ASP:OD1	7:D:8144:HOH:O	1.67	1.09
2:H:178:GLU:OE1	7:H:4929:HOH:O	1.69	1.09
1:A:47:ILE:CD1	7:A:7032:HOH:O	1.99	1.08
2:F:214:ASP:OD1	7:F:4919:HOH:O	1.73	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:MET:HB2	1:C:391:MET:HE3	1.40	1.04
1:G:480:GLU:HA	1:G:480:GLU:OE2	1.56	1.03
2:D:45[A]:GLN:HG2	7:D:7809:HOH:O	1.59	1.00
2:H:306:GLU:OE2	7:H:4859:HOH:O	1.77	1.00
1:A:209:LYS:HG2	7:A:7046:HOH:O	1.59	0.99
1:G:39:VAL:HG12	1:G:391:MET:HE1	1.45	0.98
1:G:239:ARG:HD3	2:H:23[B]:MET:SD	2.03	0.98
1:C:391:MET:CB	1:C:391:MET:SD	2.52	0.97
2:D:84:LYS:NZ	7:D:8029:HOH:O	1.96	0.95
2:D:121:ASP:O	7:D:8044:HOH:O	1.85	0.95
2:H:45[A]:GLN:HG2	7:H:3646:HOH:O	1.64	0.95
2:H:214:ASP:OD1	7:H:3806:HOH:O	1.85	0.95
2:F:477:HIS:H	2:H:499:ASN:HD21	1.15	0.94
2:B:45[B]:GLN:HG2	7:B:8147:HOH:O	1.65	0.94
1:C:391:MET:CB	1:C:391:MET:HE3	1.99	0.92
2:B:477:HIS:H	2:D:499:ASN:HD21	1.10	0.92
1:A:47:ILE:HD13	1:A:48:SER:H	1.35	0.91
1:C:473:LYS:HG2	7:C:7955:HOH:O	1.72	0.89
1:C:47:ILE:HG13	7:C:7989:HOH:O	1.73	0.89
1:E:239:ARG:HD3	2:F:23[B]:MET:SD	2.11	0.89
1:G:473:LYS:HG2	7:G:4558:HOH:O	1.70	0.89
1:C:391:MET:CB	1:C:391:MET:CE	2.50	0.89
1:C:391:MET:HB2	1:C:391:MET:CE	2.03	0.88
1:A:239:ARG:HD3	2:B:23[B]:MET:SD	2.14	0.88
1:A:47:ILE:CD1	1:A:50:LYS:HE2	2.04	0.87
2:F:404:LYS:NZ	7:F:4299:HOH:O	2.08	0.85
1:C:239:ARG:HD3	2:D:23[B]:MET:SD	2.18	0.83
1:G:479:TRP:O	1:G:480:GLU:HB2	1.77	0.83
1:G:480:GLU:OE2	1:G:480:GLU:CA	2.25	0.83
2:B:503:GLU:OE2	7:B:7745:HOH:O	1.97	0.82
1:G:473:LYS:HE2	1:G:473:LYS:HA	1.61	0.81
1:A:47:ILE:HD11	1:A:50:LYS:HE2	1.65	0.78
2:F:503:GLU:CD	7:F:4246:HOH:O	2.25	0.78
1:E:45:CYS:SG	1:E:391:MET:HE1	2.24	0.78
1:C:213:ASP:OD1	7:C:8007:HOH:O	2.00	0.77
2:D:84:LYS:CE	7:D:8029:HOH:O	2.31	0.77
1:C:139:GLU:OE2	1:C:176:LYS:HE3	1.83	0.77
5:D:6492:CA:CA	7:D:7499:HOH:O	1.62	0.76
2:B:503:GLU:CD	7:B:7976:HOH:O	2.26	0.76
1:G:39:VAL:CG1	1:G:391:MET:HE1	2.15	0.76
2:D:306:GLU:OE2	7:D:8158:HOH:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:CG2	1:A:372:MET:HE2	2.17	0.75
2:F:310:LYS:NZ	7:F:3777:HOH:O	2.20	0.75
2:F:118:MET:HE2	2:F:154[B]:MET:SD	2.27	0.74
1:A:47:ILE:HD11	7:A:7032:HOH:O	1.74	0.74
1:C:4:MET:HE2	1:C:415:ARG:NH1	2.03	0.73
2:D:124:VAL:O	2:D:124:VAL:CG2	2.37	0.73
2:D:279:GLU:OE1	7:D:7961:HOH:O	2.08	0.72
1:A:47:ILE:HD13	1:A:48:SER:N	2.06	0.71
2:H:54:GLU:OE1	7:H:4132:HOH:O	2.08	0.71
2:H:306:GLU:OE1	7:H:4032:HOH:O	2.06	0.71
2:D:125:PHE:N	7:D:8044:HOH:O	2.22	0.71
1:A:120:GLU:OE1	7:A:6934:HOH:O	2.07	0.71
1:C:479:TRP:O	1:C:480:GLU:HB2	1.91	0.71
2:D:353:ASP:OD2	7:D:8199:HOH:O	2.08	0.70
2:F:45[B]:GLN:HG2	7:F:4821:HOH:O	1.89	0.70
2:B:353:ASP:OD2	7:B:8212:HOH:O	2.09	0.70
2:B:118:MET:HE2	2:B:154[B]:MET:SD	2.31	0.70
2:D:124:VAL:O	2:D:124:VAL:HG22	1.92	0.69
1:G:31:HIS:HE1	7:G:3017:HOH:O	1.75	0.69
1:A:47:ILE:HD13	7:A:7032:HOH:O	1.78	0.68
2:H:353:ASP:OD2	7:H:5005:HOH:O	2.10	0.68
2:D:84:LYS:HE3	7:D:8029:HOH:O	1.90	0.68
2:D:503:GLU:CG	7:D:8131:HOH:O	2.40	0.68
2:D:4:GLN:OE1	7:D:8128:HOH:O	2.12	0.67
2:D:21:LYS:NZ	7:D:8014:HOH:O	2.21	0.67
2:H:84:LYS:NZ	7:H:4458:HOH:O	2.28	0.67
2:H:177:ASP:OD1	7:H:4511:HOH:O	2.13	0.67
2:H:124:VAL:HG22	2:H:124:VAL:O	1.94	0.66
1:G:209:LYS:HZ1	1:G:259:ILE:HD11	1.59	0.66
1:G:18:GLU:HG2	7:G:4205:HOH:O	1.93	0.66
2:B:120:GLU:OE2	7:B:7587:HOH:O	2.13	0.66
1:G:209:LYS:NZ	1:G:263:GLU:OE2	2.28	0.65
1:A:47:ILE:HD12	1:A:50:LYS:HE2	1.78	0.65
1:G:206:VAL:HA	1:G:209:LYS:HE2	1.78	0.65
2:F:37:GLN:HE22	2:H:513:GLN:HE22	1.45	0.65
2:F:145:ASP:OD2	7:F:3900:HOH:O	2.14	0.64
2:F:222:LYS:HE2	7:F:4730:HOH:O	1.98	0.64
2:F:391[A]:VAL:HG12	2:F:392:HIS:CE1	2.32	0.64
1:A:176:LYS:HE3	7:A:6831:HOH:O	1.97	0.64
2:D:124:VAL:CG1	7:D:8044:HOH:O	2.13	0.63
2:H:118:MET:HE2	2:H:154[B]:MET:SD	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:VAL:O	2:H:124:VAL:CG2	2.47	0.62
2:B:37:GLN:HE22	2:D:513:GLN:HE22	1.46	0.62
1:E:36:ASP:OD1	1:E:38:ALA:HB3	1.99	0.62
1:E:45:CYS:SG	1:E:391:MET:CE	2.87	0.62
5:B:7492:CA:CA	7:B:7493:HOH:O	1.77	0.62
1:C:6:ARG:NE	7:C:7884:HOH:O	1.77	0.60
2:F:503:GLU:CG	7:F:4226:HOH:O	2.50	0.60
1:E:25:ARG:HD3	7:E:3407:HOH:O	2.01	0.59
2:H:45[B]:GLN:HE22	2:H:458[B]:LYS:NZ	2.01	0.59
2:D:118:MET:HE2	2:D:154[B]:MET:SD	2.43	0.59
1:G:133:LYS:HE3	7:G:3883:HOH:O	2.02	0.59
1:G:44:LYS:NZ	7:G:3100:HOH:O	2.36	0.58
1:G:209:LYS:NZ	1:G:259:ILE:HD11	2.18	0.58
1:E:341:LYS:NZ	7:E:4543:HOH:O	2.37	0.58
2:F:478:HIS:NE2	2:H:354[B]:MET:HG3	2.19	0.58
2:B:115[B]:SER:HB2	7:B:7562:HOH:O	2.02	0.58
1:A:47:ILE:HG12	7:A:7032:HOH:O	1.97	0.57
1:C:31:HIS:HD2	1:C:402:ASP:OD2	1.87	0.57
1:A:473:LYS:HG2	7:A:6912:HOH:O	2.04	0.57
2:H:242:ARG:HD3	2:H:246:GLU:OE2	2.05	0.56
1:C:31:HIS:HE1	7:C:7601:HOH:O	1.87	0.55
1:A:209:LYS:HE2	1:A:209:LYS:N	2.22	0.55
2:H:503:GLU:CG	7:H:4772:HOH:O	2.54	0.55
7:B:7790:HOH:O	1:C:474:LYS:CE	1.89	0.55
1:C:139:GLU:CD	1:C:176:LYS:HE3	2.30	0.55
1:E:36:ASP:OD1	1:E:38:ALA:N	2.39	0.55
1:E:15[B]:GLU:OE2	7:E:4952:HOH:O	2.18	0.54
2:F:353:ASP:OD2	7:F:5006:HOH:O	2.18	0.54
2:F:120:GLU:OE2	7:F:3364:HOH:O	2.18	0.54
2:B:354[B]:MET:HG3	2:D:478:HIS:NE2	2.23	0.53
1:E:417:LYS:NZ	7:E:4120:HOH:O	2.37	0.53
1:C:480:GLU:OE2	1:C:480:GLU:HA	2.06	0.53
2:D:120:GLU:OE2	7:D:7539:HOH:O	2.19	0.53
1:A:176:LYS:NZ	7:A:6983:HOH:O	2.42	0.53
1:G:473:LYS:HE2	1:G:473:LYS:CA	2.35	0.52
2:B:478:HIS:NE2	2:D:354[B]:MET:HG3	2.25	0.52
2:H:417:LYS:NZ	7:H:4638:HOH:O	1.95	0.52
1:G:31:HIS:HD2	1:G:402:ASP:OD2	1.92	0.52
2:F:478:HIS:CD2	2:H:354[B]:MET:HG3	2.45	0.52
1:C:14:GLN:NE2	7:C:7763:HOH:O	2.43	0.52
2:F:354[B]:MET:HG3	2:H:478:HIS:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45[B]:GLN:HE22	2:H:458[B]:LYS:HZ2	1.57	0.52
1:A:473:LYS:CG	7:A:6912:HOH:O	2.57	0.51
7:B:7790:HOH:O	1:C:474:LYS:CD	2.43	0.51
1:C:39:VAL:HG12	1:C:391:MET:HE1	1.92	0.51
2:H:461:GLU:CG	7:H:4510:HOH:O	2.26	0.51
2:H:214:ASP:OD1	7:H:4825:HOH:O	2.19	0.51
2:D:354[B]:MET:SD	2:D:494:LEU:HD22	2.51	0.51
1:A:351:VAL:HG21	1:A:372:MET:HE2	1.93	0.51
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.92	0.51
2:D:503:GLU:CD	7:D:8131:HOH:O	2.52	0.51
2:F:354[B]:MET:SD	2:F:494:LEU:HD22	2.51	0.51
2:D:458[A]:LYS:HG2	2:D:462:PHE:CD2	2.46	0.51
1:C:473:LYS:HE2	1:C:473:LYS:HA	1.92	0.51
2:F:354[B]:MET:HG2	2:F:494:LEU:HD22	1.93	0.50
2:B:21:LYS:HE2	7:B:8088:HOH:O	2.10	0.50
2:H:458[A]:LYS:HE2	2:H:462:PHE:CD1	2.47	0.50
1:C:51:LYS:NZ	7:C:7861:HOH:O	2.39	0.50
1:C:417:LYS:NZ	7:C:7846:HOH:O	2.44	0.50
1:E:442:HIS:HB3	3:E:8494:HCA:O5	2.12	0.50
2:D:354[B]:MET:HG2	2:D:494:LEU:HD22	1.94	0.49
2:B:478:HIS:CD2	2:D:354[B]:MET:HG3	2.47	0.49
2:B:503:GLU:CG	7:B:7976:HOH:O	2.58	0.49
1:C:480:GLU:OE2	1:C:480:GLU:CA	2.61	0.49
1:G:206:VAL:HA	1:G:209:LYS:CE	2.41	0.49
1:G:139:GLU:CD	1:G:176:LYS:HE3	2.37	0.49
1:E:50:LYS:NZ	7:E:4377:HOH:O	2.33	0.49
2:H:151:THR:HG23	2:H:162:LEU:HD11	1.94	0.48
2:H:354[B]:MET:HG2	2:H:494:LEU:HD22	1.94	0.48
1:G:351:VAL:CG2	1:G:372:MET:HE2	2.43	0.48
2:D:206:ARG:HG2	7:D:8053:HOH:O	2.12	0.48
2:D:391[A]:VAL:HG12	2:D:392:HIS:CE1	2.48	0.48
2:F:243[B]:MET:HE2	2:F:329:LEU:HD21	1.96	0.48
2:B:391[A]:VAL:HG12	2:B:392:HIS:CE1	2.48	0.48
2:H:354[B]:MET:SD	2:H:494:LEU:HD22	2.53	0.48
1:A:415:ARG:HD2	7:A:7036:HOH:O	2.13	0.48
2:B:354[B]:MET:HG2	2:B:494:LEU:HD22	1.96	0.48
2:F:151:THR:HG23	2:F:162:LEU:HD11	1.94	0.48
2:F:128:GLN:HE22	2:F:165:PHE:HA	1.78	0.48
1:G:7:GLU:CD	1:G:7:GLU:H	2.23	0.47
1:C:479:TRP:O	1:C:480:GLU:CB	2.60	0.47
1:A:208:GLY:C	1:A:209:LYS:HE2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:THR:HG21	7:C:7911:HOH:O	2.15	0.47
2:F:194:VAL:HB	2:F:297:HIS:CG	2.50	0.47
1:G:442:HIS:HB3	3:G:9494:HCA:O5	2.14	0.47
2:H:411:ALA:HB3	7:H:3114:HOH:O	2.15	0.47
1:C:4:MET:HE2	1:C:415:ARG:CZ	2.45	0.47
1:C:203[A]:ARG:HD2	1:C:204:ASP:OD1	2.14	0.47
2:F:503:GLU:HG3	7:F:4226:HOH:O	2.13	0.47
2:H:503:GLU:CD	7:H:4772:HOH:O	2.57	0.46
2:B:354[B]:MET:HG3	2:D:478:HIS:CD2	2.51	0.46
1:A:22:GLU:HG3	1:A:26:LYS:HE3	1.97	0.46
1:A:76:LYS:O	1:A:108:ALA:HA	2.16	0.46
1:E:134:LEU:C	1:E:134:LEU:HD23	2.41	0.46
1:G:14:GLN:NE2	7:G:3719:HOH:O	2.45	0.46
2:D:417:LYS:NZ	7:D:8090:HOH:O	1.96	0.45
2:H:354[B]:MET:HG2	2:H:494:LEU:CD2	2.46	0.45
1:A:351:VAL:CG2	1:A:372:MET:CE	2.92	0.45
1:E:176:LYS:NZ	7:E:4742:HOH:O	2.49	0.45
2:B:128:GLN:HE22	2:B:165:PHE:HA	1.81	0.45
2:B:354[B]:MET:CG	2:B:494:LEU:HD22	2.47	0.45
2:B:354[B]:MET:SD	2:B:494:LEU:HD22	2.57	0.45
2:F:354[B]:MET:HG2	2:F:494:LEU:CD2	2.46	0.45
2:D:128:GLN:HE22	2:D:165:PHE:HA	1.82	0.45
2:F:45[B]:GLN:CG	7:F:4821:HOH:O	2.59	0.45
1:G:4:MET:HE2	1:G:415:ARG:NH1	2.31	0.45
2:H:128:GLN:HE22	2:H:165:PHE:HA	1.82	0.45
1:A:47:ILE:HD12	1:A:50:LYS:CE	2.47	0.44
2:D:194:VAL:HB	2:D:297:HIS:CG	2.52	0.44
1:G:391:MET:HE3	1:G:391:MET:HB2	1.56	0.44
2:D:494:LEU:C	2:D:494:LEU:HD23	2.43	0.44
2:H:458[A]:LYS:HE2	2:H:462:PHE:CE1	2.52	0.44
1:A:134:LEU:HD23	1:A:134:LEU:C	2.42	0.44
2:B:494:LEU:C	2:B:494:LEU:HD23	2.42	0.44
1:C:17:LEU:N	1:C:17:LEU:CD1	2.80	0.44
1:G:100:TYR:CE1	1:G:110:VAL:HB	2.52	0.44
2:H:178:GLU:CD	2:H:178:GLU:H	2.25	0.44
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.52	0.44
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.44
1:C:6:ARG:NH2	7:C:7884:HOH:O	2.47	0.44
1:E:36:ASP:OD1	1:E:38:ALA:CB	2.66	0.44
1:G:253:TRP:HA	1:G:254:SER:HA	1.78	0.44
2:H:154[B]:MET:HE2	2:H:154[B]:MET:HB2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ARG:HD3	2:B:246:GLU:OE2	2.18	0.44
2:D:21:LYS:HB2	2:D:21:LYS:HE2	1.56	0.44
1:G:219:THR:HB	1:G:220:PRO:HD2	1.99	0.43
1:C:76:LYS:O	1:C:108:ALA:HA	2.18	0.43
2:D:503:GLU:HG3	7:D:8131:HOH:O	2.10	0.43
2:D:391[A]:VAL:HG13	7:D:7918:HOH:O	2.18	0.43
1:A:442:HIS:CG	3:A:6494:HCA:H52	2.54	0.43
2:B:478:HIS:CE1	2:D:354[B]:MET:HG3	2.54	0.43
2:D:121:ASP:O	2:D:125:PHE:CE1	2.72	0.43
2:D:400:LYS:HB3	7:D:8152:HOH:O	2.18	0.43
2:F:247[B]:MET:HE1	2:F:332:VAL:CG1	2.49	0.43
1:G:442:HIS:CG	3:G:9494:HCA:H52	2.54	0.43
2:B:168:ASN:ND2	7:B:8105:HOH:O	2.52	0.42
1:C:442:HIS:CG	3:C:7494:HCA:H52	2.54	0.42
2:B:354[B]:MET:HG2	2:B:494:LEU:CD2	2.49	0.42
1:C:209:LYS:NZ	1:C:263:GLU:OE2	2.43	0.42
2:D:354[B]:MET:HG2	2:D:494:LEU:CD2	2.48	0.42
2:H:168:ASN:ND2	2:H:171:LYS:NZ	2.67	0.42
1:C:391:MET:CG	1:C:391:MET:CA	2.81	0.42
2:F:130:ASN:HD22	2:F:130:ASN:H	1.67	0.42
2:F:478:HIS:CE1	2:H:354[B]:MET:HG3	2.55	0.42
2:H:494:LEU:HD23	2:H:494:LEU:C	2.44	0.42
2:F:417:LYS:CG	7:F:4979:HOH:O	2.67	0.42
2:H:376:VAL:HG21	2:H:395[B]:CYS:SG	2.60	0.42
2:B:504:ARG:NH2	7:B:7973:HOH:O	2.52	0.42
2:D:124:VAL:HG23	2:D:124:VAL:O	2.19	0.42
2:H:21:LYS:HB2	2:H:21:LYS:HE2	1.49	0.42
1:C:262:ILE:HD13	1:C:262:ILE:HG21	1.83	0.42
1:C:382:ALA:HB1	1:C:386:ASP:HB2	2.02	0.42
1:E:53:GLN:HB2	1:E:56:LEU:HD12	2.02	0.42
1:E:253:TRP:HA	1:E:254:SER:HA	1.86	0.42
2:F:317:ASN:ND2	7:F:2832:HOH:O	2.47	0.42
2:H:354[B]:MET:CG	2:H:494:LEU:HD22	2.49	0.41
1:A:442:HIS:HB3	3:A:6494:HCA:O5	2.20	0.41
1:C:442:HIS:HB3	3:C:7494:HCA:O5	2.21	0.41
2:F:70:CYS:HB2	2:F:188:SER:HB2	2.02	0.41
2:B:70:CYS:HB2	2:B:188:SER:HB2	2.03	0.41
2:F:354[B]:MET:HG3	2:H:478:HIS:CD2	2.55	0.41
2:F:354[B]:MET:CG	2:F:494:LEU:HD22	2.50	0.41
2:H:45[A]:GLN:CG	7:H:3646:HOH:O	2.42	0.41
1:G:480:GLU:OE2	1:G:480:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:ARG:HH11	2:F:401:ARG:HD2	1.69	0.41
2:F:242:ARG:HD3	2:F:246:GLU:OE2	2.21	0.41
1:G:134:LEU:C	1:G:134:LEU:HD23	2.46	0.41
2:H:503:GLU:HG3	7:H:4772:HOH:O	2.19	0.41
2:B:37:GLN:NE2	2:D:513:GLN:HE22	2.17	0.41
2:D:45[A]:GLN:CG	7:D:7809:HOH:O	2.37	0.41
1:A:391:MET:HB2	1:A:391:MET:HE3	1.38	0.40
2:D:404:LYS:HE3	2:D:404:LYS:HB3	1.31	0.40
1:G:76:LYS:O	1:G:108:ALA:HA	2.20	0.40
2:F:143:LYS:N	2:F:144:PRO:CD	2.84	0.40
1:G:133:LYS:CE	7:G:3883:HOH:O	2.66	0.40
2:H:194:VAL:HB	2:H:297:HIS:CG	2.57	0.40
2:D:354[B]:MET:CG	2:D:494:LEU:HD22	2.50	0.40
2:F:26:LYS:HE3	2:F:26:LYS:HB3	1.80	0.40
1:G:479:TRP:O	1:G:480:GLU:CB	2.58	0.40
1:G:68:LYS:C	1:G:68:LYS:HD3	2.46	0.40

All (20) 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)
7:G:3329:HOH:O	7:H:4423:HOH:O[2_756]	0.55	1.65
7:C:8019:HOH:O	7:D:8052:HOH:O[2_545]	0.56	1.64
7:A:6891:HOH:O	7:B:8141:HOH:O[2_655]	0.71	1.49
7:C:7897:HOH:O	7:F:4626:HOH:O[1_454]	0.84	1.36
7:C:7978:HOH:O	7:H:4816:HOH:O[1_454]	0.98	1.22
7:C:8023:HOH:O	7:H:4818:HOH:O[1_454]	1.11	1.09
7:C:8014:HOH:O	7:D:7911:HOH:O[2_545]	1.28	0.92
7:G:4892:HOH:O	7:H:4841:HOH:O[2_756]	1.30	0.90
1:C:288:GLU:OE2	7:A:6735:HOH:O[1_455]	1.33	0.87
7:A:6860:HOH:O	7:B:8174:HOH:O[2_655]	1.42	0.78
7:C:8015:HOH:O	7:F:4519:HOH:O[1_454]	1.57	0.63
7:C:8051:HOH:O	7:D:8116:HOH:O[2_545]	1.61	0.59
7:C:7911:HOH:O	7:F:4562:HOH:O[1_454]	1.64	0.56
7:G:4874:HOH:O	7:H:4641:HOH:O[2_756]	1.67	0.53
7:C:7808:HOH:O	7:D:8152:HOH:O[2_545]	1.72	0.48
7:C:8028:HOH:O	7:D:7858:HOH:O[2_545]	1.83	0.37
7:A:7018:HOH:O	7:C:7937:HOH:O[1_655]	1.90	0.30
1:C:288:GLU:CD	7:A:6735:HOH:O[1_455]	2.11	0.09
7:D:8175:HOH:O	7:G:5020:HOH:O[1_455]	2.16	0.04
7:C:7911:HOH:O	7:F:4799:HOH:O[1_454]	2.18	0.02

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	481/491 (98%)	463 (96%)	18 (4%)	0	100	100
1	C	481/491 (98%)	461 (96%)	20 (4%)	0	100	100
1	E	482/491 (98%)	462 (96%)	20 (4%)	0	100	100
1	G	482/491 (98%)	462 (96%)	20 (4%)	0	100	100
2	B	538/522 (103%)	529 (98%)	8 (2%)	1 (0%)	43	13
2	D	535/522 (102%)	525 (98%)	9 (2%)	1 (0%)	43	13
2	F	537/522 (103%)	527 (98%)	9 (2%)	1 (0%)	43	13
2	H	533/522 (102%)	524 (98%)	8 (2%)	1 (0%)	43	13
All	All	4069/4052 (100%)	3953 (97%)	112 (3%)	4 (0%)	48	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	255	SER
2	D	255	SER
2	F	255	SER
2	H	255	SER

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	413/414 (100%)	403 (98%)	10 (2%)	43 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	413/414 (100%)	403 (98%)	10 (2%)	43 7
1	E	414/414 (100%)	407 (98%)	7 (2%)	53 15
1	G	414/414 (100%)	404 (98%)	10 (2%)	43 7
2	B	472/454 (104%)	470 (100%)	2 (0%)	84 64
2	D	469/454 (103%)	461 (98%)	8 (2%)	53 15
2	F	471/454 (104%)	467 (99%)	4 (1%)	73 41
2	H	467/454 (103%)	464 (99%)	3 (1%)	78 53
All	All	3533/3472 (102%)	3479 (98%)	54 (2%)	57 18

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	CYS
1	A	47	ILE
1	A	98	ASN
1	A	121	LYS
1	A	209	LYS
1	A	355	ILE
1	A	362	HIS
1	A	392	LYS
1	A	445	ASP
1	A	473	LYS
2	B	7	LYS
2	B	26	LYS
1	C	45[A]	CYS
1	C	45[B]	CYS
1	C	47	ILE
1	C	98	ASN
1	C	355	ILE
1	C	362	HIS
1	C	392	LYS
1	C	445	ASP
1	C	473	LYS
1	C	480	GLU
2	D	4	GLN
2	D	21	LYS
2	D	26	LYS
2	D	38[A]	ASP
2	D	38[B]	ASP
2	D	124	VAL

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Mol	Chain	Res	Type
2	D	125	PHE
2	D	258	GLU
1	E	40	THR
1	E	45	CYS
1	E	98	ASN
1	E	355	ILE
1	E	362	HIS
1	E	445	ASP
1	E	473	LYS
2	F	13	PRO
2	F	121	ASP
2	F	177	ASP
2	F	258	GLU
1	G	45[A]	CYS
1	G	45[B]	CYS
1	G	98	ASN
1	G	176	LYS
1	G	355	ILE
1	G	362	HIS
1	G	392	LYS
1	G	445	ASP
1	G	473	LYS
1	G	480	GLU
2	H	21	LYS
2	H	178	GLU
2	H	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	35	ASN
1	A	271	ASN
1	A	476	GLN
2	B	37	GLN
2	B	93	GLN
2	B	104	ASN
2	B	128	GLN
2	B	130	ASN
2	B	168	ASN
2	B	338	GLN

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Mol	Chain	Res	Type
2	B	418	ASN
1	C	31	HIS
1	C	35	ASN
1	C	49	ASN
1	C	271	ASN
2	D	104	ASN
2	D	128	GLN
2	D	130	ASN
2	D	168	ASN
2	D	294	GLN
2	D	499	ASN
1	E	35	ASN
1	E	271	ASN
2	F	18	GLN
2	F	37	GLN
2	F	104	ASN
2	F	128	GLN
2	F	130	ASN
2	F	168	ASN
2	F	418	ASN
1	G	31	HIS
1	G	35	ASN
1	G	49	ASN
1	G	271	ASN
2	H	104	ASN
2	H	128	GLN
2	H	130	ASN
2	H	168	ASN
2	H	418	ASN
2	H	499	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
4	CFN	A	6496	1	18,30,30	1.99	6 (33%)	-		
3	HCA	C	7494	-	13,13,13	1.76	2 (15%)	15,18,18	1.96	4 (26%)
6	CLF	B	6498	2,1	0,24,24	-	-	-		
6	CLF	H	9498	2,1	0,24,24	-	-	-		
3	HCA	G	9494	-	13,13,13	2.40	6 (46%)	15,18,18	2.15	4 (26%)
3	HCA	A	6494	-	13,13,13	3.25	6 (46%)	15,18,18	2.73	6 (40%)
4	CFN	E	8496	1	18,30,30	1.99	7 (38%)	-		
3	HCA	E	8494	-	13,13,13	2.16	4 (30%)	15,18,18	2.08	4 (26%)
6	CLF	F	8498	2,1	0,24,24	-	-	-		
6	CLF	D	7498	2,1	0,24,24	-	-	-		
4	CFN	G	9496	1	18,30,30	2.04	7 (38%)	-		
4	CFN	C	7496	1	18,30,30	2.07	7 (38%)	-		

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
3	HCA	C	7494	-	-	0/17/17/17	-
6	CLF	B	6498	2,1	-	-	0/12/10/10
6	CLF	H	9498	2,1	-	-	0/12/10/10
3	HCA	G	9494	-	-	0/17/17/17	-
3	HCA	A	6494	-	-	0/17/17/17	-
3	HCA	E	8494	-	-	0/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLF	F	8498	2,1	-	-	0/12/10/10
6	CLF	D	7498	2,1	-	-	0/12/10/10

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6494	HCA	C3-C7	9.24	1.63	1.53
3	G	9494	HCA	C5-C6	-4.30	1.40	1.50
4	G	9496	CFN	S4B-FE7	-4.25	2.21	2.29
4	E	8496	CFN	S3B-FE6	-4.21	2.21	2.29
4	A	6496	CFN	S4B-FE7	-4.05	2.21	2.29
3	G	9494	HCA	C3-C7	4.03	1.57	1.53
4	G	9496	CFN	S3B-FE6	-4.01	2.21	2.29
3	E	8494	HCA	C3-C7	3.95	1.57	1.53
4	C	7496	CFN	S4B-FE7	-3.87	2.22	2.29
4	C	7496	CFN	S1B-FE6	-3.73	2.22	2.29
4	A	6496	CFN	S3B-FE6	-3.73	2.22	2.29
3	E	8494	HCA	O3-C6	3.73	1.34	1.22
4	C	7496	CFN	S3B-FE6	-3.70	2.22	2.29
3	C	7494	HCA	O3-C6	3.62	1.33	1.22
3	A	6494	HCA	C5-C6	-3.51	1.42	1.50
3	A	6494	HCA	O6-C7	-3.45	1.18	1.30
3	G	9494	HCA	O5-C7	3.44	1.32	1.22
4	E	8496	CFN	S4B-FE7	-3.44	2.22	2.29
4	E	8496	CFN	S1B-FE6	-3.28	2.23	2.29
4	A	6496	CFN	S1B-FE6	-3.08	2.23	2.29
3	C	7494	HCA	O5-C7	3.07	1.31	1.22
4	G	9496	CFN	S1B-FE6	-2.90	2.23	2.29
4	C	7496	CFN	S4B-FE5	-2.89	2.23	2.29
3	E	8494	HCA	O5-C7	2.86	1.31	1.22
3	A	6494	HCA	O3-C6	2.81	1.31	1.22
3	G	9494	HCA	O3-C6	2.70	1.30	1.22
4	G	9496	CFN	S4B-FE5	-2.59	2.24	2.29
3	E	8494	HCA	O6-C7	-2.57	1.21	1.30
4	A	6496	CFN	S2B-FE6	-2.54	2.17	2.24
4	E	8496	CFN	S4B-FE5	-2.53	2.24	2.29
3	A	6494	HCA	O5-C7	2.50	1.29	1.22
4	C	7496	CFN	S1A-FE2	-2.47	2.24	2.29
4	A	6496	CFN	S4B-FE5	-2.46	2.24	2.29
3	G	9494	HCA	O6-C7	-2.38	1.21	1.30
4	G	9496	CFN	S2B-FE6	-2.36	2.17	2.24
4	C	7496	CFN	S4A-FE3	-2.35	2.24	2.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	9496	CFN	S2A-FE2	-2.34	2.24	2.29
4	E	8496	CFN	S4A-FE3	-2.27	2.25	2.29
4	A	6496	CFN	S2A-FE2	-2.23	2.25	2.29
4	E	8496	CFN	S3B-FE7	-2.16	2.25	2.29
4	G	9496	CFN	S3B-FE7	-2.12	2.25	2.29
4	E	8496	CFN	S2A-FE2	-2.09	2.25	2.29
3	G	9494	HCA	O1-C1	2.08	1.28	1.22
4	C	7496	CFN	S2A-FE2	-2.02	2.25	2.29
3	A	6494	HCA	O1-C1	2.02	1.28	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	6494	HCA	O5-C7-C3	-7.75	107.08	122.09
3	G	9494	HCA	O5-C7-C3	-5.67	111.10	122.09
3	E	8494	HCA	O5-C7-C3	-5.60	111.24	122.09
3	C	7494	HCA	O5-C7-C3	-4.83	112.74	122.09
3	G	9494	HCA	C4-C5-C6	3.48	120.84	112.77
3	C	7494	HCA	O6-C7-C3	3.43	119.71	113.14
3	A	6494	HCA	C4-C5-C6	3.33	120.49	112.77
3	A	6494	HCA	O6-C7-C3	3.28	119.42	113.14
3	C	7494	HCA	C4-C5-C6	3.19	120.17	112.77
3	G	9494	HCA	O6-C7-C3	3.11	119.11	113.14
3	E	8494	HCA	O6-C7-C3	2.99	118.88	113.14
3	A	6494	HCA	O6-C7-O5	2.89	133.11	123.86
3	E	8494	HCA	C4-C5-C6	2.49	118.54	112.77
3	A	6494	HCA	O1-C1-C2	-2.49	115.90	122.95
3	G	9494	HCA	O4-C6-O3	-2.43	117.07	123.33
3	E	8494	HCA	O4-C6-C5	2.34	121.38	114.00
3	C	7494	HCA	O4-C6-C5	2.15	120.80	114.00
3	A	6494	HCA	O4-C6-C5	2.14	120.76	114.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

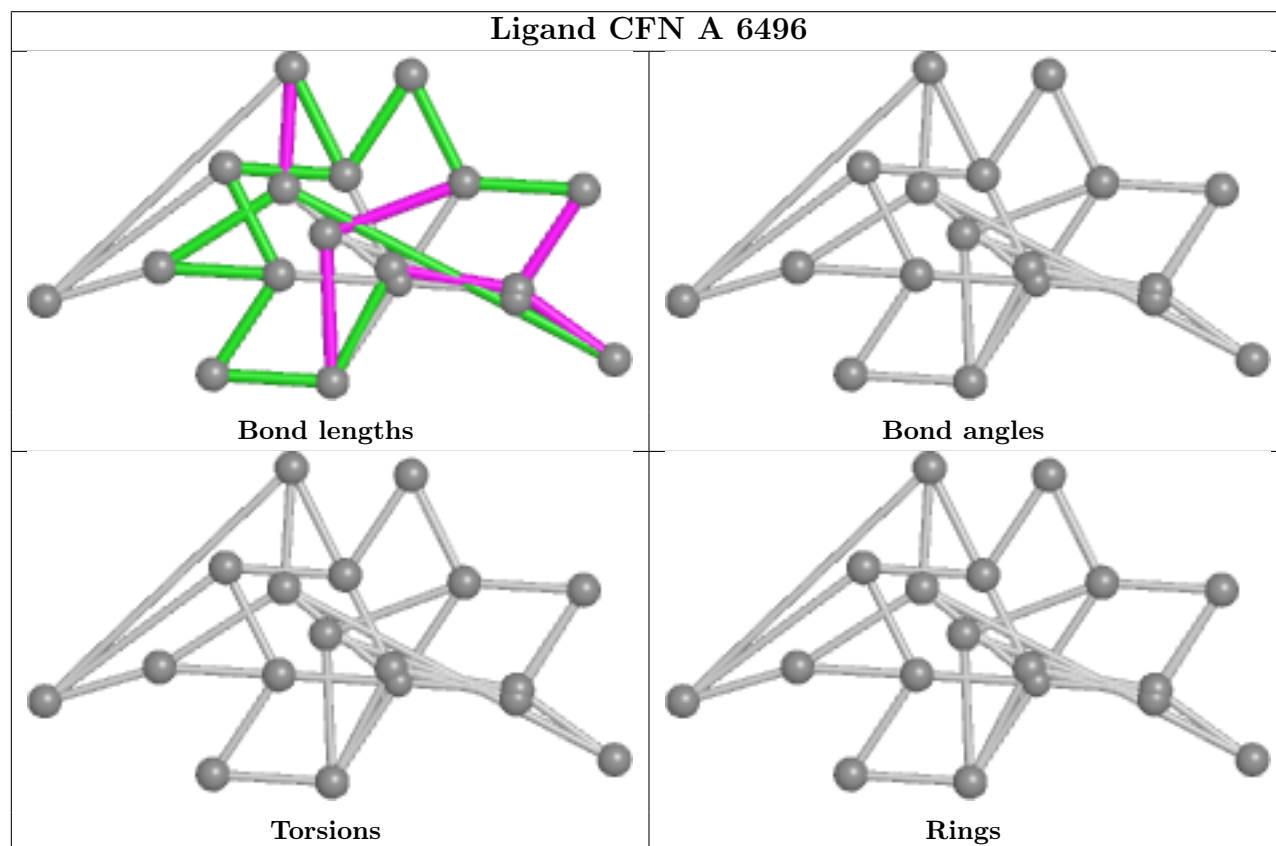
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	7494	HCA	2	0
3	G	9494	HCA	2	0
3	A	6494	HCA	2	0

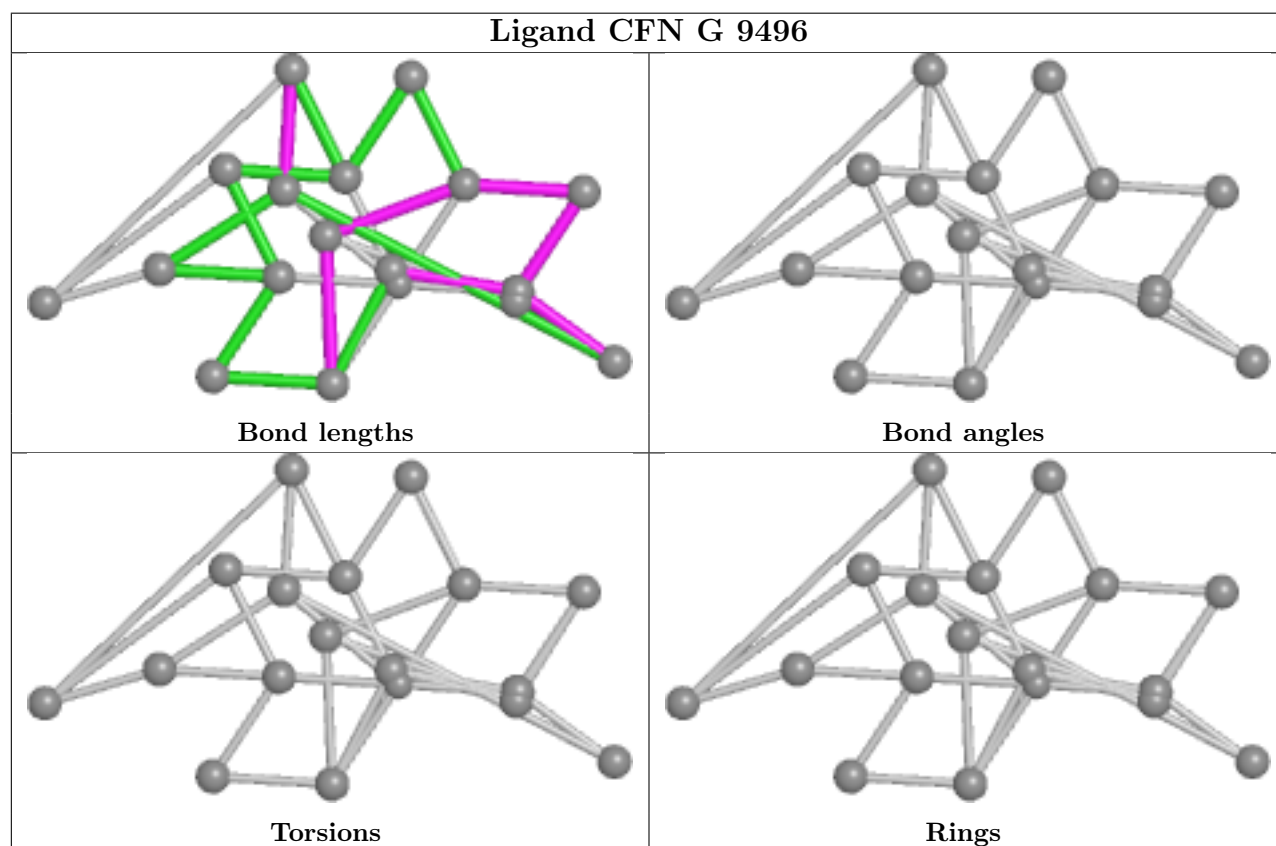
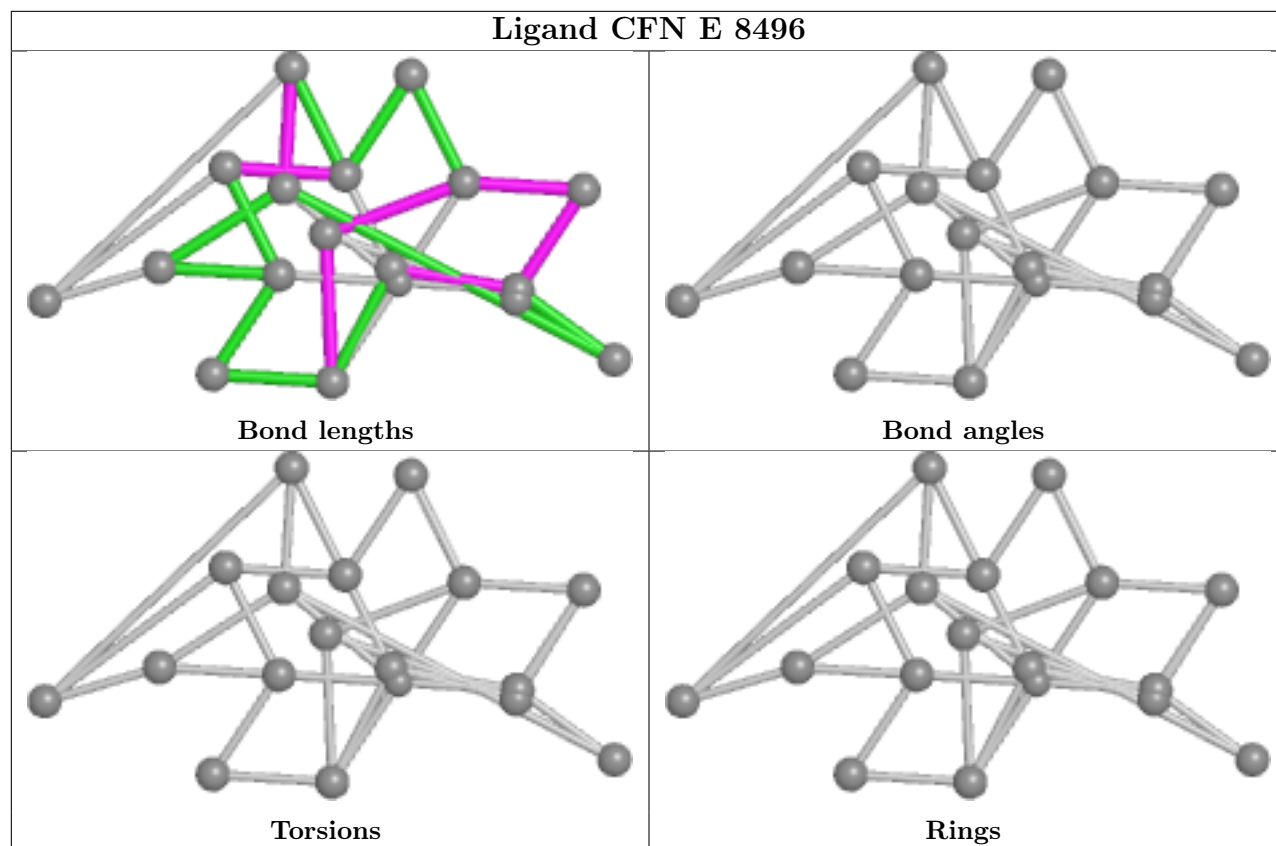
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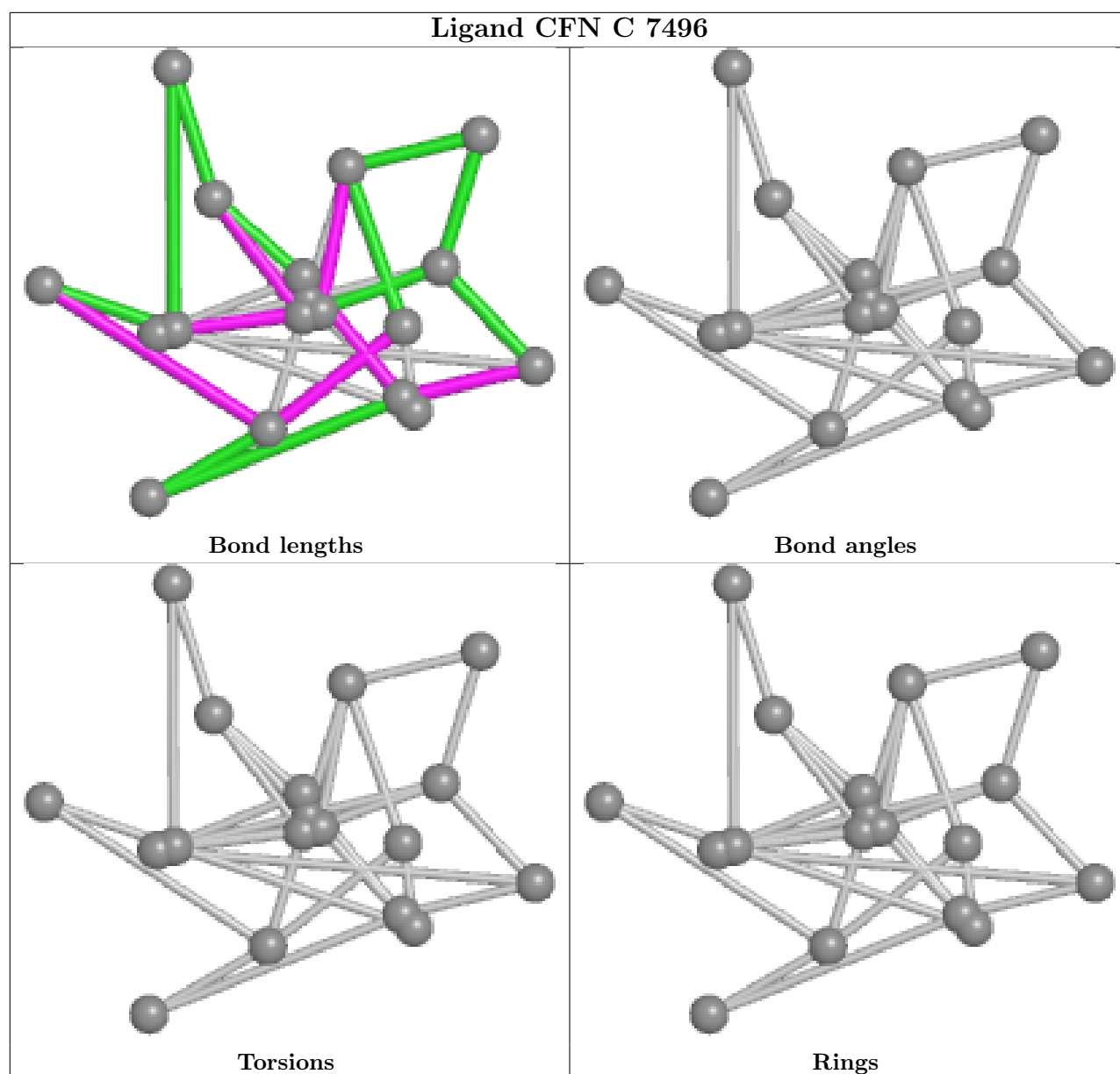
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	8494	HCA	1	0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.