



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:12 am BST

PDB ID : 5JQU
Title : Crystal structure of Cytochrome P450 BM3 heme domain G265F/T269V/L272 W/L322I/F405M/A406S (WIVS-FM) variant with iron(III) deuteroporphyrin IX bound
Authors : Reynolds, E.W.; McHenry, M.W.; Cannac, F.; Gober, J.G.; Snow, C.D.; Brustad, E.M.
Deposited on : 2016-05-05
Resolution : 2.16 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 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

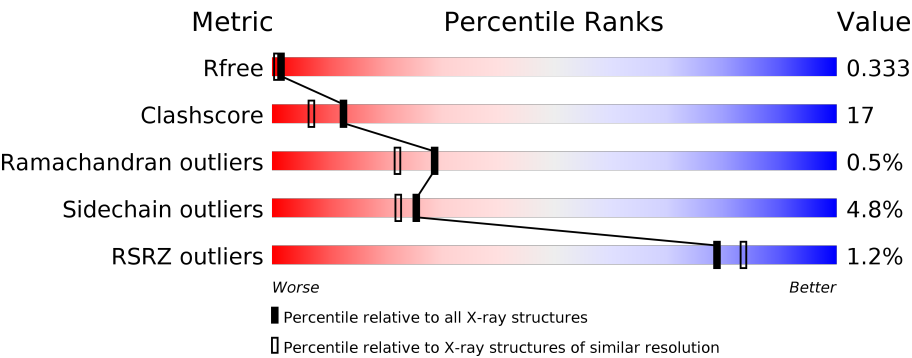
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	471	
1	B	471	
1	C	471	
1	D	471	
1	E	471	
1	F	471	

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Mol	Chain	Length	Quality of chain
1	G	471	<div><div><div>%</div><div><div></div></div><div>59%34%</div><div><div></div><div></div></div></div></div>
1	H	471	<div><div><div>%</div><div><div></div></div><div>62%32%</div><div><div></div><div></div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29916 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3554	2284	606	646	18			
1	B	453	Total	C	N	O	S	0	0	0
			3578	2293	607	660	18			
1	C	453	Total	C	N	O	S	0	0	0
			3552	2281	604	650	17			
1	D	454	Total	C	N	O	S	0	0	0
			3485	2243	591	633	18			
1	E	451	Total	C	N	O	S	0	1	0
			3579	2299	606	656	18			
1	F	455	Total	C	N	O	S	0	0	0
			3543	2275	602	648	18			
1	G	451	Total	C	N	O	S	0	2	0
			3546	2274	600	655	17			
1	H	450	Total	C	N	O	S	0	0	0
			3571	2294	605	654	18			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	PHE	GLY	engineered mutation	UNP P14779
A	269	VAL	THR	engineered mutation	UNP P14779
A	272	TRP	LEU	engineered mutation	UNP P14779
A	322	ILE	LEU	engineered mutation	UNP P14779
A	405	MET	PHE	engineered mutation	UNP P14779
A	406	SER	ALA	engineered mutation	UNP P14779
A	464	LEU	-	expression tag	UNP P14779
A	465	GLU	-	expression tag	UNP P14779
A	466	HIS	-	expression tag	UNP P14779
A	467	HIS	-	expression tag	UNP P14779
A	468	HIS	-	expression tag	UNP P14779
A	469	HIS	-	expression tag	UNP P14779
A	470	HIS	-	expression tag	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
A	471	HIS	-	expression tag	UNP P14779
B	265	PHE	GLY	engineered mutation	UNP P14779
B	269	VAL	THR	engineered mutation	UNP P14779
B	272	TRP	LEU	engineered mutation	UNP P14779
B	322	ILE	LEU	engineered mutation	UNP P14779
B	405	MET	PHE	engineered mutation	UNP P14779
B	406	SER	ALA	engineered mutation	UNP P14779
B	464	LEU	-	expression tag	UNP P14779
B	465	GLU	-	expression tag	UNP P14779
B	466	HIS	-	expression tag	UNP P14779
B	467	HIS	-	expression tag	UNP P14779
B	468	HIS	-	expression tag	UNP P14779
B	469	HIS	-	expression tag	UNP P14779
B	470	HIS	-	expression tag	UNP P14779
B	471	HIS	-	expression tag	UNP P14779
C	265	PHE	GLY	engineered mutation	UNP P14779
C	269	VAL	THR	engineered mutation	UNP P14779
C	272	TRP	LEU	engineered mutation	UNP P14779
C	322	ILE	LEU	engineered mutation	UNP P14779
C	405	MET	PHE	engineered mutation	UNP P14779
C	406	SER	ALA	engineered mutation	UNP P14779
C	464	LEU	-	expression tag	UNP P14779
C	465	GLU	-	expression tag	UNP P14779
C	466	HIS	-	expression tag	UNP P14779
C	467	HIS	-	expression tag	UNP P14779
C	468	HIS	-	expression tag	UNP P14779
C	469	HIS	-	expression tag	UNP P14779
C	470	HIS	-	expression tag	UNP P14779
C	471	HIS	-	expression tag	UNP P14779
D	265	PHE	GLY	engineered mutation	UNP P14779
D	269	VAL	THR	engineered mutation	UNP P14779
D	272	TRP	LEU	engineered mutation	UNP P14779
D	322	ILE	LEU	engineered mutation	UNP P14779
D	405	MET	PHE	engineered mutation	UNP P14779
D	406	SER	ALA	engineered mutation	UNP P14779
D	464	LEU	-	expression tag	UNP P14779
D	465	GLU	-	expression tag	UNP P14779
D	466	HIS	-	expression tag	UNP P14779
D	467	HIS	-	expression tag	UNP P14779
D	468	HIS	-	expression tag	UNP P14779
D	469	HIS	-	expression tag	UNP P14779
D	470	HIS	-	expression tag	UNP P14779

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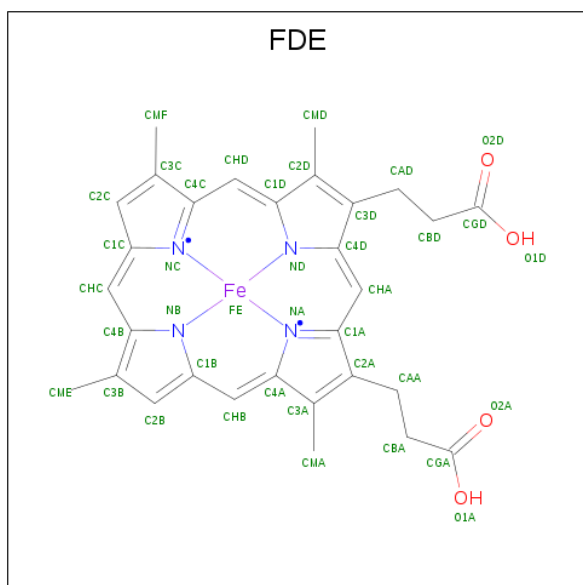
Chain	Residue	Modelled	Actual	Comment	Reference
D	471	HIS	-	expression tag	UNP P14779
E	265	PHE	GLY	engineered mutation	UNP P14779
E	269	VAL	THR	engineered mutation	UNP P14779
E	272	TRP	LEU	engineered mutation	UNP P14779
E	322	ILE	LEU	engineered mutation	UNP P14779
E	405	MET	PHE	engineered mutation	UNP P14779
E	406	SER	ALA	engineered mutation	UNP P14779
E	464	LEU	-	expression tag	UNP P14779
E	465	GLU	-	expression tag	UNP P14779
E	466	HIS	-	expression tag	UNP P14779
E	467	HIS	-	expression tag	UNP P14779
E	468	HIS	-	expression tag	UNP P14779
E	469	HIS	-	expression tag	UNP P14779
E	470	HIS	-	expression tag	UNP P14779
E	471	HIS	-	expression tag	UNP P14779
F	265	PHE	GLY	engineered mutation	UNP P14779
F	269	VAL	THR	engineered mutation	UNP P14779
F	272	TRP	LEU	engineered mutation	UNP P14779
F	322	ILE	LEU	engineered mutation	UNP P14779
F	405	MET	PHE	engineered mutation	UNP P14779
F	406	SER	ALA	engineered mutation	UNP P14779
F	464	LEU	-	expression tag	UNP P14779
F	465	GLU	-	expression tag	UNP P14779
F	466	HIS	-	expression tag	UNP P14779
F	467	HIS	-	expression tag	UNP P14779
F	468	HIS	-	expression tag	UNP P14779
F	469	HIS	-	expression tag	UNP P14779
F	470	HIS	-	expression tag	UNP P14779
F	471	HIS	-	expression tag	UNP P14779
G	265	PHE	GLY	engineered mutation	UNP P14779
G	269	VAL	THR	engineered mutation	UNP P14779
G	272	TRP	LEU	engineered mutation	UNP P14779
G	322	ILE	LEU	engineered mutation	UNP P14779
G	405	MET	PHE	engineered mutation	UNP P14779
G	406	SER	ALA	engineered mutation	UNP P14779
G	464	LEU	-	expression tag	UNP P14779
G	465	GLU	-	expression tag	UNP P14779
G	466	HIS	-	expression tag	UNP P14779
G	467	HIS	-	expression tag	UNP P14779
G	468	HIS	-	expression tag	UNP P14779
G	469	HIS	-	expression tag	UNP P14779
G	470	HIS	-	expression tag	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
G	471	HIS	-	expression tag	UNP P14779
H	265	PHE	GLY	engineered mutation	UNP P14779
H	269	VAL	THR	engineered mutation	UNP P14779
H	272	TRP	LEU	engineered mutation	UNP P14779
H	322	ILE	LEU	engineered mutation	UNP P14779
H	405	MET	PHE	engineered mutation	UNP P14779
H	406	SER	ALA	engineered mutation	UNP P14779
H	464	LEU	-	expression tag	UNP P14779
H	465	GLU	-	expression tag	UNP P14779
H	466	HIS	-	expression tag	UNP P14779
H	467	HIS	-	expression tag	UNP P14779
H	468	HIS	-	expression tag	UNP P14779
H	469	HIS	-	expression tag	UNP P14779
H	470	HIS	-	expression tag	UNP P14779
H	471	HIS	-	expression tag	UNP P14779

- Molecule 2 is FE(III) DEUTEROPORPHYRIN IX (three-letter code: FDE) (formula: $C_{30}H_{28}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	B	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	C	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	D	1	Total 39	C 30	Fe 1	N 4	O 4	0	0

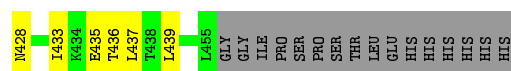
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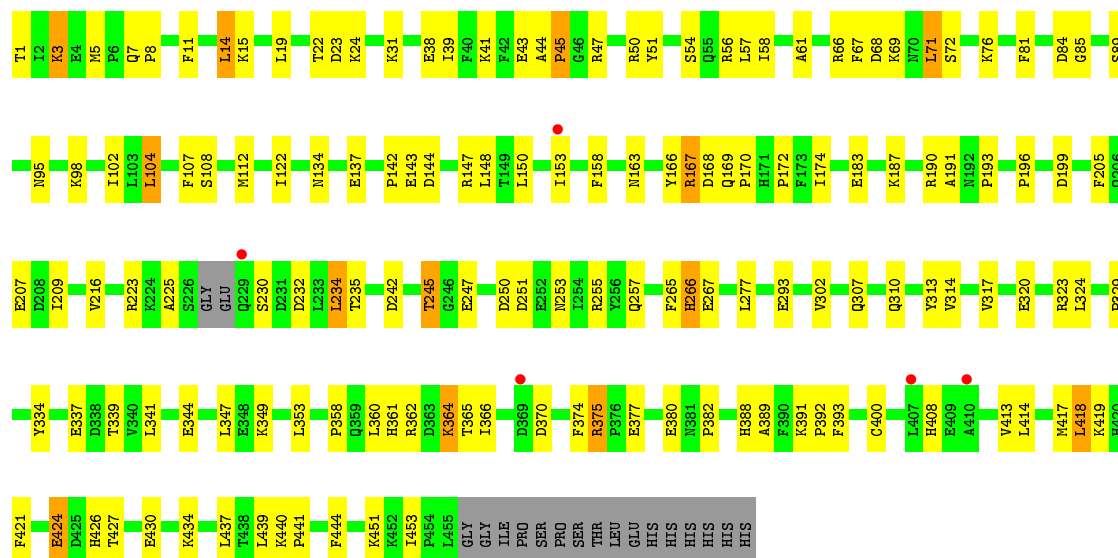
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	Fe	N	O	0	0
			39	30	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			39	30	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			39	30	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			39	30	1	4	4		

- Molecule 3 is water.

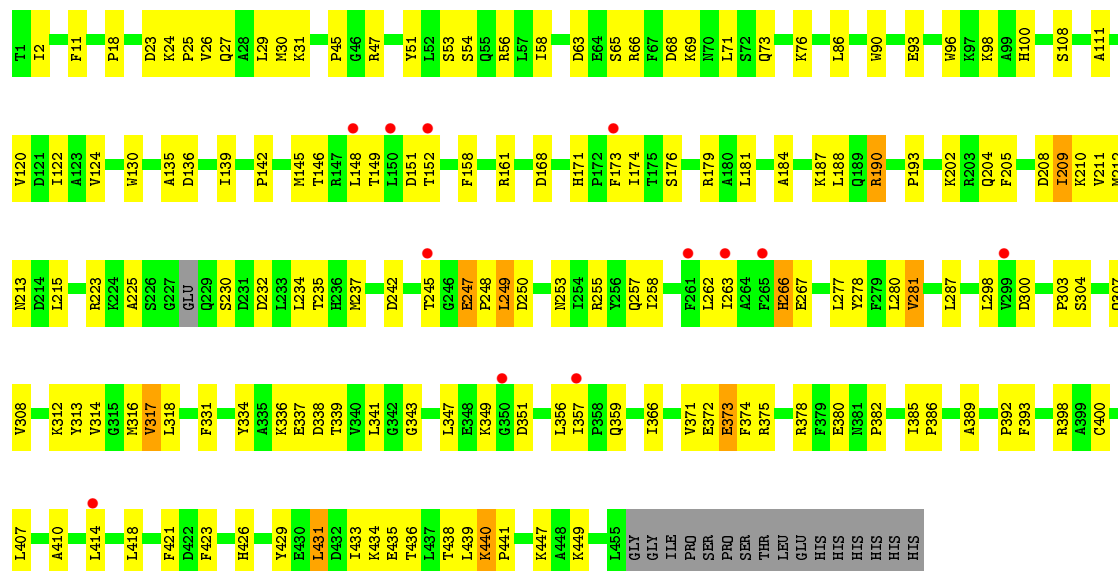
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	189	Total	O	0	0
			189	189		
3	C	165	Total	O	0	0
			165	165		
3	D	112	Total	O	0	0
			112	112		
3	E	155	Total	O	0	0
			155	155		
3	F	117	Total	O	0	0
			117	117		
3	G	138	Total	O	0	0
			138	138		
3	H	171	Total	O	0	0
			171	171		



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

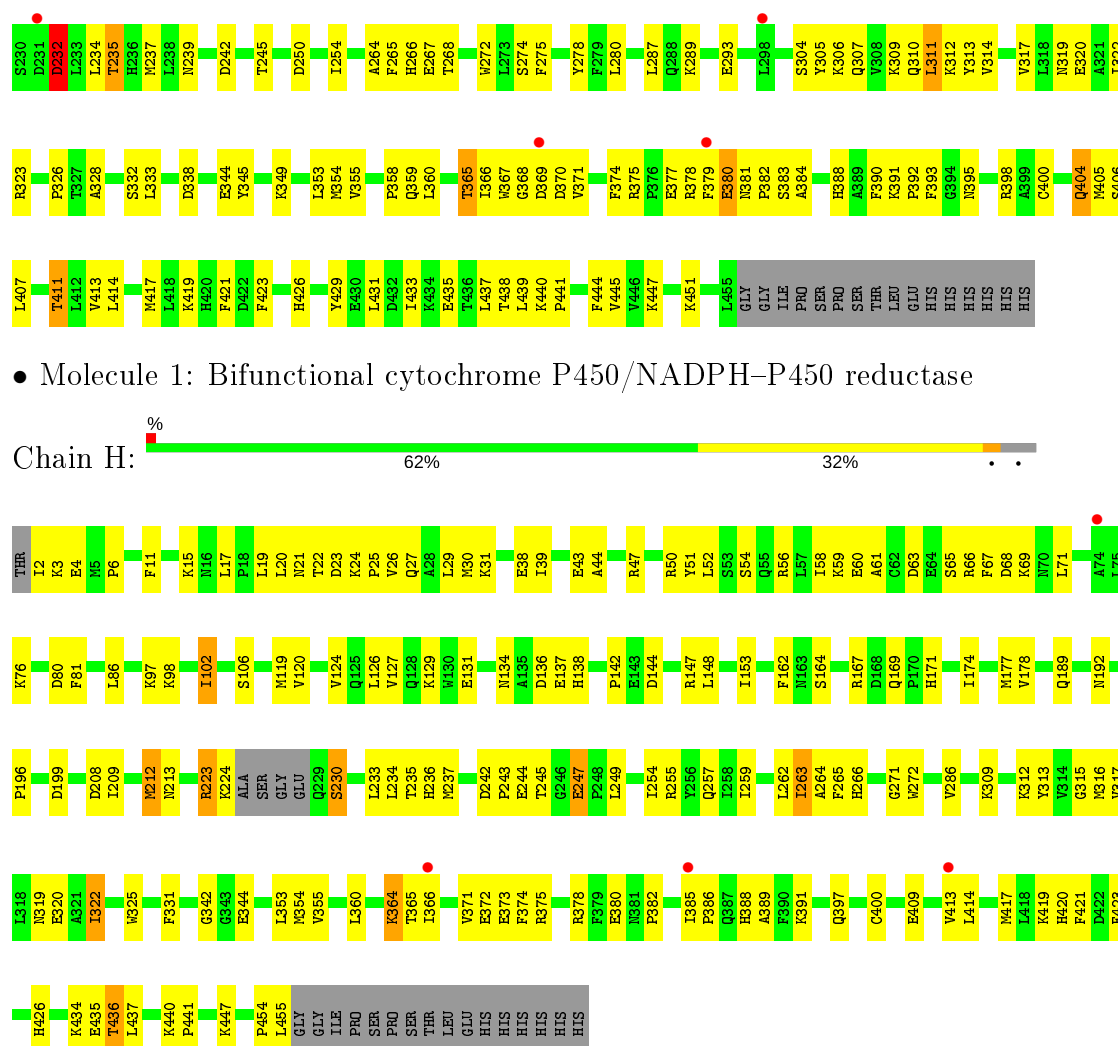


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.06 Å 166.30 Å 229.33 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.85 – 2.16 28.85 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.85-2.16) 98.9 (28.85-2.16)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.16 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.258 , 0.334 0.259 , 0.333	Depositor DCC
R_{free} test set	2000 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	29916	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.37% 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: FDE

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	0.53	0/3640	0.70	3/4939 (0.1%)
1	B	0.56	0/3665	0.72	1/4972 (0.0%)
1	C	0.53	0/3637	0.72	3/4936 (0.1%)
1	D	0.51	0/3571	0.69	2/4855 (0.0%)
1	E	0.54	1/3668 (0.0%)	0.70	1/4974 (0.0%)
1	F	0.54	2/3629 (0.1%)	0.68	1/4930 (0.0%)
1	G	0.53	0/3638	0.70	1/4939 (0.0%)
1	H	0.51	0/3657	0.70	0/4955
All	All	0.53	3/29105 (0.0%)	0.70	12/39500 (0.0%)

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	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	156	CYS	CB-SG	-6.66	1.71	1.82
1	F	400	CYS	CB-SG	-6.36	1.71	1.82
1	F	156	CYS	CB-SG	-5.72	1.72	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	C	168	ASP	C-N-CA	6.84	138.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	232	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	356	LEU	CA-CB-CG	6.11	129.36	115.30
1	C	71	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	14	LEU	CA-CB-CG	5.75	128.53	115.30
1	E	356	LEU	CA-CB-CG	5.72	128.47	115.30
1	A	436	THR	C-N-CA	-5.53	107.87	121.70
1	D	188	LEU	CA-CB-CG	5.51	127.97	115.30
1	C	14	LEU	CA-CB-CG	5.40	127.72	115.30
1	D	431	LEU	CA-CB-CG	5.37	127.65	115.30
1	F	195	ASP	CB-CG-OD1	5.25	123.03	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	ILE	Peptide

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	3554	0	3443	121	0
1	B	3578	0	3463	114	0
1	C	3552	0	3444	109	0
1	D	3485	0	3286	116	0
1	E	3579	0	3482	90	0
1	F	3543	0	3387	138	0
1	G	3546	0	3392	143	0
1	H	3571	0	3480	121	0
2	A	39	0	25	2	0
2	B	39	0	25	2	0
2	C	39	0	25	2	0
2	D	39	0	25	2	0
2	E	39	0	25	3	0
2	F	39	0	25	1	0
2	G	39	0	25	4	0
2	H	39	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	149	0	0	27	0
3	B	189	0	0	21	0
3	C	165	0	0	19	1
3	D	112	0	0	10	0
3	E	155	0	0	10	2
3	F	117	0	0	12	0
3	G	138	0	0	21	0
3	H	171	0	0	23	1
All	All	29916	0	27577	941	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (941) 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:G:272:TRP:CD1	1:G:322:ILE:CD1	2.39	1.05
1:G:272:TRP:NE1	1:G:322:ILE:HD13	1.75	1.02
1:G:391:LYS:NZ	3:G:601:HOH:O	1.92	1.02
1:A:68:ASP:HB2	1:A:336:LYS:NZ	1.75	1.01
1:G:272:TRP:CD1	1:G:322:ILE:HD13	1.99	0.96
1:H:106:SER:HG	1:H:236:HIS:HD1	1.10	0.96
1:G:272:TRP:CD1	1:G:322:ILE:HD11	2.00	0.95
1:F:223:ARG:NH2	1:F:232:ASP:OD2	2.00	0.94
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.31	0.94
1:E:218:LYS:NZ	3:E:602:HOH:O	2.02	0.92
1:A:277:LEU:HD21	1:A:417:MET:HE1	1.49	0.91
1:H:162:PHE:O	1:H:167:ARG:NH2	2.02	0.91
1:D:312:LYS:HE3	1:D:380:GLU:HG3	1.52	0.91
1:C:440:LYS:NZ	3:C:601:HOH:O	2.02	0.91
1:C:223:ARG:HH12	1:C:235:THR:HG23	1.37	0.86
1:F:282:LYS:NZ	1:F:425:ASP:OD2	2.09	0.86
1:A:68:ASP:HB2	1:A:336:LYS:HZ3	1.40	0.85
1:H:373:GLU:OE2	1:H:375:ARG:NE	2.10	0.84
1:H:436:THR:OG1	1:H:437:LEU:N	2.06	0.84
1:B:302:VAL:O	3:B:601:HOH:O	1.96	0.84
1:C:358:PRO:O	1:C:362:ARG:NH1	2.10	0.83
1:A:296:ARG:NH2	3:A:604:HOH:O	2.11	0.83
1:E:170:PRO:O	3:E:601:HOH:O	1.97	0.82
1:D:122:ILE:HG22	1:D:148:LEU:HD12	1.61	0.82
1:G:237:MET:HE2	1:G:254:ILE:HG23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:NZ	1:F:21:ASN:HD21	1.78	0.82
1:F:91:THR:HB	1:F:398:ARG:HH11	1.45	0.82
1:D:98:LYS:HG3	1:D:242:ASP:HB3	1.62	0.81
1:C:324:LEU:O	1:C:362:ARG:NH2	2.12	0.81
1:A:86:LEU:H	1:A:257:GLN:HE22	1.29	0.80
1:B:48:VAL:O	3:B:602:HOH:O	1.98	0.80
1:H:17:LEU:O	3:H:601:HOH:O	2.00	0.79
1:F:50:ARG:NH1	3:F:604:HOH:O	2.14	0.79
1:H:385:ILE:HD12	1:H:386:PRO:HD2	1.64	0.79
1:C:223:ARG:NH1	1:C:235:THR:HG23	1.97	0.79
1:B:86:LEU:H	1:B:257:GLN:HE22	1.28	0.78
1:H:189:GLN:OE1	3:H:601:HOH:O	1.99	0.78
1:G:93:GLU:HG2	3:G:606:HOH:O	1.82	0.78
1:E:247:GLU:HG3	1:E:248:PRO:HD2	1.64	0.77
1:B:26:VAL:N	1:B:435:GLU:OE2	2.17	0.77
1:E:179:ARG:NH1	1:E:208:ASP:OD1	2.18	0.77
1:B:223:ARG:NH1	1:B:223:ARG:HG3	1.91	0.77
1:F:277:LEU:HD21	1:F:417:MET:HE1	1.67	0.76
1:G:433:ILE:HD12	1:G:440:LYS:O	1.85	0.76
1:B:20:LEU:HD13	1:B:25:PRO:HB3	1.67	0.76
1:D:142:PRO:O	3:D:602:HOH:O	2.04	0.75
1:A:424:GLU:OE2	3:A:601:HOH:O	2.03	0.75
1:E:267:GLU:O	3:E:603:HOH:O	2.04	0.75
1:C:150:LEU:HD22	1:C:174:ILE:HD11	1.68	0.75
1:D:136:ASP:OD1	3:D:601:HOH:O	2.04	0.75
1:F:132:ARG:NH1	1:G:125:GLN:OE1	2.20	0.74
1:H:56:ARG:NH2	1:H:344:GLU:OE2	2.21	0.74
1:C:183:GLU:HG3	1:C:187:LYS:HD2	1.68	0.74
1:G:25:PRO:HG2	1:G:185:MET:HE2	1.69	0.74
1:B:132:ARG:NH1	1:C:166:TYR:OH	2.21	0.74
1:B:196:PRO:HG3	1:G:11:PHE:CE2	2.23	0.74
1:D:375:ARG:H	1:D:378:ARG:HH12	1.36	0.74
1:D:267:GLU:OE1	1:D:438:THR:OG1	2.05	0.74
1:C:216:VAL:HG11	1:C:255:ARG:HG3	1.68	0.73
1:C:230:SER:O	1:C:235:THR:HG21	1.87	0.73
1:B:211:VAL:O	3:B:603:HOH:O	2.05	0.73
1:F:43:GLU:HG2	1:F:48:VAL:HG22	1.70	0.73
1:E:81:PHE:HB3	1:E:209:ILE:HG12	1.70	0.73
1:G:223:ARG:HD2	1:G:234:LEU:HD22	1.71	0.73
1:B:43:GLU:HG2	1:B:48:VAL:HG22	1.69	0.73
1:E:280:LEU:HB3	1:E:287:LEU:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:N	3:A:612:HOH:O	2.22	0.72
1:G:407:LEU:O	1:G:411:THR:OG1	2.06	0.72
1:B:277:LEU:HD22	1:B:417:MET:HE1	1.72	0.72
1:E:173:PHE:HE2	1:E:177:MET:HE2	1.55	0.71
1:A:94:LYS:HZ3	1:F:21:ASN:HD21	1.38	0.71
1:H:315:GLY:O	1:H:319:ASN:ND2	2.21	0.71
1:A:223:ARG:NH2	1:A:232:ASP:OD2	2.24	0.71
1:D:317:VAL:HG23	1:D:374:PHE:HZ	1.55	0.71
1:B:143:GLU:N	1:B:143:GLU:OE2	2.24	0.71
1:H:119:MET:SD	3:H:677:HOH:O	2.48	0.71
1:A:64:GLU:OE1	3:A:603:HOH:O	2.08	0.71
1:B:223:ARG:HE	1:B:235:THR:HG23	1.53	0.71
1:C:143:GLU:O	3:C:602:HOH:O	2.09	0.71
1:H:120:VAL:O	1:H:124:VAL:HG23	1.91	0.71
1:A:223:ARG:HE	1:A:234:LEU:HD23	1.55	0.70
1:F:223:ARG:C	1:F:225:ALA:H	1.93	0.70
1:G:250:ASP:OD1	3:G:602:HOH:O	2.08	0.70
1:G:95:ASN:N	3:G:606:HOH:O	2.19	0.70
1:G:323:ARG:NH1	1:G:371:VAL:O	2.25	0.70
1:G:34:ASP:OD1	1:G:359:GLN:NE2	2.25	0.70
1:C:148:LEU:HD21	1:C:413:VAL:HG21	1.74	0.69
1:C:421:PHE:N	1:C:451:LYS:HZ1	1.90	0.69
1:E:414:LEU:HA	1:E:417:MET:HE2	1.74	0.69
1:A:431:LEU:O	3:A:602:HOH:O	2.08	0.69
1:E:404:GLN:OE1	1:E:405:MET:N	2.25	0.69
1:H:167:ARG:NH2	1:H:171:HIS:HD2	1.91	0.69
1:D:426:HIS:CG	1:D:447:LYS:HD2	2.28	0.68
1:B:308:VAL:HA	3:B:620:HOH:O	1.93	0.68
1:B:192:ASN:HB3	1:G:14:LEU:HD11	1.76	0.68
1:G:232:ASP:OD1	1:G:234:LEU:N	2.26	0.68
1:C:122:ILE:HG22	1:C:148:LEU:HD12	1.75	0.68
1:G:272:TRP:CG	1:G:322:ILE:HD11	2.28	0.68
1:H:80:ASP:OD2	3:H:602:HOH:O	2.11	0.68
1:C:8:PRO:O	3:C:604:HOH:O	2.11	0.68
1:C:134:ASN:OD1	3:C:603:HOH:O	2.11	0.68
1:D:51:TYR:HB3	1:D:356:LEU:HD11	1.76	0.68
1:A:119:MET:O	3:A:605:HOH:O	2.11	0.68
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.06	0.67
1:E:404:GLN:NE2	3:E:609:HOH:O	2.27	0.67
1:H:21:ASN:OD1	3:H:603:HOH:O	2.12	0.67
1:D:213:ASN:HB3	1:D:255:ARG:HH21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:ARG:HG2	1:H:164:SER:HB3	1.77	0.67
1:B:296:ARG:HD2	3:B:616:HOH:O	1.93	0.67
1:D:375:ARG:N	1:D:378:ARG:HH12	1.93	0.67
1:C:134:ASN:N	1:C:137:GLU:OE1	2.22	0.66
1:B:169:GLN:HG2	3:B:683:HOH:O	1.94	0.66
1:E:167:ARG:NH1	3:E:601:HOH:O	2.29	0.66
1:E:173:PHE:HB2	1:E:215[B]:LEU:HD22	1.76	0.66
1:F:20:LEU:HD11	1:F:29:LEU:HG	1.77	0.66
1:A:436:THR:OG1	1:A:437:LEU:N	2.28	0.66
1:G:179:ARG:HD2	1:G:208:ASP:OD2	1.95	0.66
1:F:223:ARG:O	1:F:225:ALA:N	2.29	0.66
1:F:280:LEU:HD21	1:F:317:VAL:HG11	1.78	0.66
1:H:153:ILE:HG12	3:H:631:HOH:O	1.96	0.66
1:C:68:ASP:HB3	1:C:334:TYR:CE1	2.31	0.65
1:D:25:PRO:HD2	1:D:435:GLU:OE2	1.96	0.65
1:D:27:GLN:NE2	1:D:433:ILE:HB	2.11	0.65
1:A:196:PRO:HG3	1:H:11:PHE:CE2	2.31	0.65
1:G:272:TRP:NE1	1:G:322:ILE:CD1	2.48	0.65
1:B:436:THR:OG1	1:B:437:LEU:N	2.30	0.65
1:C:329:PRO:HB3	1:C:439:LEU:HD11	1.77	0.65
1:F:75:LEU:HA	1:F:78:VAL:HG22	1.78	0.65
1:G:395:ASN:O	3:G:604:HOH:O	2.14	0.65
1:D:314:VAL:HG13	1:D:414:LEU:HD22	1.79	0.65
1:E:43:GLU:HG3	1:E:48:VAL:HG22	1.79	0.65
1:E:366:ILE:HG21	1:E:389:ALA:HB1	1.79	0.64
1:E:112:MET:HE1	1:E:405:MET:HG3	1.80	0.64
1:E:66:ARG:NH1	1:E:339:THR:OG1	2.30	0.64
1:H:265:PHE:HB3	3:H:631:HOH:O	1.97	0.64
1:D:47:ARG:HD2	1:D:73:GLN:HG2	1.79	0.64
1:F:122:ILE:HG22	1:F:148:LEU:HD12	1.80	0.64
1:B:245:THR:HG23	1:B:247:GLU:H	1.62	0.64
1:D:312:LYS:CE	1:D:380:GLU:HG3	2.25	0.64
1:D:414:LEU:O	1:D:418:LEU:HD22	1.97	0.64
1:D:375:ARG:H	1:D:378:ARG:NH1	1.95	0.63
1:E:90:TRP:HB2	1:E:93:GLU:HG3	1.80	0.63
1:H:38:GLU:HG3	1:H:39:ILE:HG22	1.79	0.63
1:G:58:ILE:HG13	1:G:360:LEU:HD13	1.79	0.63
1:G:370:ASP:OD2	1:G:375:ARG:NH2	2.31	0.63
1:A:288:GLN:O	1:A:292:GLU:HG2	1.99	0.63
1:G:74:ALA:O	1:G:78:VAL:HG23	1.99	0.63
1:H:171:HIS:HB3	1:H:174:ILE:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:OE2	1:E:341:LEU:HD12	1.98	0.63
1:B:203:ARG:NH1	3:B:608:HOH:O	2.32	0.63
1:C:71:LEU:HD13	1:C:76:LYS:HG2	1.80	0.63
1:D:69:LYS:HD2	1:D:398:ARG:HE	1.63	0.63
1:E:173:PHE:CE2	1:E:177:MET:HE2	2.34	0.63
1:F:296:ARG:NH2	3:F:601:HOH:O	2.10	0.63
1:E:436:THR:OG1	1:E:437:LEU:N	2.32	0.63
1:B:181:LEU:HD22	1:B:437:LEU:HB2	1.80	0.62
1:A:167:ARG:NH1	1:A:171:HIS:HD2	1.96	0.62
1:F:242:ASP:HB3	3:F:608:HOH:O	1.99	0.62
1:D:249:LEU:O	3:D:603:HOH:O	2.16	0.62
1:A:51:TYR:HB3	1:A:356:LEU:HD11	1.81	0.62
1:F:20:LEU:HD12	1:F:25:PRO:HB3	1.81	0.62
1:F:253:ASN:O	1:F:257:GLN:HG2	2.00	0.62
1:B:250:ASP:OD1	1:B:253:ASN:N	2.32	0.62
1:B:38:GLU:OE1	1:B:56:ARG:NH1	2.33	0.62
1:H:426:HIS:CD2	1:H:447:LYS:HE2	2.34	0.62
1:H:47:ARG:NH2	3:H:617:HOH:O	2.33	0.62
1:A:51:TYR:CE2	1:A:354:MET:HG2	2.34	0.62
1:G:313:TYR:O	1:G:317:VAL:HG23	2.00	0.62
1:C:167:ARG:HH21	1:C:172:PRO:HD3	1.65	0.62
1:G:317:VAL:HG13	1:G:374:PHE:HZ	1.64	0.62
1:H:223:ARG:NH1	1:H:234:LEU:HD23	2.15	0.62
1:B:173:PHE:CD1	1:B:215:LEU:HD21	2.35	0.61
1:D:171:HIS:HB2	1:D:174:ILE:HG12	1.82	0.61
1:E:380:GLU:OE2	1:E:380:GLU:HA	1.98	0.61
1:A:101:ASN:O	3:A:606:HOH:O	2.16	0.61
1:B:242:ASP:OD2	1:B:245:THR:HG22	2.00	0.61
1:H:263:ILE:HG13	1:H:264:ALA:N	2.15	0.61
1:F:26:VAL:N	1:F:435:GLU:OE2	2.34	0.61
1:F:313:TYR:O	1:F:317:VAL:HG23	2.01	0.61
1:A:367:TRP:N	3:A:611:HOH:O	2.19	0.61
1:B:260:THR:HA	3:B:736:HOH:O	2.00	0.61
1:A:405:MET:O	3:A:608:HOH:O	2.16	0.61
1:B:223:ARG:NH2	1:B:230:SER:HB2	2.16	0.61
1:D:179:ARG:HH21	1:D:204:GLN:HB2	1.65	0.60
1:G:55:GLN:OE1	3:G:605:HOH:O	2.17	0.60
1:H:2:ILE:N	3:H:618:HOH:O	2.33	0.60
1:H:265:PHE:HB2	2:H:501:FDE:HMF3	1.83	0.60
1:G:344:GLU:HG3	1:G:345:TYR:CE2	2.35	0.60
1:H:366:ILE:HG21	1:H:389:ALA:HB1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ARG:NH2	3:H:613:HOH:O	2.30	0.60
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.84	0.60
1:C:69:LYS:NZ	3:C:605:HOH:O	2.15	0.60
1:D:312:LYS:NZ	1:D:380:GLU:HA	2.16	0.60
1:D:27:GLN:HE22	1:D:433:ILE:HB	1.65	0.60
1:C:380:GLU:O	1:C:382:PRO:HD3	2.02	0.60
1:B:223:ARG:NE	1:B:235:THR:HG23	2.16	0.60
1:C:15:LYS:NZ	1:C:43:GLU:OE2	2.35	0.60
1:H:129:LYS:NZ	1:H:144:ASP:OD1	2.29	0.60
1:G:69:LYS:NZ	3:G:615:HOH:O	2.34	0.59
1:D:277:LEU:O	1:D:281:VAL:HG23	2.02	0.59
1:D:69:LYS:HD2	1:D:398:ARG:NE	2.16	0.59
1:F:429:TYR:CE2	1:F:444:PHE:HD1	2.20	0.59
1:C:250:ASP:OD2	3:C:606:HOH:O	2.17	0.59
1:C:57:LEU:HD22	1:C:341:LEU:HG	1.84	0.59
1:H:124:VAL:HG13	1:H:455:LEU:HD13	1.84	0.59
1:D:280:LEU:HB3	1:D:287:LEU:HD13	1.83	0.59
1:C:187:LYS:HE3	3:C:691:HOH:O	2.03	0.59
1:E:18:PRO:HA	1:E:21:ASN:OD1	2.03	0.59
1:F:177:MET:HE2	1:F:263:ILE:HG23	1.83	0.59
1:F:421:PHE:HB2	1:F:423:PHE:CZ	2.37	0.59
1:G:51:TYR:CE2	1:G:354:MET:HG2	2.38	0.59
1:H:419:LYS:HE2	1:H:420:HIS:NE2	2.18	0.59
1:A:171:HIS:HB3	1:A:174:ILE:HG22	1.84	0.59
1:G:305:TYR:CZ	1:G:309:LYS:HE2	2.38	0.59
1:B:313:TYR:O	1:B:317:VAL:HG23	2.03	0.59
1:D:304:SER:OG	1:D:307:GLN:HG2	2.03	0.59
1:F:141:VAL:HB	1:F:444:PHE:HD2	1.67	0.59
1:A:52:LEU:HD11	1:A:353:LEU:HD22	1.85	0.58
1:H:388:HIS:HA	1:H:391:LYS:HD3	1.85	0.58
1:G:268:THR:HG22	3:G:646:HOH:O	2.02	0.58
1:E:203:ARG:NH1	3:E:618:HOH:O	2.36	0.58
1:H:196:PRO:HA	1:H:199:ASP:OD2	2.04	0.58
1:A:257:GLN:HB3	1:A:261:PHE:HE2	1.69	0.58
1:A:312:LYS:HZ1	1:A:380:GLU:HG2	1.68	0.58
1:A:378:ARG:O	3:A:609:HOH:O	2.17	0.58
1:B:21:ASN:HB2	1:B:189:GLN:OE1	2.03	0.58
1:B:329:PRO:HB3	1:B:439:LEU:HD11	1.84	0.58
1:F:66:ARG:HH11	1:F:339:THR:HG21	1.68	0.58
1:D:223:ARG:HE	1:D:234:LEU:HD23	1.67	0.58
1:E:122:ILE:HG22	1:E:148:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:GLU:O	1:E:382:PRO:HD3	2.03	0.58
1:G:13:GLU:CD	1:G:13:GLU:H	2.05	0.58
1:H:382:PRO:O	1:H:385:ILE:HG22	2.03	0.58
1:D:230:SER:O	1:D:235:THR:HG21	2.02	0.58
1:H:25:PRO:HD2	1:H:435:GLU:OE2	2.04	0.58
1:B:223:ARG:NH1	1:B:234:LEU:HD22	2.18	0.58
1:G:280:LEU:HB3	1:G:287:LEU:HD12	1.85	0.58
1:E:363:ASP:OD2	1:E:366:ILE:HD13	2.04	0.57
1:G:167:ARG:HD3	3:G:665:HOH:O	2.03	0.57
1:A:90:TRP:HB2	1:A:93:GLU:HG3	1.86	0.57
1:D:146:THR:N	3:D:602:HOH:O	2.37	0.57
1:H:142:PRO:HB3	3:H:675:HOH:O	2.04	0.57
1:A:404:GLN:NE2	3:A:620:HOH:O	2.35	0.57
1:B:120:VAL:O	1:B:124:VAL:HG23	2.04	0.57
1:B:68:ASP:HB3	1:B:334:TYR:CE1	2.39	0.57
1:G:61:ALA:HA	1:G:67:PHE:CD2	2.37	0.57
1:H:414:LEU:HA	1:H:417:MET:HE2	1.86	0.57
1:A:368:GLY:O	1:A:371:VAL:HG13	2.05	0.57
1:C:107:PHE:HB3	3:C:688:HOH:O	2.04	0.57
1:C:5:MET:HG2	1:C:41:LYS:HB2	1.85	0.57
1:C:58:ILE:HG13	1:C:360:LEU:HD13	1.85	0.57
1:D:212:MET:HE1	1:D:263:ILE:HD11	1.87	0.57
1:C:56:ARG:NE	3:C:620:HOH:O	2.37	0.57
1:G:86:LEU:O	1:G:398:ARG:NH2	2.38	0.57
1:C:235:THR:HG22	3:C:654:HOH:O	2.03	0.57
1:H:414:LEU:HA	1:H:417:MET:CE	2.35	0.57
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.87	0.57
1:B:337:GLU:HA	1:B:349:LYS:HG3	1.87	0.57
1:B:119:MET:HE3	1:B:409:GLU:OE2	2.05	0.57
1:D:382:PRO:O	1:D:385:ILE:HG22	2.04	0.57
1:C:11:PHE:CZ	1:H:244:GLU:HG3	2.39	0.57
1:F:153:ILE:HB	1:F:265:PHE:CD1	2.40	0.56
1:E:275:PHE:CE2	1:E:441:PRO:HD3	2.40	0.56
1:F:293:GLU:OE2	1:F:314:VAL:HG23	2.05	0.56
1:G:27:GLN:HE22	1:G:433:ILE:HG23	1.70	0.56
1:H:81:PHE:HB3	1:H:209:ILE:HG12	1.87	0.56
1:B:69:LYS:HG3	3:B:660:HOH:O	2.04	0.56
1:B:79:ARG:NH2	1:B:93:GLU:OE1	2.32	0.56
1:G:433:ILE:HD11	1:G:439:LEU:HB3	1.87	0.56
1:H:138:HIS:ND1	3:H:616:HOH:O	2.32	0.56
1:H:177:MET:SD	1:H:263:ILE:HG22	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:CG	1:C:344:GLU:HB3	2.34	0.56
1:E:124:VAL:O	1:E:128:GLN:HG2	2.05	0.56
1:E:12:GLY:HA2	1:F:4:GLU:HG2	1.88	0.56
1:G:148:LEU:HD21	1:G:413:VAL:HG21	1.88	0.56
1:H:259:ILE:O	1:H:263:ILE:HG23	2.05	0.56
1:C:337:GLU:HA	1:C:349:LYS:HB2	1.87	0.56
1:D:434:LYS:N	1:D:440:LYS:O	2.38	0.56
1:F:404:GLN:NE2	1:F:405:MET:H	2.04	0.56
1:G:54:SER:O	1:G:58:ILE:HG12	2.06	0.56
1:A:167:ARG:HH12	1:A:171:HIS:HD2	1.54	0.55
1:A:46:GLY:O	3:A:610:HOH:O	2.18	0.55
1:D:66:ARG:HH21	1:D:339:THR:HB	1.70	0.55
1:E:237:MET:HB3	1:E:254:ILE:HD12	1.88	0.55
1:H:317:VAL:HG13	1:H:374:PHE:HZ	1.71	0.55
1:A:391:LYS:HE3	1:A:394:GLY:O	2.06	0.55
1:C:370:ASP:OD2	1:C:375:ARG:HD3	2.06	0.55
1:F:124:VAL:HG13	1:F:455:LEU:HD13	1.88	0.55
1:E:375:ARG:O	1:E:378:ARG:HG3	2.07	0.55
1:B:103:LEU:HD21	1:B:237:MET:HG3	1.86	0.55
1:D:158:PHE:CE1	1:D:258:ILE:HD13	2.41	0.55
1:F:343:GLY:HA3	3:F:610:HOH:O	2.06	0.55
1:G:22:THR:HB	1:G:24:LYS:H	1.69	0.55
1:B:385:ILE:HB	3:B:662:HOH:O	2.06	0.55
1:H:409:GLU:HA	3:H:677:HOH:O	2.07	0.55
1:D:181:LEU:HB3	1:D:436:THR:HG21	1.89	0.55
1:G:27:GLN:NE2	1:G:433:ILE:HG23	2.21	0.55
1:B:380:GLU:N	1:B:380:GLU:OE1	2.39	0.55
1:C:191:ALA:O	1:C:193:PRO:HD3	2.06	0.55
1:D:176:SER:OG	1:D:211:VAL:HG11	2.06	0.55
1:D:366:ILE:HG21	1:D:389:ALA:HB1	1.89	0.55
1:F:215:LEU:O	1:F:218:LYS:HG2	2.07	0.55
1:F:310:GLN:O	1:F:312:LYS:N	2.40	0.55
1:G:421:PHE:HB2	1:G:423:PHE:CZ	2.42	0.55
1:A:289:LYS:HA	1:A:292:GLU:HG2	1.88	0.55
1:A:375:ARG:O	1:A:378:ARG:HG3	2.05	0.55
1:H:68:ASP:OD1	1:H:69:LYS:N	2.39	0.55
1:E:391:LYS:HE2	1:E:395:ASN:HB2	1.88	0.55
1:F:104:LEU:HA	1:F:401:ILE:HD11	1.89	0.55
1:A:304:SER:HA	3:A:615:HOH:O	2.06	0.55
1:A:7:GLN:OE1	1:A:41:LYS:HD2	2.07	0.55
1:G:122:ILE:HG22	1:G:148:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:371:VAL:HG23	1:H:372:GLU:HG2	1.88	0.55
1:B:121:ASP:OD2	1:B:161:ARG:NH2	2.40	0.54
1:B:209:ILE:HG23	3:B:661:HOH:O	2.06	0.54
1:E:388:HIS:HA	1:E:391:LYS:HD2	1.88	0.54
1:G:264:ALA:O	1:G:268:THR:HG23	2.08	0.54
1:A:155:LEU:HD13	1:A:161:ARG:HG2	1.89	0.54
1:C:277:LEU:HD22	1:C:417:MET:HE1	1.90	0.54
1:D:23:ASP:OD2	1:D:24:LYS:HG3	2.07	0.54
1:F:81:PHE:HB3	1:F:209:ILE:HG12	1.89	0.54
1:A:23:ASP:OD1	1:A:23:ASP:N	2.31	0.54
1:F:166:TYR:HE2	1:G:129:LYS:HB2	1.72	0.54
1:G:70:ASN:O	1:G:332:SER:HB3	2.08	0.54
1:B:171:HIS:HD2	1:B:173:PHE:HB3	1.73	0.54
1:A:257:GLN:HB3	1:A:261:PHE:CE2	2.43	0.54
1:E:392:PRO:HG2	1:E:393:PHE:CD2	2.42	0.54
1:G:381:ASN:HB3	3:G:648:HOH:O	2.07	0.54
1:G:69:LYS:HG3	3:G:643:HOH:O	2.07	0.54
1:H:50:ARG:HB2	1:H:353:LEU:HD23	1.89	0.54
1:F:50:ARG:HB2	1:F:353:LEU:HD23	1.90	0.54
1:F:177:MET:HE1	1:F:267:GLU:HG2	1.90	0.54
1:G:365:THR:HG22	1:G:366:ILE:HG12	1.90	0.54
1:F:404:GLN:CD	1:F:404:GLN:H	2.11	0.54
1:G:293:GLU:OE2	1:G:313:TYR:N	2.36	0.54
1:H:58:ILE:HD13	1:H:360:LEU:HD13	1.90	0.54
1:F:215:LEU:H	1:F:215:LEU:HD23	1.72	0.53
1:A:216:VAL:O	1:A:220:ILE:HD12	2.09	0.53
1:B:187:LYS:HG2	1:B:190:ARG:NH1	2.23	0.53
1:C:242:ASP:HB3	1:C:245:THR:HG22	1.90	0.53
1:F:223:ARG:HE	1:F:234:LEU:HD23	1.73	0.53
1:B:109:GLN:HG2	1:B:404:GLN:NE2	2.24	0.53
1:C:3:LYS:HG2	1:C:344:GLU:HB3	1.91	0.53
1:C:85:GLY:O	1:C:89:SER:OG	2.22	0.53
1:H:20:LEU:HD21	1:H:29:LEU:HD11	1.90	0.53
1:C:427:THR:HG22	3:C:660:HOH:O	2.08	0.53
1:G:167:ARG:HG3	1:G:171:HIS:CE1	2.44	0.53
1:C:98:LYS:O	1:C:102:ILE:HG13	2.07	0.53
1:D:205:PHE:O	1:D:209:ILE:HG23	2.08	0.53
1:E:51:TYR:CE2	1:E:354:MET:HG2	2.44	0.53
1:A:68:ASP:OD1	1:A:69:LYS:N	2.39	0.53
1:C:183:GLU:O	1:C:187:LYS:HG3	2.08	0.53
1:E:22:THR:OG1	1:E:23:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:ASP:HB3	1:F:234:LEU:H	1.72	0.53
1:H:378:ARG:NH1	3:H:604:HOH:O	2.14	0.53
1:C:419:LYS:O	1:C:451:LYS:HE2	2.09	0.53
1:F:136:ASP:OD1	3:F:605:HOH:O	2.19	0.53
1:F:237:MET:HE1	1:F:257:GLN:HB2	1.91	0.53
1:G:235:THR:O	1:G:239:ASN:HB3	2.09	0.53
1:B:311:LEU:HG	3:B:620:HOH:O	2.08	0.53
1:C:392:PRO:HG2	1:C:393:PHE:CD2	2.44	0.53
1:A:314:VAL:O	1:A:317:VAL:HG22	2.09	0.53
1:C:22:THR:HB	1:C:24:LYS:H	1.74	0.53
1:F:232:ASP:HB3	1:F:234:LEU:N	2.23	0.53
1:F:371:VAL:HG23	1:F:372:GLU:H	1.73	0.53
1:H:98:LYS:O	1:H:102:ILE:HG13	2.09	0.53
1:A:436:THR:HG21	3:A:623:HOH:O	2.08	0.53
1:H:26:VAL:HG12	1:H:30:MET:HE2	1.90	0.53
1:H:331:PHE:CE2	1:H:355:VAL:HG21	2.44	0.53
1:F:289:LYS:HG2	3:F:602:HOH:O	2.08	0.52
1:G:131:GLU:HG3	3:G:682:HOH:O	2.09	0.52
1:F:216:VAL:HG21	1:F:259:ILE:HG13	1.91	0.52
1:G:242:ASP:CB	1:G:245:THR:HG22	2.39	0.52
1:A:173:PHE:CE1	1:A:212:MET:HG2	2.44	0.52
1:B:277:LEU:O	1:B:281:VAL:HG23	2.09	0.52
1:B:39:ILE:HA	1:B:51:TYR:O	2.10	0.52
1:H:441:PRO:HD2	3:H:675:HOH:O	2.08	0.52
1:A:16:ASN:HB2	1:A:19:LEU:HD12	1.92	0.52
1:C:323:ARG:HA	1:C:361:HIS:HD1	1.73	0.52
1:F:2:ILE:HG23	1:F:346:PRO:HG3	1.90	0.52
1:E:196:PRO:HA	1:E:199:ASP:OD2	2.10	0.52
1:F:78:VAL:HG23	1:F:88:THR:HG21	1.92	0.52
1:G:167:ARG:HG3	1:G:171:HIS:HE1	1.75	0.52
1:G:3:LYS:HB2	1:G:344:GLU:HB2	1.91	0.52
1:H:54:SER:O	1:H:58:ILE:HD12	2.10	0.52
1:D:68:ASP:OD1	1:D:69:LYS:N	2.41	0.52
1:E:85:GLY:HA2	1:E:257:GLN:NE2	2.25	0.52
1:C:223:ARG:NH2	1:C:232:ASP:OD2	2.42	0.52
1:B:297:VAL:O	1:B:299:VAL:HG13	2.10	0.52
1:C:366:ILE:HG21	1:C:389:ALA:HB1	1.91	0.52
1:E:318:LEU:HD22	1:E:410:ALA:HB1	1.92	0.52
1:H:30:MET:HE1	1:H:325:TRP:HZ3	1.75	0.52
1:A:337:GLU:HA	1:A:349:LYS:HE3	1.92	0.51
1:B:137:GLU:OE2	1:B:138:HIS:ND1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:LYS:HD3	1:E:94:LYS:H	1.74	0.51
1:F:316:MET:HG2	1:F:379:PHE:O	2.10	0.51
1:H:22:THR:HB	1:H:24:LYS:H	1.74	0.51
1:H:60:GLU:OE2	1:H:342:GLY:N	2.41	0.51
1:A:403:GLN:HG2	3:A:690:HOH:O	2.09	0.51
1:C:158:PHE:HD1	1:C:234:LEU:HG	1.75	0.51
1:C:419:LYS:HE2	1:C:453:ILE:HG21	1.91	0.51
1:B:150:LEU:HD22	1:B:174:ILE:HD12	1.92	0.51
1:F:166:TYR:CE2	1:G:129:LYS:HB2	2.46	0.51
1:H:23:ASP:OD1	1:H:23:ASP:N	2.34	0.51
1:D:120:VAL:O	1:D:124:VAL:HG23	2.10	0.51
1:F:297:VAL:HG11	1:F:310:GLN:HB2	1.92	0.51
1:D:312:LYS:HZ2	1:D:380:GLU:HA	1.76	0.51
1:H:106:SER:OG	1:H:236:HIS:ND1	2.18	0.51
1:D:90:TRP:HB2	1:D:93:GLU:HG3	1.92	0.51
1:E:120:VAL:O	1:E:124:VAL:HG23	2.11	0.51
1:E:168:ASP:N	1:E:168:ASP:OD1	2.37	0.51
1:H:375:ARG:O	1:H:378:ARG:HG3	2.11	0.51
1:C:170:PRO:HG3	3:C:704:HOH:O	2.10	0.51
1:B:215:LEU:O	1:B:219:ILE:HG13	2.11	0.51
1:B:392:PRO:HG2	1:B:393:PHE:CD2	2.44	0.51
1:B:428:ASN:O	3:B:604:HOH:O	2.19	0.51
1:A:167:ARG:HD3	1:A:169:GLN:O	2.11	0.51
1:H:245:THR:HG23	1:H:247:GLU:HG3	1.93	0.51
1:A:348:GLU:N	1:A:351:ASP:OD2	2.44	0.51
1:G:414:LEU:HA	1:G:417:MET:HE2	1.92	0.51
1:H:271:GLY:HA2	1:H:440:LYS:HG3	1.93	0.51
1:G:405:MET:N	3:G:607:HOH:O	2.21	0.50
1:H:400:CYS:HB2	2:H:501:FDE:NA	2.26	0.50
1:H:167:ARG:CZ	1:H:171:HIS:HD2	2.24	0.50
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.92	0.50
1:B:392:PRO:HG2	1:B:393:PHE:HD2	1.77	0.50
1:B:4:GLU:HG3	3:B:735:HOH:O	2.12	0.50
1:F:237:MET:HE2	1:F:254:ILE:HG23	1.94	0.50
1:F:33:ALA:HB3	1:F:359:GLN:HE21	1.76	0.50
1:G:275:PHE:CZ	1:G:433:ILE:HD13	2.47	0.50
1:H:397:GLN:N	3:H:621:HOH:O	2.44	0.50
1:E:85:GLY:O	1:E:89:SER:OG	2.21	0.50
1:E:94:LYS:H	1:E:94:LYS:CD	2.24	0.50
1:A:27:GLN:HE22	1:A:433:ILE:HB	1.75	0.50
1:H:242:ASP:OD1	1:H:243:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:MET:HE1	1:E:405:MET:HA	1.94	0.50
1:F:233:LEU:HD21	1:F:261:PHE:CG	2.47	0.50
1:G:25:PRO:HG2	1:G:185:MET:CE	2.40	0.50
1:B:375:ARG:O	1:B:378:ARG:HG3	2.11	0.50
1:F:215:LEU:HG	1:F:216:VAL:N	2.26	0.50
1:H:434:LYS:N	1:H:440:LYS:O	2.43	0.50
1:B:213:ASN:OD1	1:B:255:ARG:HD3	2.12	0.50
1:B:223:ARG:HH21	1:B:230:SER:HB2	1.75	0.50
1:E:366:ILE:HG21	1:E:389:ALA:CB	2.40	0.50
1:G:275:PHE:HZ	1:G:433:ILE:HD13	1.75	0.50
1:H:312:LYS:NZ	1:H:380:GLU:OE2	2.45	0.50
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.93	0.49
1:H:171:HIS:O	1:H:174:ILE:HG22	2.12	0.49
1:A:24:LYS:NZ	3:A:629:HOH:O	2.43	0.49
1:A:370:ASP:O	1:A:378:ARG:NH2	2.46	0.49
1:C:364:LYS:HE3	1:C:365:THR:HG23	1.94	0.49
1:E:93:GLU:O	3:E:606:HOH:O	2.20	0.49
1:F:140:GLU:HB3	1:F:143:GLU:OE2	2.12	0.49
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.94	0.49
1:C:108:SER:O	1:C:112:MET:HG2	2.12	0.49
1:C:245:THR:HG23	1:C:247:GLU:H	1.77	0.49
1:D:253:ASN:O	1:D:257:GLN:HG2	2.12	0.49
1:D:69:LYS:NZ	3:D:608:HOH:O	2.31	0.49
1:F:375:ARG:HG3	1:F:378:ARG:HG3	1.94	0.49
1:D:135:ALA:O	3:D:604:HOH:O	2.20	0.49
1:D:371:VAL:HG23	1:D:372:GLU:HG2	1.94	0.49
1:F:223:ARG:C	1:F:225:ALA:N	2.61	0.49
1:F:289:LYS:HD3	1:F:313:TYR:CZ	2.47	0.49
1:G:168:ASP:N	1:G:168:ASP:OD1	2.38	0.49
1:D:429:TYR:CE2	1:D:431:LEU:HA	2.48	0.49
1:B:86:LEU:N	1:B:257:GLN:HE22	2.05	0.49
1:C:421:PHE:CA	1:C:451:LYS:HZ1	2.26	0.49
1:D:25:PRO:CD	1:D:435:GLU:OE2	2.61	0.49
1:B:179:ARG:HD2	1:B:208:ASP:OD2	2.13	0.49
1:G:265:PHE:HB2	2:G:501:FDE:HMF3	1.95	0.49
1:H:320:GLU:HG3	1:H:374:PHE:CD1	2.48	0.49
1:C:424:GLU:OE1	1:C:426:HIS:HB3	2.13	0.49
1:D:181:LEU:HB3	1:D:436:THR:CG2	2.42	0.49
1:G:388:HIS:HA	1:G:391:LYS:HD2	1.95	0.49
1:G:69:LYS:HA	1:G:333:LEU:HD23	1.93	0.49
1:E:367:TRP:HB2	1:E:371:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:LEU:HD21	1:H:353:LEU:HD22	1.94	0.48
1:A:452:LYS:HE2	3:A:683:HOH:O	2.13	0.48
1:A:64:GLU:OE2	1:A:397:GLN:HG2	2.13	0.48
1:B:214:ASP:HB2	3:B:603:HOH:O	2.13	0.48
1:D:151:ASP:OD2	3:D:605:HOH:O	2.20	0.48
1:H:272:TRP:CE2	1:H:322:ILE:HD12	2.48	0.48
1:F:14:LEU:CD1	1:F:18:PRO:HD3	2.43	0.48
1:A:47:ARG:NH1	3:A:633:HOH:O	2.44	0.48
1:B:223:ARG:NH2	1:B:232:ASP:OD1	2.46	0.48
1:G:112:MET:SD	1:G:405:MET:HA	2.53	0.48
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.95	0.48
1:B:223:ARG:HE	1:B:235:THR:CG2	2.22	0.48
1:F:224:LYS:HD2	3:F:707:HOH:O	2.14	0.48
1:F:329:PRO:HB3	1:F:439:LEU:HD11	1.95	0.48
1:F:403:GLN:NE2	3:F:612:HOH:O	2.37	0.48
1:A:68:ASP:CB	1:A:336:LYS:HZ3	2.21	0.48
1:C:38:GLU:HB2	1:C:54:SER:HB3	1.95	0.48
1:F:118:MET:HB3	1:F:155:LEU:HD23	1.95	0.48
1:E:434:LYS:N	1:E:440:LYS:O	2.44	0.48
1:F:99:ALA:HA	1:F:102:ILE:HD11	1.95	0.48
1:H:20:LEU:HD11	1:H:29:LEU:HG	1.96	0.48
1:H:56:ARG:O	1:H:59:LYS:HG2	2.13	0.48
1:A:289:LYS:HA	1:A:292:GLU:CG	2.43	0.48
1:A:1:THR:HA	1:A:346:PRO:HG3	1.95	0.48
1:C:408:HIS:ND1	3:C:611:HOH:O	2.28	0.48
1:D:334:TYR:HA	1:D:351:ASP:O	2.13	0.48
1:E:148:LEU:HD21	1:E:413:VAL:HG21	1.95	0.48
1:F:307:GLN:HA	1:F:310:GLN:HG3	1.95	0.48
1:G:391:LYS:HE2	1:G:395:ASN:HB2	1.95	0.48
1:H:264:ALA:HB1	3:H:687:HOH:O	2.13	0.48
1:B:391:LYS:NZ	3:B:625:HOH:O	2.46	0.48
1:D:71:LEU:O	1:D:76:LYS:NZ	2.42	0.48
1:E:253:ASN:O	1:E:257:GLN:HG2	2.14	0.48
1:G:438:THR:HB	3:G:620:HOH:O	2.14	0.48
1:A:20:LEU:HD22	1:A:42:PHE:CZ	2.48	0.48
2:G:501:FDE:HBA1	3:G:616:HOH:O	2.13	0.48
1:A:119:MET:HG2	1:A:412:LEU:HD23	1.96	0.47
1:B:183:GLU:CD	1:B:190:ARG:HH22	2.17	0.47
1:C:196:PRO:HA	1:C:199:ASP:OD2	2.13	0.47
1:D:184:ALA:HA	1:D:187:LYS:HG2	1.95	0.47
1:H:20:LEU:HG	1:H:25:PRO:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:SER:OG	1:A:307:GLN:HG3	2.14	0.47
1:F:238:LEU:HD12	1:F:254:ILE:HD13	1.96	0.47
1:A:206:GLN:HG2	3:A:674:HOH:O	2.15	0.47
1:C:61:ALA:HA	1:C:67:PHE:CD2	2.49	0.47
1:G:310:GLN:O	1:G:312:LYS:N	2.46	0.47
1:H:61:ALA:HA	1:H:67:PHE:CD2	2.50	0.47
1:A:173:PHE:CE1	1:A:212:MET:HA	2.49	0.47
1:B:249:LEU:HD13	1:B:253:ASN:OD1	2.14	0.47
1:H:11:PHE:HE1	1:H:19:LEU:CD1	2.27	0.47
1:A:112:MET:SD	1:A:405:MET:HA	2.55	0.47
1:B:108:SER:O	1:B:112:MET:HG2	2.14	0.47
1:D:298:LEU:HD22	1:D:303:PRO:HB3	1.96	0.47
1:E:173:PHE:HB2	1:E:215[B]:LEU:CD2	2.41	0.47
1:E:69:LYS:HG3	3:E:615:HOH:O	2.14	0.47
1:H:167:ARG:HG2	1:H:169:GLN:O	2.14	0.47
1:H:286:VAL:HG13	1:H:313:TYR:OH	2.13	0.47
1:C:44:ALA:HB1	1:C:45:PRO:HD2	1.96	0.47
1:F:107:PHE:HB3	1:F:404:GLN:NE2	2.30	0.47
1:F:119:MET:HE1	1:F:409:GLU:HA	1.97	0.47
1:H:421:PHE:HB2	1:H:423:PHE:CZ	2.49	0.47
1:A:337:GLU:HA	1:A:349:LYS:CE	2.45	0.47
1:A:62:CYS:HB3	1:A:395:ASN:OD1	2.15	0.47
1:D:149:THR:HA	1:D:152:THR:HG22	1.96	0.47
1:D:190:ARG:HE	1:D:190:ARG:HB3	1.33	0.47
1:F:186:ASN:HB3	1:F:190:ARG:NH1	2.30	0.47
1:F:146:THR:HG23	1:F:266:HIS:HE2	1.79	0.47
1:F:44:ALA:HB1	1:F:45:PRO:HD2	1.95	0.47
1:F:99:ALA:HA	1:F:102:ILE:CD1	2.44	0.47
1:G:267:GLU:HB3	1:G:438:THR:HG21	1.96	0.47
1:A:173:PHE:HE2	1:A:262:LEU:HD13	1.80	0.47
1:A:27:GLN:NE2	1:A:435:GLU:OE2	2.45	0.47
1:B:400:CYS:HB2	2:B:501:FDE:NA	2.30	0.47
1:C:253:ASN:O	1:C:257:GLN:HG2	2.15	0.47
1:D:96:TRP:CD1	1:D:398:ARG:NH1	2.82	0.47
1:F:245:THR:CB	1:F:247:GLU:OE1	2.63	0.47
1:F:69:LYS:HA	1:F:333:LEU:HD23	1.97	0.47
1:A:173:PHE:HE1	1:A:212:MET:HA	1.80	0.47
1:C:1:THR:HG22	3:C:627:HOH:O	2.14	0.47
1:D:337:GLU:HA	1:D:349:LYS:HB2	1.96	0.47
1:G:437:LEU:HD23	1:G:437:LEU:HA	1.79	0.47
1:H:234:LEU:HA	1:H:237:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:LEU:HA	1:E:417:MET:CE	2.44	0.47
1:E:58:ILE:HG13	1:E:360:LEU:HD13	1.97	0.47
1:G:384:ALA:HB3	3:G:648:HOH:O	2.15	0.47
1:G:26:VAL:N	1:G:435:GLU:OE1	2.40	0.47
1:A:2:ILE:HG13	1:A:3:LYS:HG3	1.97	0.47
1:D:209:ILE:HG13	1:D:210:LYS:N	2.29	0.47
1:E:69:LYS:O	3:E:607:HOH:O	2.21	0.47
1:G:44:ALA:HB1	1:G:45:PRO:HD2	1.96	0.47
1:H:71:LEU:O	1:H:76:LYS:HE2	2.15	0.47
1:B:242:ASP:HB3	1:B:245:THR:HG22	1.96	0.46
1:B:412:LEU:HD23	1:B:413:VAL:N	2.31	0.46
1:E:14:LEU:HD23	1:E:14:LEU:HA	1.71	0.46
1:A:280:LEU:HB3	1:A:287:LEU:HD13	1.97	0.46
1:C:223:ARG:HA	1:C:223:ARG:HD3	1.61	0.46
1:D:161:ARG:HA	3:D:607:HOH:O	2.15	0.46
1:E:400:CYS:HB2	2:E:501:FDE:NA	2.30	0.46
1:F:272:TRP:CD1	1:F:322:ILE:HD13	2.49	0.46
1:C:400:CYS:HB2	2:C:501:FDE:NA	2.30	0.46
1:D:54:SER:O	1:D:58:ILE:HG12	2.16	0.46
1:E:298:LEU:HD11	1:E:311:LEU:HD11	1.97	0.46
1:F:366:ILE:HG21	1:F:389:ALA:HB1	1.97	0.46
1:G:413:VAL:HG12	1:G:417:MET:HE2	1.97	0.46
1:G:15:LYS:HB3	1:G:43:GLU:HG3	1.96	0.46
1:C:323:ARG:HA	1:C:361:HIS:ND1	2.30	0.46
1:D:68:ASP:HB3	1:D:334:TYR:CE1	2.50	0.46
1:G:289:LYS:HE2	1:G:313:TYR:CE1	2.51	0.46
1:G:406:SER:OG	2:G:501:FDE:HHC	2.15	0.46
1:G:278:TYR:HA	1:G:444:PHE:CZ	2.51	0.46
1:B:27:GLN:O	1:B:31:LYS:HG3	2.16	0.46
1:C:153:ILE:HB	1:C:265:PHE:CD2	2.51	0.46
1:D:51:TYR:HB3	1:D:356:LEU:CD1	2.44	0.46
1:F:293:GLU:OE1	1:F:312:LYS:N	2.49	0.46
1:F:335:ALA:HB2	1:F:347:LEU:HD13	1.97	0.46
1:H:242:ASP:HB3	1:H:245:THR:HG22	1.98	0.46
1:A:293:GLU:OE2	1:A:312:LYS:N	2.39	0.46
1:D:375:ARG:CB	1:D:378:ARG:NH1	2.79	0.46
1:F:61:ALA:HA	1:F:67:PHE:CE2	2.50	0.46
1:H:262:LEU:HA	3:H:631:HOH:O	2.16	0.46
1:C:183:GLU:HG2	1:C:205:PHE:CD1	2.51	0.46
1:C:7:GLN:NE2	1:C:43:GLU:OE1	2.33	0.46
1:G:381:ASN:ND2	1:G:384:ALA:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:HB3	1:A:334:TYR:CE1	2.51	0.46
1:B:60:GLU:HB3	1:B:66:ARG:NH1	2.31	0.46
1:C:223:ARG:HH22	1:C:232:ASP:CG	2.19	0.46
1:D:392:PRO:HG2	1:D:393:PHE:CD2	2.50	0.46
1:F:212:MET:HA	1:F:215:LEU:HD21	1.97	0.46
1:G:429:TYR:CE2	1:G:431:LEU:HA	2.51	0.46
1:A:102:ILE:HG12	1:A:102:ILE:H	1.60	0.46
1:F:66:ARG:HH11	1:F:339:THR:CG2	2.28	0.46
1:B:287:LEU:HD21	3:B:645:HOH:O	2.16	0.46
1:C:190:ARG:NH1	3:C:614:HOH:O	2.31	0.46
1:C:81:PHE:HB3	1:C:209:ILE:HG12	1.98	0.46
1:D:145:MET:O	1:D:149:THR:HG23	2.16	0.46
1:D:336:LYS:O	1:D:349:LYS:HG3	2.16	0.46
1:E:293:GLU:OE2	1:E:313:TYR:N	2.43	0.46
1:G:272:TRP:HE1	1:G:322:ILE:HD13	1.74	0.46
1:H:86:LEU:HD23	1:H:86:LEU:HA	1.77	0.46
1:A:231:ASP:N	3:A:640:HOH:O	2.49	0.45
1:D:278:TYR:CE1	1:D:431:LEU:HB2	2.50	0.45
1:E:94:LYS:HD3	1:E:94:LYS:N	2.30	0.45
1:F:91:THR:HB	1:F:398:ARG:HD3	1.98	0.45
1:G:280:LEU:HD23	1:G:280:LEU:HA	1.66	0.45
1:A:147:ARG:HG2	1:A:164:SER:HB3	1.98	0.45
1:A:174:ILE:HD11	1:A:266:HIS:NE2	2.32	0.45
1:A:158:PHE:CE1	1:A:258:ILE:HG12	2.52	0.45
1:B:103:LEU:HD21	1:B:237:MET:CG	2.46	0.45
1:E:422:ASP:O	1:E:448:ALA:HA	2.16	0.45
1:A:143:GLU:N	1:A:143:GLU:OE1	2.44	0.45
1:F:211:VAL:O	1:F:215:LEU:HD23	2.16	0.45
1:F:160:TYR:OH	1:F:218:LYS:HD3	2.17	0.45
1:H:148:LEU:HD21	1:H:413:VAL:HG21	1.98	0.45
1:A:51:TYR:HB3	1:A:356:LEU:CD1	2.47	0.45
1:B:112:MET:HE1	1:B:405:MET:HG3	1.99	0.45
1:B:69:LYS:HA	1:B:333:LEU:HD23	1.99	0.45
1:E:87:PHE:CZ	2:E:501:FDE:HBA1	2.52	0.45
1:F:148:LEU:HD21	1:F:413:VAL:HG21	1.97	0.45
1:C:414:LEU:O	1:C:418:LEU:HD13	2.15	0.45
1:C:69:LYS:HG3	3:C:622:HOH:O	2.16	0.45
1:D:266:HIS:NE2	1:D:267:GLU:HG2	2.32	0.45
1:D:304:SER:O	1:D:308:VAL:HG23	2.16	0.45
1:D:313:TYR:HA	1:D:316:MET:HE2	1.98	0.45
1:D:447:LYS:HD3	3:D:642:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:TRP:O	1:D:93:GLU:HB2	2.17	0.45
1:F:61:ALA:HA	1:F:67:PHE:CD2	2.51	0.45
1:G:419:LYS:O	1:G:451:LYS:HD3	2.16	0.45
2:H:501:FDE:HAD2	3:H:667:HOH:O	2.16	0.45
1:A:242:ASP:O	1:A:246:GLY:N	2.47	0.45
1:B:437:LEU:HD12	1:B:437:LEU:HA	1.75	0.45
1:C:163:ASN:HB2	3:C:709:HOH:O	2.15	0.45
1:F:217:ASP:OD1	3:F:606:HOH:O	2.21	0.45
1:F:26:VAL:O	1:F:30:MET:HG3	2.16	0.45
1:G:319:ASN:HB3	1:G:379:PHE:CE1	2.51	0.45
1:G:47:ARG:NH2	3:G:623:HOH:O	2.49	0.45
1:C:320:GLU:HG3	1:C:374:PHE:CE1	2.51	0.45
1:C:421:PHE:C	1:C:451:LYS:HZ1	2.20	0.45
1:D:373:GLU:O	1:D:378:ARG:NH2	2.50	0.45
1:E:60:GLU:OE1	1:E:342:GLY:HA2	2.16	0.45
1:A:305:TYR:CE2	1:A:309:LYS:HD2	2.52	0.45
1:D:108:SER:O	1:D:111:ALA:N	2.33	0.45
1:D:11:PHE:HB2	1:D:18:PRO:HG2	1.99	0.45
1:F:108:SER:HB2	3:F:621:HOH:O	2.17	0.45
1:B:16:ASN:O	1:B:19:LEU:HB2	2.17	0.45
1:C:71:LEU:CD1	1:C:76:LYS:HG2	2.45	0.45
1:D:331:PHE:HD1	1:D:357:ILE:HD11	1.81	0.45
1:D:440:LYS:HG3	1:D:441:PRO:HD2	1.98	0.45
1:E:54:SER:O	1:E:58:ILE:HG12	2.16	0.45
1:F:371:VAL:HG23	1:F:372:GLU:N	2.32	0.45
1:A:250:ASP:HB3	1:A:253:ASN:H	1.82	0.44
1:G:368:GLY:O	1:G:371:VAL:HG13	2.17	0.44
1:G:68:ASP:OD1	1:G:69:LYS:N	2.50	0.44
1:H:233:LEU:O	1:H:233:LEU:HD13	2.17	0.44
1:H:312:LYS:HG2	1:H:316:MET:CE	2.47	0.44
1:F:293:GLU:HG3	1:F:296:ARG:NH2	2.32	0.44
1:F:456:GLY:O	3:F:607:HOH:O	2.21	0.44
1:G:317:VAL:HG13	1:G:374:PHE:CZ	2.49	0.44
1:D:51:TYR:CD1	1:D:356:LEU:HD11	2.52	0.44
1:G:62:CYS:HB3	1:G:395:ASN:OD1	2.18	0.44
1:H:454:PRO:O	3:H:607:HOH:O	2.21	0.44
1:F:400:CYS:HB2	2:F:501:FDE:NA	2.31	0.44
1:G:320:GLU:HG3	1:G:374:PHE:CD1	2.52	0.44
1:G:426:HIS:CE1	1:G:447:LYS:HG3	2.53	0.44
1:G:81:PHE:HB3	1:G:209:ILE:HG12	1.99	0.44
1:A:178:VAL:HG23	3:A:623:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:C	3:A:612:HOH:O	2.55	0.44
1:C:71:LEU:HD12	1:C:71:LEU:O	2.17	0.44
1:D:313:TYR:O	1:D:317:VAL:HG12	2.17	0.44
1:D:385:ILE:HD12	1:D:386:PRO:HD2	1.99	0.44
1:F:303:PRO:HA	1:F:307:GLN:OE1	2.18	0.44
1:G:110:GLN:CD	1:G:110:GLN:H	2.21	0.44
1:G:268:THR:HA	3:G:620:HOH:O	2.16	0.44
1:G:274:SER:HB3	1:G:441:PRO:HG2	1.99	0.44
1:C:266:HIS:CD2	1:C:267:GLU:HG2	2.53	0.44
2:C:501:FDE:HMF1	3:C:745:HOH:O	2.17	0.44
1:C:5:MET:CE	1:C:50:ARG:HG2	2.48	0.44
1:D:318:LEU:HD22	1:D:410:ALA:HB1	1.99	0.44
1:E:203:ARG:HG3	1:E:204:GLN:N	2.32	0.44
1:F:223:ARG:HE	1:F:234:LEU:CD2	2.30	0.44
1:F:177:MET:HE1	1:F:267:GLU:CG	2.48	0.44
1:G:121:ASP:O	1:G:124:VAL:HG22	2.18	0.44
1:H:167:ARG:NH2	1:H:171:HIS:CD2	2.80	0.44
1:C:104:LEU:O	1:C:104:LEU:HD22	2.17	0.44
1:D:208:ASP:HA	1:D:211:VAL:HG12	1.99	0.44
1:D:209:ILE:HD12	1:D:213:ASN:ND2	2.33	0.44
1:G:338:ASP:OD1	1:G:349:LYS:N	2.43	0.44
1:G:378:ARG:HB2	1:G:379:PHE:HD2	1.83	0.44
1:G:377:GLU:O	1:G:380:GLU:HG3	2.17	0.44
1:H:223:ARG:HH21	1:H:235:THR:HG23	1.82	0.44
1:A:400:CYS:HB2	2:A:501:FDE:NA	2.33	0.44
1:C:364:LYS:HD2	1:C:365:THR:N	2.33	0.44
1:F:58:ILE:HG13	1:F:360:LEU:HD13	2.00	0.44
1:F:404:GLN:CD	1:F:404:GLN:N	2.71	0.44
1:G:136:ASP:N	1:G:136:ASP:OD1	2.51	0.44
1:A:349:LYS:HE3	1:A:349:LYS:HB2	1.89	0.43
1:A:16:ASN:HD21	1:A:43:GLU:H	1.66	0.43
1:B:78:VAL:HG13	1:B:81:PHE:CZ	2.53	0.43
1:C:8:PRO:HB2	1:C:19:LEU:CD2	2.48	0.43
1:C:84:ASP:OD2	1:C:95:ASN:ND2	2.33	0.43
1:A:268:THR:HB	2:A:501:FDE:HME3	1.99	0.43
1:B:116:HIS:N	3:B:628:HOH:O	2.50	0.43
1:B:162:PHE:O	1:B:167:ARG:NH1	2.52	0.43
1:B:273:LEU:HD21	1:B:410:ALA:HA	2.00	0.43
1:D:120:VAL:HB	3:D:613:HOH:O	2.17	0.43
1:D:168:ASP:N	1:D:168:ASP:OD1	2.44	0.43
1:G:17:LEU:HD11	1:G:189:GLN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:LYS:HB2	3:G:659:HOH:O	2.19	0.43
1:H:63:ASP:OD2	1:H:66:ARG:HG3	2.18	0.43
1:A:300:ASP:HB2	1:A:302:VAL:O	2.18	0.43
1:B:282:LYS:HD2	3:B:647:HOH:O	2.17	0.43
1:B:58:ILE:HD12	1:B:355:VAL:HG13	2.00	0.43
1:C:144:ASP:OD1	1:C:147:ARG:NH1	2.51	0.43
1:C:72:SER:O	1:C:76:LYS:HG3	2.17	0.43
1:E:153:ILE:HB	1:E:265:PHE:CD2	2.54	0.43
1:E:265:PHE:HB2	2:E:501:FDE:HMF3	1.99	0.43
1:G:328:ALA:HB2	3:G:646:HOH:O	2.18	0.43
1:G:72:SER:OG	1:G:75:LEU:HD13	2.18	0.43
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.77	0.43
1:D:234:LEU:HA	1:D:237:MET:HE3	2.01	0.43
1:E:75:LEU:HD21	1:E:87:PHE:HE1	1.84	0.43
1:F:147:ARG:HG2	1:F:164:SER:HB3	2.01	0.43
1:A:94:LYS:HZ1	1:F:21:ASN:HD21	1.59	0.43
1:F:102:ILE:HD11	1:F:249:LEU:HD21	2.01	0.43
1:H:380:GLU:O	1:H:382:PRO:HD3	2.17	0.43
1:A:22:THR:HB	1:A:24:LYS:H	1.83	0.43
1:F:135:ALA:N	3:F:622:HOH:O	2.50	0.43
1:F:79:ARG:HG3	1:F:83:GLY:O	2.19	0.43
1:G:404:GLN:H	1:G:404:GLN:CD	2.21	0.43
1:A:215:LEU:O	1:A:219:ILE:HG13	2.19	0.43
1:A:257:GLN:HA	1:A:257:GLN:HE21	1.84	0.43
1:A:377:GLU:OE1	1:A:377:GLU:N	2.51	0.43
1:A:68:ASP:HB2	1:A:336:LYS:HZ1	1.76	0.43
1:H:208:ASP:O	1:H:212:MET:HG2	2.19	0.43
1:H:272:TRP:CD2	1:H:322:ILE:HD12	2.53	0.43
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.69	0.43
1:C:11:PHE:HE2	1:C:19:LEU:CD1	2.31	0.43
1:D:407:LEU:HD12	1:D:407:LEU:HA	1.81	0.43
1:F:121:ASP:C	1:F:121:ASP:OD2	2.56	0.43
1:G:344:GLU:HG3	1:G:345:TYR:CD2	2.53	0.43
1:G:392:PRO:HG2	1:G:393:PHE:CD2	2.54	0.43
1:G:393:PHE:HB3	1:G:400:CYS:HB3	1.99	0.43
1:B:10:THR:HG23	1:B:15:LYS:HA	2.01	0.43
1:C:393:PHE:HB3	1:C:400:CYS:HB3	2.01	0.43
1:E:254:ILE:HD13	1:E:254:ILE:HA	1.78	0.43
1:G:311:LEU:HB3	1:G:314:VAL:HB	2.00	0.43
1:G:86:LEU:HA	1:G:86:LEU:HD23	1.73	0.43
1:H:3:LYS:CB	1:H:344:GLU:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:PRO:O	1:D:202:LYS:NZ	2.40	0.43
1:D:247:GLU:CB	1:D:248:PRO:HD3	2.49	0.43
1:H:44:ALA:HB3	1:H:47:ARG:HG3	2.01	0.43
1:C:22:THR:HG22	1:C:23:ASP:N	2.34	0.42
1:C:66:ARG:NH2	1:C:339:THR:OG1	2.40	0.42
1:D:29:LEU:HB3	1:D:356:LEU:HD21	2.00	0.42
1:B:223:ARG:CZ	1:B:234:LEU:HD22	2.49	0.42
1:B:61:ALA:O	1:B:333:LEU:HD13	2.20	0.42
1:C:250:ASP:OD1	1:C:251:ASP:N	2.52	0.42
1:C:293:GLU:OE2	1:C:314:VAL:HG23	2.19	0.42
1:C:347:LEU:HD13	1:C:353:LEU:HD11	2.00	0.42
1:F:305:TYR:O	1:F:309:LYS:NZ	2.52	0.42
1:F:382:PRO:HA	1:F:385:ILE:HD12	2.00	0.42
1:F:413:VAL:O	1:F:417:MET:HG3	2.20	0.42
1:G:390:PHE:CZ	1:G:392:PRO:HG3	2.54	0.42
1:H:98:LYS:HE2	1:H:249:LEU:HD23	1.99	0.42
1:A:174:ILE:HD11	1:A:266:HIS:CE1	2.54	0.42
1:E:426:HIS:CG	1:E:447:LYS:HG3	2.54	0.42
1:E:440:LYS:HG3	3:E:603:HOH:O	2.19	0.42
1:G:22:THR:HG22	1:G:23:ASP:N	2.34	0.42
1:G:39:ILE:HA	1:G:51:TYR:O	2.18	0.42
1:H:372:GLU:OE2	3:H:608:HOH:O	2.21	0.42
1:B:418:LEU:HD23	1:B:418:LEU:HA	1.77	0.42
1:B:54:SER:O	1:B:58:ILE:HG12	2.20	0.42
1:D:30:MET:HG2	1:D:359:GLN:HG2	2.00	0.42
1:D:375:ARG:N	1:D:378:ARG:NH1	2.62	0.42
1:D:400:CYS:HB2	2:D:501:FDE:NA	2.33	0.42
1:F:263:ILE:HD13	1:F:263:ILE:N	2.34	0.42
1:G:50:ARG:HB2	1:G:353:LEU:HD23	2.01	0.42
1:D:262:LEU:HD23	1:D:262:LEU:HA	1.83	0.42
1:F:250:ASP:N	1:F:250:ASP:OD1	2.50	0.42
1:G:125:GLN:HE21	1:G:165:PHE:HD2	1.67	0.42
1:G:55:GLN:HA	1:G:58:ILE:HB	2.00	0.42
1:H:230:SER:O	1:H:235:THR:HG21	2.18	0.42
1:A:158:PHE:HE1	1:A:258:ILE:HG12	1.85	0.42
1:A:187:LYS:O	1:A:189:GLN:N	2.53	0.42
1:B:24:LYS:HB2	3:B:665:HOH:O	2.19	0.42
1:C:142:PRO:HD3	1:C:444:PHE:HB3	2.01	0.42
1:D:449:LYS:HA	1:D:449:LYS:HD3	1.75	0.42
1:A:245:THR:HG22	1:F:18:PRO:O	2.20	0.42
1:A:203:ARG:HG3	3:A:672:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HA	1:C:51:TYR:O	2.20	0.42
1:H:254:ILE:O	1:H:257:GLN:N	2.52	0.42
1:B:280:LEU:HD21	1:B:317:VAL:HG11	2.00	0.42
1:D:341:LEU:HD22	1:D:347:LEU:HD11	2.01	0.42
1:D:63:ASP:OD2	1:D:65:SER:OG	2.19	0.42
1:E:280:LEU:O	1:E:287:LEU:HD22	2.19	0.42
1:E:304:SER:N	1:E:307:GLN:OE1	2.42	0.42
1:E:98:LYS:O	1:E:102:ILE:HG13	2.19	0.42
1:F:119:MET:HE3	1:F:409:GLU:OE2	2.20	0.42
1:F:271:GLY:HA3	1:F:327:THR:HG21	2.02	0.42
1:G:118:MET:HB3	1:G:155:LEU:HD23	2.01	0.42
1:G:237:MET:CE	1:G:254:ILE:HG23	2.40	0.42
1:G:380:GLU:OE2	1:G:381:ASN:N	2.51	0.42
1:G:433:ILE:CD1	1:G:440:LYS:O	2.63	0.42
1:B:107:PHE:CE1	1:B:233:LEU:HD21	2.55	0.42
1:B:289:LYS:HD2	1:B:313:TYR:CE1	2.55	0.42
1:B:8:PRO:HB2	1:B:19:LEU:HD21	2.01	0.42
1:C:313:TYR:O	1:C:317:VAL:HG23	2.19	0.42
1:C:421:PHE:N	1:C:451:LYS:NZ	2.66	0.42
1:E:174:ILE:HD13	1:E:177:MET:HE3	2.02	0.42
1:E:280:LEU:HA	1:E:280:LEU:HD23	1.72	0.42
1:F:335:ALA:CB	1:F:347:LEU:CD1	2.97	0.42
1:A:409:GLU:N	3:A:608:HOH:O	2.52	0.42
1:B:129:LYS:HB2	1:C:166:TYR:CE2	2.55	0.42
1:D:173:PHE:CZ	1:D:215:LEU:HD12	2.55	0.42
1:D:86:LEU:HD23	1:D:86:LEU:HA	1.86	0.42
1:F:2:ILE:HG23	1:F:346:PRO:CG	2.50	0.42
1:F:440:LYS:HB3	1:F:440:LYS:HE3	1.74	0.42
1:G:224:LYS:H	1:G:224:LYS:HD3	1.84	0.42
1:G:319:ASN:HB3	1:G:379:PHE:CD1	2.55	0.42
1:G:39:ILE:HG21	1:G:345:TYR:CE2	2.54	0.42
1:H:455:LEU:HA	3:H:607:HOH:O	2.19	0.42
1:A:130:TRP:CE2	1:A:139:ILE:HD13	2.54	0.41
1:A:280:LEU:HA	1:A:280:LEU:HD23	1.66	0.41
1:B:173:PHE:HD1	1:B:215:LEU:HD21	1.84	0.41
1:D:398:ARG:HH11	1:D:398:ARG:HD2	1.68	0.41
1:D:421:PHE:HB2	1:D:423:PHE:CZ	2.55	0.41
1:G:265:PHE:HD1	2:G:501:FDE:H2C	1.85	0.41
1:G:267:GLU:OE2	1:G:438:THR:OG1	2.25	0.41
1:G:66:ARG:NH1	3:G:613:HOH:O	2.30	0.41
1:H:136:ASP:OD2	3:H:609:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:ASN:OD1	1:H:255:ARG:HD3	2.20	0.41
1:H:437:LEU:HA	1:H:437:LEU:HD23	1.81	0.41
1:A:271:GLY:CA	1:A:440:LYS:HG2	2.51	0.41
1:B:122:ILE:HG22	1:B:148:LEU:HD12	2.01	0.41
1:B:433:ILE:HD11	1:B:439:LEU:HD22	2.01	0.41
2:B:501:FDE:HAD2	3:B:640:HOH:O	2.19	0.41
1:C:440:LYS:HG3	1:C:441:PRO:O	2.21	0.41
1:C:54:SER:O	1:C:58:ILE:HG12	2.19	0.41
1:D:278:TYR:CD2	1:D:278:TYR:C	2.94	0.41
1:F:234:LEU:HD13	1:F:258:ILE:HD11	2.01	0.41
1:H:50:ARG:O	1:H:354:MET:N	2.44	0.41
1:B:22:THR:HB	1:B:24:LYS:H	1.85	0.41
1:C:47:ARG:NH1	3:C:640:HOH:O	2.53	0.41
1:E:266:HIS:CD2	1:E:267:GLU:HG2	2.54	0.41
1:G:377:GLU:N	1:G:377:GLU:OE2	2.51	0.41
1:D:331:PHE:HB3	2:D:501:FDE:HBA2	2.01	0.41
1:E:128:GLN:HB3	1:E:132:ARG:HE	1.85	0.41
1:F:426:HIS:CG	1:F:447:LYS:HG3	2.56	0.41
1:A:24:LYS:HA	1:A:435:GLU:CD	2.41	0.41
1:G:326:PRO:HG2	1:G:358:PRO:HG3	2.03	0.41
1:H:127:VAL:O	1:H:131:GLU:HG3	2.21	0.41
1:H:20:LEU:C	1:H:22:THR:H	2.24	0.41
1:H:59:LYS:HE3	1:H:59:LYS:HB2	1.85	0.41
1:A:278:TYR:CZ	1:A:431:LEU:HB2	2.55	0.41
1:D:380:GLU:O	1:D:382:PRO:HD3	2.21	0.41
1:E:11:PHE:CD1	1:E:11:PHE:N	2.89	0.41
1:F:194:ASP:CG	1:F:195:ASP:H	2.24	0.41
1:F:218:LYS:HE3	1:F:218:LYS:HB2	1.76	0.41
1:G:378:ARG:HB2	1:G:379:PHE:CD2	2.54	0.41
1:G:58:ILE:HD12	1:G:355:VAL:HG13	2.02	0.41
1:D:338:ASP:O	1:D:339:THR:HG23	2.21	0.41
1:E:234:LEU:O	1:E:238:LEU:HD13	2.21	0.41
1:E:55:GLN:HA	1:E:58:ILE:HB	2.02	0.41
1:F:173:PHE:CD1	1:F:215:LEU:HD21	2.55	0.41
1:A:167:ARG:NH1	1:A:171:HIS:CD2	2.84	0.41
1:A:364:LYS:HA	3:A:611:HOH:O	2.19	0.41
1:C:377:GLU:N	1:C:377:GLU:OE1	2.52	0.41
1:C:57:LEU:HD23	1:C:57:LEU:HA	1.78	0.41
1:D:343:GLY:HA2	1:F:206:GLN:NE2	2.36	0.41
1:F:63:ASP:OD2	1:F:66:ARG:HG3	2.20	0.41
1:B:191:ALA:O	1:B:193:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:LEU:HA	1:E:262:LEU:HD23	1.80	0.41
1:F:154:GLY:HA2	1:F:158:PHE:HD2	1.86	0.41
1:F:312:LYS:O	1:F:316:MET:HG3	2.21	0.41
1:F:391:LYS:HZ1	1:F:395:ASN:HA	1.85	0.41
1:H:59:LYS:HG3	1:H:60:GLU:N	2.36	0.41
1:A:87:PHE:HE2	3:A:675:HOH:O	2.03	0.41
1:B:132:ARG:HH11	1:B:132:ARG:HD3	1.73	0.41
1:B:189:GLN:O	1:B:189:GLN:HG3	2.21	0.41
1:C:167:ARG:HG2	1:C:169:GLN:O	2.21	0.41
1:E:118:MET:HB3	1:E:155:LEU:HD23	2.02	0.41
1:E:5:MET:SD	1:E:50:ARG:HG2	2.61	0.41
1:G:122:ILE:HG13	1:G:152:THR:HA	2.02	0.41
1:G:367:TRP:HB2	1:G:371:VAL:HG12	2.03	0.41
1:H:39:ILE:HA	1:H:51:TYR:O	2.21	0.41
1:D:439:LEU:O	1:D:440:LYS:HB2	2.21	0.41
1:E:44:ALA:HB1	1:E:45:PRO:HD2	2.03	0.41
1:F:331:PHE:CD2	1:F:357:ILE:HD11	2.55	0.41
1:F:54:SER:O	1:F:58:ILE:HG12	2.21	0.41
1:F:66:ARG:HD2	1:F:339:THR:HG21	2.03	0.41
1:G:304:SER:OG	1:G:307:GLN:HG3	2.21	0.41
1:H:27:GLN:O	1:H:31:LYS:HG3	2.21	0.41
1:C:388:HIS:HA	1:C:391:LYS:HD3	2.03	0.40
1:E:198:TYR:O	1:E:202:LYS:HG3	2.21	0.40
1:F:234:LEU:O	1:F:238:LEU:HD22	2.21	0.40
1:G:127:VAL:O	1:G:131:GLU:HB2	2.21	0.40
1:H:15:LYS:HD3	1:H:43:GLU:OE1	2.22	0.40
1:B:109:GLN:HG2	1:B:404:GLN:HE22	1.86	0.40
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.78	0.40
1:B:96:TRP:CE3	1:B:97:LYS:N	2.89	0.40
1:G:22:THR:HG22	1:G:23:ASP:H	1.86	0.40
1:G:52:LEU:HB2	1:G:58:ILE:HD11	2.02	0.40
1:H:134:ASN:ND2	1:H:137:GLU:OE2	2.32	0.40
1:A:119:MET:SD	3:A:608:HOH:O	2.63	0.40
1:B:371:VAL:HG23	1:B:372:GLU:HG2	2.02	0.40
1:F:232:ASP:CB	1:F:235:THR:H	2.35	0.40
1:H:364:LYS:HG2	1:H:365:THR:N	2.36	0.40
1:H:360:LEU:HD21	1:H:391:LYS:HG2	2.03	0.40
1:B:128:GLN:O	1:B:132:ARG:HD2	2.21	0.40
1:D:130:TRP:CD2	1:D:139:ILE:HD13	2.57	0.40
1:D:223:ARG:NH2	1:D:232:ASP:OD2	2.54	0.40
1:D:331:PHE:CD1	1:D:357:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:GLU:H	1:E:252:GLU:CD	2.24	0.40
1:F:250:ASP:HB2	1:F:252:GLU:OE1	2.21	0.40
1:F:437:LEU:HA	1:F:437:LEU:HD23	1.92	0.40
1:F:77:PHE:CE1	1:F:187:LYS:HE2	2.56	0.40
1:A:39:ILE:HA	1:A:51:TYR:O	2.21	0.40
1:A:78:VAL:HG13	1:A:81:PHE:CZ	2.56	0.40
1:B:118:MET:H	1:B:118:MET:HG3	1.63	0.40
1:C:307:GLN:HA	1:C:310:GLN:OE1	2.21	0.40
1:D:26:VAL:O	1:D:30:MET:HG3	2.21	0.40
1:E:297:VAL:HG23	1:E:298:LEU:HG	2.03	0.40
1:F:91:THR:HB	1:F:398:ARG:NH1	2.23	0.40
1:G:130:TRP:CD2	1:G:139:ILE:HD13	2.56	0.40
1:H:414:LEU:HD12	1:H:417:MET:HE3	2.04	0.40
1:H:26:VAL:HG23	1:H:435:GLU:OE2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:715:HOH:O	3:H:734:HOH:O[2_455]	2.02	0.18
3:C:741:HOH:O	3:E:719:HOH:O[2_354]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/471 (95%)	429 (96%)	18 (4%)	1 (0%)	47	46
1	B	451/471 (96%)	437 (97%)	13 (3%)	1 (0%)	47	46
1	C	449/471 (95%)	426 (95%)	21 (5%)	2 (0%)	34	29
1	D	450/471 (96%)	427 (95%)	18 (4%)	5 (1%)	14	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	448/471 (95%)	426 (95%)	19 (4%)	3 (1%)	22	15
1	F	451/471 (96%)	427 (95%)	19 (4%)	5 (1%)	14	8
1	G	449/471 (95%)	431 (96%)	17 (4%)	1 (0%)	47	46
1	H	446/471 (95%)	428 (96%)	18 (4%)	0	100	100
All	All	3592/3768 (95%)	3431 (96%)	143 (4%)	18 (0%)	29	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	247	GLU
1	E	225	ALA
1	E	311	LEU
1	F	224	LYS
1	D	245	THR
1	G	311	LEU
1	A	188	LEU
1	C	225	ALA
1	B	96	TRP
1	D	225	ALA
1	F	12	GLY
1	F	311	LEU
1	E	403	GLN
1	F	238	LEU
1	F	45	PRO
1	D	45	PRO
1	C	45	PRO
1	D	440	LYS

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	367/415 (88%)	348 (95%)	19 (5%)	23	19
1	B	374/415 (90%)	361 (96%)	13 (4%)	36	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	368/415 (89%)	351 (95%)	17 (5%)	27	23
1	D	343/415 (83%)	330 (96%)	13 (4%)	33	31
1	E	375/415 (90%)	358 (96%)	17 (4%)	27	24
1	F	360/415 (87%)	337 (94%)	23 (6%)	17	12
1	G	364/415 (88%)	344 (94%)	20 (6%)	21	17
1	H	375/415 (90%)	356 (95%)	19 (5%)	24	20
All	All	2926/3320 (88%)	2785 (95%)	141 (5%)	25	22

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	20	LEU
1	A	23	ASP
1	A	49	THR
1	A	102	ILE
1	A	156	CYS
1	A	181	LEU
1	A	203	ARG
1	A	235	THR
1	A	242	ASP
1	A	251	ASP
1	A	266	HIS
1	A	336	LYS
1	A	369	ASP
1	A	383	SER
1	A	407	LEU
1	A	427	THR
1	A	436	THR
1	A	445	VAL
1	B	19	LEU
1	B	59	LYS
1	B	126	LEU
1	B	159	ASN
1	B	169	GLN
1	B	173	PHE
1	B	174	ILE
1	B	215	LEU
1	B	223	ARG
1	B	266	HIS

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Mol	Chain	Res	Type
1	B	302	VAL
1	B	314	VAL
1	B	324	LEU
1	C	3	LYS
1	C	14	LEU
1	C	31	LYS
1	C	104	LEU
1	C	167	ARG
1	C	207	GLU
1	C	234	LEU
1	C	245	THR
1	C	266	HIS
1	C	302	VAL
1	C	364	LYS
1	C	375	ARG
1	C	418	LEU
1	C	424	GLU
1	C	430	GLU
1	C	434	LYS
1	C	437	LEU
1	D	31	LYS
1	D	53	SER
1	D	56	ARG
1	D	100	HIS
1	D	190	ARG
1	D	209	ILE
1	D	249	LEU
1	D	250	ASP
1	D	266	HIS
1	D	281	VAL
1	D	300	ASP
1	D	317	VAL
1	D	373	GLU
1	E	11	PHE
1	E	22	THR
1	E	94	LYS
1	E	102	ILE
1	E	178	VAL
1	E	189	GLN
1	E	230	SER
1	E	238	LEU
1	E	247	GLU

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Mol	Chain	Res	Type
1	E	266	HIS
1	E	300	ASP
1	E	327	THR
1	E	369	ASP
1	E	404	GLN
1	E	427	THR
1	E	440	LYS
1	E	445	VAL
1	F	10	THR
1	F	17	LEU
1	F	47	ARG
1	F	80	ASP
1	F	91	THR
1	F	102	ILE
1	F	178	VAL
1	F	195	ASP
1	F	199	ASP
1	F	215	LEU
1	F	222	ASP
1	F	230	SER
1	F	238	LEU
1	F	247	GLU
1	F	252	GLU
1	F	263	ILE
1	F	309	LYS
1	F	381	ASN
1	F	404	GLN
1	F	427	THR
1	F	436	THR
1	F	440	LYS
1	F	445	VAL
1	G	23	ASP
1	G	47	ARG
1	G	131	GLU
1	G	159	ASN
1	G	175	THR
1	G	178	VAL
1	G	204	GLN
1	G	224	LYS
1	G	232	ASP
1	G	235	THR
1	G	266	HIS

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Mol	Chain	Res	Type
1	G	306	LYS
1	G	365	THR
1	G	369	ASP
1	G	380	GLU
1	G	382	PRO
1	G	383	SER
1	G	404	GLN
1	G	411	THR
1	G	445	VAL
1	H	4	GLU
1	H	6	PRO
1	H	65	SER
1	H	97	LYS
1	H	102	ILE
1	H	126	LEU
1	H	178	VAL
1	H	192	ASN
1	H	212	MET
1	H	223	ARG
1	H	224	LYS
1	H	230	SER
1	H	247	GLU
1	H	263	ILE
1	H	266	HIS
1	H	309	LYS
1	H	322	ILE
1	H	364	LYS
1	H	436	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	B	100	HIS
1	B	257	GLN
1	D	266	HIS
1	D	403	GLN
1	E	110	GLN
1	E	266	HIS
1	F	21	ASN
1	F	359	GLN
1	F	387	GLN

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Mol	Chain	Res	Type
1	F	408	HIS
1	H	189	GLN

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 ⓘ

8 ligands are modelled in this entry.

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	$\# Z > 2$
2	FDE	H	501	1	32,46,46	6.93	19 (59%)	20,76,76	3.33	10 (50%)
2	FDE	C	501	1	32,46,46	6.44	18 (56%)	20,76,76	3.43	11 (55%)
2	FDE	E	501	1,3	32,46,46	6.69	16 (50%)	20,76,76	3.57	9 (45%)
2	FDE	A	501	1,3	32,46,46	6.46	16 (50%)	20,76,76	3.80	11 (55%)
2	FDE	G	501	1	32,46,46	6.67	18 (56%)	20,76,76	3.51	10 (50%)
2	FDE	D	501	1	32,46,46	6.51	18 (56%)	20,76,76	3.50	10 (50%)
2	FDE	F	501	1	32,46,46	6.51	18 (56%)	20,76,76	3.79	10 (50%)
2	FDE	B	501	1	32,46,46	6.77	17 (53%)	20,76,76	3.22	10 (50%)

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
2	FDE	H	501	1	-	0/6/86/86	-
2	FDE	C	501	1	-	0/6/86/86	-
2	FDE	E	501	1,3	-	1/6/86/86	-
2	FDE	A	501	1,3	-	0/6/86/86	-
2	FDE	G	501	1	-	0/6/86/86	-
2	FDE	D	501	1	-	2/6/86/86	-
2	FDE	F	501	1	-	0/6/86/86	-
2	FDE	B	501	1	-	1/6/86/86	-

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	FDE	C3A-C2A	19.14	1.49	1.34
2	H	501	FDE	C3A-C2A	18.70	1.49	1.34
2	E	501	FDE	C3A-C2A	18.64	1.49	1.34
2	B	501	FDE	C3A-C2A	18.31	1.48	1.34
2	D	501	FDE	C3A-C2A	18.25	1.48	1.34
2	F	501	FDE	C3A-C2A	18.12	1.48	1.34
2	A	501	FDE	C3A-C2A	17.67	1.48	1.34
2	C	501	FDE	C3A-C2A	16.71	1.47	1.34
2	H	501	FDE	C1C-NC	-14.37	1.30	1.49
2	E	501	FDE	C1C-NC	-13.30	1.31	1.49
2	F	501	FDE	CHD-C4C	-13.16	1.30	1.53
2	B	501	FDE	CHD-C4C	-13.07	1.30	1.53
2	H	501	FDE	CHD-C4C	-13.06	1.30	1.53
2	A	501	FDE	CHD-C4C	-13.05	1.30	1.53
2	E	501	FDE	CHD-C4C	-12.99	1.31	1.53
2	D	501	FDE	CHD-C4C	-12.84	1.31	1.53
2	G	501	FDE	CHD-C4C	-12.78	1.31	1.53
2	C	501	FDE	C1C-NC	-12.76	1.32	1.49
2	B	501	FDE	C1C-NC	-12.73	1.32	1.49
2	G	501	FDE	C1C-NC	-12.69	1.32	1.49
2	H	501	FDE	C1A-NA	-12.66	1.32	1.49
2	F	501	FDE	C1C-NC	-12.64	1.32	1.49
2	C	501	FDE	C4C-NC	-12.62	1.32	1.49
2	G	501	FDE	CHB-C4A	-12.42	1.32	1.53
2	C	501	FDE	CHD-C4C	-12.31	1.32	1.53
2	D	501	FDE	C1C-NC	-12.27	1.32	1.49
2	A	501	FDE	C4C-NC	-12.13	1.33	1.49
2	B	501	FDE	C4A-NA	-11.99	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FDE	C1A-NA	-11.93	1.33	1.49
2	H	501	FDE	C4C-NC	-11.85	1.33	1.49
2	F	501	FDE	C4C-NC	-11.71	1.33	1.49
2	H	501	FDE	C4A-NA	-11.70	1.33	1.49
2	A	501	FDE	C1C-NC	-11.56	1.33	1.49
2	A	501	FDE	C1A-NA	-11.55	1.33	1.49
2	C	501	FDE	C1A-NA	-11.51	1.34	1.49
2	F	501	FDE	C1A-NA	-11.46	1.34	1.49
2	B	501	FDE	C4C-NC	-11.40	1.34	1.49
2	D	501	FDE	C4C-NC	-11.30	1.34	1.49
2	E	501	FDE	C4C-NC	-11.29	1.34	1.49
2	E	501	FDE	C4A-NA	-11.25	1.34	1.49
2	H	501	FDE	CHB-C4A	-11.23	1.34	1.53
2	D	501	FDE	C1A-NA	-11.22	1.34	1.49
2	E	501	FDE	CHB-C4A	-11.19	1.34	1.53
2	A	501	FDE	CHB-C4A	-11.15	1.34	1.53
2	G	501	FDE	C1A-NA	-11.09	1.34	1.49
2	G	501	FDE	C4C-NC	-11.06	1.34	1.49
2	E	501	FDE	C1A-NA	-10.98	1.34	1.49
2	D	501	FDE	CHB-C4A	-10.71	1.34	1.53
2	C	501	FDE	CHB-C4A	-10.68	1.34	1.53
2	F	501	FDE	CHB-C4A	-10.61	1.35	1.53
2	D	501	FDE	C4A-NA	-10.61	1.35	1.49
2	G	501	FDE	C4A-NA	-10.60	1.35	1.49
2	B	501	FDE	CHB-C4A	-10.51	1.35	1.53
2	C	501	FDE	C4A-NA	-10.35	1.35	1.49
2	F	501	FDE	C4A-NA	-9.97	1.36	1.49
2	A	501	FDE	C4A-NA	-9.82	1.36	1.49
2	F	501	FDE	CHD-C1D	-8.04	1.31	1.51
2	B	501	FDE	C1B-NB	-7.72	1.30	1.35
2	B	501	FDE	CHD-C1D	-7.72	1.32	1.51
2	H	501	FDE	CHD-C1D	-7.60	1.32	1.51
2	D	501	FDE	CHD-C1D	-7.56	1.32	1.51
2	E	501	FDE	CHD-C1D	-7.55	1.32	1.51
2	A	501	FDE	CHD-C1D	-7.30	1.33	1.51
2	G	501	FDE	CHD-C1D	-7.21	1.33	1.51
2	C	501	FDE	CHD-C1D	-7.05	1.33	1.51
2	E	501	FDE	C1B-NB	-6.85	1.31	1.35
2	G	501	FDE	CHB-C1B	-6.52	1.34	1.50
2	A	501	FDE	CHB-C1B	-6.33	1.35	1.50
2	H	501	FDE	CHB-C1B	-6.32	1.35	1.50
2	H	501	FDE	C1B-NB	-6.23	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	FDE	C2C-C3C	6.12	1.41	1.33
2	C	501	FDE	CHB-C1B	-6.12	1.35	1.50
2	D	501	FDE	CHB-C1B	-5.93	1.35	1.50
2	F	501	FDE	C2C-C3C	5.90	1.41	1.33
2	B	501	FDE	C2C-C3C	5.84	1.41	1.33
2	E	501	FDE	CHB-C1B	-5.81	1.36	1.50
2	B	501	FDE	CHB-C1B	-5.66	1.36	1.50
2	D	501	FDE	C2C-C3C	5.58	1.41	1.33
2	D	501	FDE	C1B-NB	-5.54	1.31	1.35
2	A	501	FDE	C4B-C3B	5.53	1.45	1.38
2	F	501	FDE	CHB-C1B	-5.42	1.37	1.50
2	C	501	FDE	C2C-C3C	4.96	1.40	1.33
2	E	501	FDE	C2C-C3C	4.87	1.40	1.33
2	H	501	FDE	C2C-C3C	4.85	1.40	1.33
2	A	501	FDE	C2C-C3C	4.77	1.39	1.33
2	C	501	FDE	C4B-C3B	4.69	1.44	1.38
2	H	501	FDE	CHA-C1A	-4.50	1.45	1.53
2	B	501	FDE	CHA-C1A	-4.43	1.45	1.53
2	C	501	FDE	C1B-NB	-4.40	1.32	1.35
2	C	501	FDE	CHA-C1A	-4.36	1.45	1.53
2	G	501	FDE	C4B-C3B	4.34	1.44	1.38
2	F	501	FDE	C4B-C3B	4.27	1.44	1.38
2	B	501	FDE	C4B-C3B	4.26	1.44	1.38
2	F	501	FDE	CHA-C1A	-4.14	1.46	1.53
2	D	501	FDE	C3D-C2D	3.93	1.49	1.37
2	E	501	FDE	C4B-C3B	3.92	1.43	1.38
2	E	501	FDE	CHA-C1A	-3.79	1.46	1.53
2	A	501	FDE	C1B-NB	-3.79	1.32	1.35
2	G	501	FDE	CHC-C1C	-3.79	1.46	1.53
2	D	501	FDE	C4B-C3B	3.78	1.43	1.38
2	H	501	FDE	C4B-C3B	3.69	1.43	1.38
2	B	501	FDE	CHC-C1C	-3.57	1.46	1.53
2	E	501	FDE	CHC-C1C	-3.55	1.46	1.53
2	G	501	FDE	C3D-C2D	3.54	1.48	1.37
2	B	501	FDE	C3D-C2D	3.54	1.48	1.37
2	C	501	FDE	CHC-C1C	-3.51	1.46	1.53
2	E	501	FDE	C3D-C2D	3.44	1.47	1.37
2	A	501	FDE	C3D-C2D	3.42	1.47	1.37
2	H	501	FDE	C3D-C2D	3.42	1.47	1.37
2	H	501	FDE	CHC-C1C	-3.38	1.46	1.53
2	A	501	FDE	CHA-C1A	-3.31	1.47	1.53
2	A	501	FDE	CHC-C1C	-3.27	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FDE	CHC-C1C	-3.23	1.47	1.53
2	G	501	FDE	CHA-C1A	-3.15	1.47	1.53
2	F	501	FDE	CHC-C1C	-3.14	1.47	1.53
2	F	501	FDE	C3D-C2D	3.11	1.46	1.37
2	C	501	FDE	C3D-C2D	2.90	1.46	1.37
2	D	501	FDE	CHA-C1A	-2.86	1.48	1.53
2	G	501	FDE	C1B-NB	-2.70	1.33	1.35
2	G	501	FDE	CHC-C4B	-2.65	1.44	1.51
2	C	501	FDE	C1C-C2C	-2.48	1.38	1.48
2	B	501	FDE	C1C-C2C	-2.41	1.38	1.48
2	H	501	FDE	C1C-C2C	-2.40	1.38	1.48
2	D	501	FDE	C1C-C2C	-2.34	1.39	1.48
2	F	501	FDE	FE-NB	2.30	2.12	1.95
2	A	501	FDE	C1C-C2C	-2.29	1.39	1.48
2	E	501	FDE	C1C-C2C	-2.27	1.39	1.48
2	C	501	FDE	CHA-C4D	-2.26	1.45	1.51
2	C	501	FDE	FE-NB	2.19	2.11	1.95
2	G	501	FDE	C1C-C2C	-2.18	1.39	1.48
2	D	501	FDE	FE-ND	2.07	2.10	1.95
2	G	501	FDE	FE-NB	2.06	2.10	1.95
2	F	501	FDE	C1B-NB	-2.06	1.33	1.35
2	D	501	FDE	FE-NB	2.05	2.10	1.95
2	B	501	FDE	CHA-C4D	-2.05	1.46	1.51
2	H	501	FDE	CHC-C4B	-2.03	1.46	1.51
2	H	501	FDE	CHA-C4D	-2.02	1.46	1.51
2	F	501	FDE	C1C-C2C	-2.02	1.40	1.48
2	F	501	FDE	CHC-C4B	-2.01	1.46	1.51
2	H	501	FDE	FE-ND	2.00	2.10	1.95

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FDE	CBD-CAD-C3D	-9.95	94.14	112.49
2	H	501	FDE	CHA-C1A-NA	7.33	124.58	110.75
2	E	501	FDE	CHA-C1A-NA	7.16	124.25	110.75
2	A	501	FDE	CHC-C1C-NC	7.02	123.99	110.75
2	G	501	FDE	CHA-C1A-NA	6.77	123.53	110.75
2	D	501	FDE	CHA-C1A-NA	6.70	123.38	110.75
2	G	501	FDE	C2B-C1B-NB	6.59	117.34	108.63
2	D	501	FDE	CHC-C1C-NC	6.47	122.96	110.75
2	C	501	FDE	C2B-C1B-NB	6.40	117.09	108.63
2	A	501	FDE	CHA-C1A-NA	6.39	122.80	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FDE	CHA-C1A-NA	6.35	122.73	110.75
2	F	501	FDE	CHC-C1C-NC	6.33	122.68	110.75
2	A	501	FDE	C2B-C1B-NB	6.31	116.97	108.63
2	C	501	FDE	CMF-C3C-C2C	-6.25	116.67	127.69
2	C	501	FDE	CHC-C1C-NC	6.25	122.55	110.75
2	G	501	FDE	CHC-C1C-NC	6.25	122.53	110.75
2	E	501	FDE	CHC-C1C-NC	6.24	122.52	110.75
2	A	501	FDE	CAD-CBD-CGD	-6.22	102.23	112.67
2	H	501	FDE	CHC-C1C-NC	6.05	122.16	110.75
2	D	501	FDE	C2B-C1B-NB	5.94	116.49	108.63
2	B	501	FDE	CHC-C1C-NC	5.93	121.94	110.75
2	C	501	FDE	CHA-C1A-NA	5.85	121.78	110.75
2	B	501	FDE	C2B-C1B-NB	5.76	116.25	108.63
2	F	501	FDE	C2B-C1B-NB	5.72	116.20	108.63
2	E	501	FDE	C2B-C1B-NB	5.71	116.18	108.63
2	A	501	FDE	CBD-CAD-C3D	-5.66	102.05	112.49
2	A	501	FDE	CMF-C3C-C2C	-5.59	117.84	127.69
2	E	501	FDE	CMF-C3C-C2C	-5.58	117.85	127.69
2	G	501	FDE	CMF-C3C-C2C	-5.53	117.94	127.69
2	H	501	FDE	CMF-C3C-C2C	-5.51	117.97	127.69
2	E	501	FDE	CBD-CAD-C3D	-5.51	102.33	112.49
2	H	501	FDE	C2B-C1B-NB	5.47	115.87	108.63
2	F	501	FDE	CHA-C1A-NA	5.40	120.94	110.75
2	D	501	FDE	CMF-C3C-C2C	-5.33	118.30	127.69
2	C	501	FDE	CBD-CAD-C3D	-5.19	102.91	112.49
2	F	501	FDE	C1D-C2D-C3D	-5.11	100.37	105.81
2	D	501	FDE	CAA-CBA-CGA	-5.06	104.18	112.67
2	E	501	FDE	CBA-CAA-C2A	-4.65	106.11	114.35
2	F	501	FDE	CMF-C3C-C2C	-4.41	119.91	127.69
2	A	501	FDE	C1D-C2D-C3D	-4.39	101.13	105.81
2	G	501	FDE	CAD-CBD-CGD	-4.25	105.54	112.67
2	D	501	FDE	CBD-CAD-C3D	-4.19	104.76	112.49
2	H	501	FDE	CBD-CAD-C3D	-4.18	104.78	112.49
2	E	501	FDE	C1D-C2D-C3D	-4.10	101.44	105.81
2	H	501	FDE	C1D-C2D-C3D	-4.10	101.45	105.81
2	B	501	FDE	CAA-CBA-CGA	-4.04	105.89	112.67
2	G	501	FDE	C1D-C2D-C3D	-3.98	101.57	105.81
2	B	501	FDE	C1D-C2D-C3D	-3.97	101.59	105.81
2	B	501	FDE	CBD-CAD-C3D	-3.92	105.25	112.49
2	G	501	FDE	CBD-CAD-C3D	-3.87	105.35	112.49
2	B	501	FDE	CMF-C3C-C2C	-3.86	120.89	127.69
2	G	501	FDE	C1B-C2B-C3B	-3.69	100.53	106.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FDE	C1D-C2D-C3D	-3.68	101.90	105.81
2	C	501	FDE	C1B-C2B-C3B	-3.48	100.86	106.09
2	C	501	FDE	C1D-C2D-C3D	-3.35	102.25	105.81
2	D	501	FDE	C1B-C2B-C3B	-3.29	101.14	106.09
2	E	501	FDE	C1B-C2B-C3B	-3.14	101.37	106.09
2	F	501	FDE	C1B-C2B-C3B	-3.13	101.38	106.09
2	H	501	FDE	C1B-C2B-C3B	-2.99	101.59	106.09
2	H	501	FDE	CAD-C3D-C4D	2.98	129.39	127.30
2	B	501	FDE	C1B-C2B-C3B	-2.96	101.64	106.09
2	A	501	FDE	CHC-C4B-C3B	-2.91	124.50	129.62
2	D	501	FDE	CHC-C4B-C3B	-2.86	124.60	129.62
2	C	501	FDE	CAA-CBA-CGA	-2.86	107.88	112.67
2	A	501	FDE	C1B-C2B-C3B	-2.76	101.94	106.09
2	C	501	FDE	CHC-C4B-C3B	-2.73	124.83	129.62
2	F	501	FDE	CHC-C4B-C3B	-2.62	125.02	129.62
2	G	501	FDE	CHC-C4B-C3B	-2.59	125.08	129.62
2	E	501	FDE	CHC-C4B-C3B	-2.54	125.16	129.62
2	B	501	FDE	CHC-C4B-C3B	-2.47	125.29	129.62
2	H	501	FDE	CHC-C4B-C3B	-2.40	125.41	129.62
2	D	501	FDE	CMD-C2D-C3D	2.34	129.34	124.94
2	A	501	FDE	CBA-CAA-C2A	-2.27	110.33	114.35
2	F	501	FDE	CAD-C3D-C4D	2.26	128.88	127.30
2	C	501	FDE	CMA-C3A-C2A	-2.23	125.33	128.33
2	A	501	FDE	CAA-CBA-CGA	-2.23	108.94	112.67
2	F	501	FDE	CAD-CBD-CGD	-2.15	109.07	112.67
2	B	501	FDE	CHD-C4C-NC	2.11	114.72	110.75
2	G	501	FDE	CBA-CAA-C2A	-2.11	110.62	114.35
2	H	501	FDE	CHD-C4C-NC	2.10	114.70	110.75
2	C	501	FDE	CHD-C1D-C2D	2.09	133.06	129.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

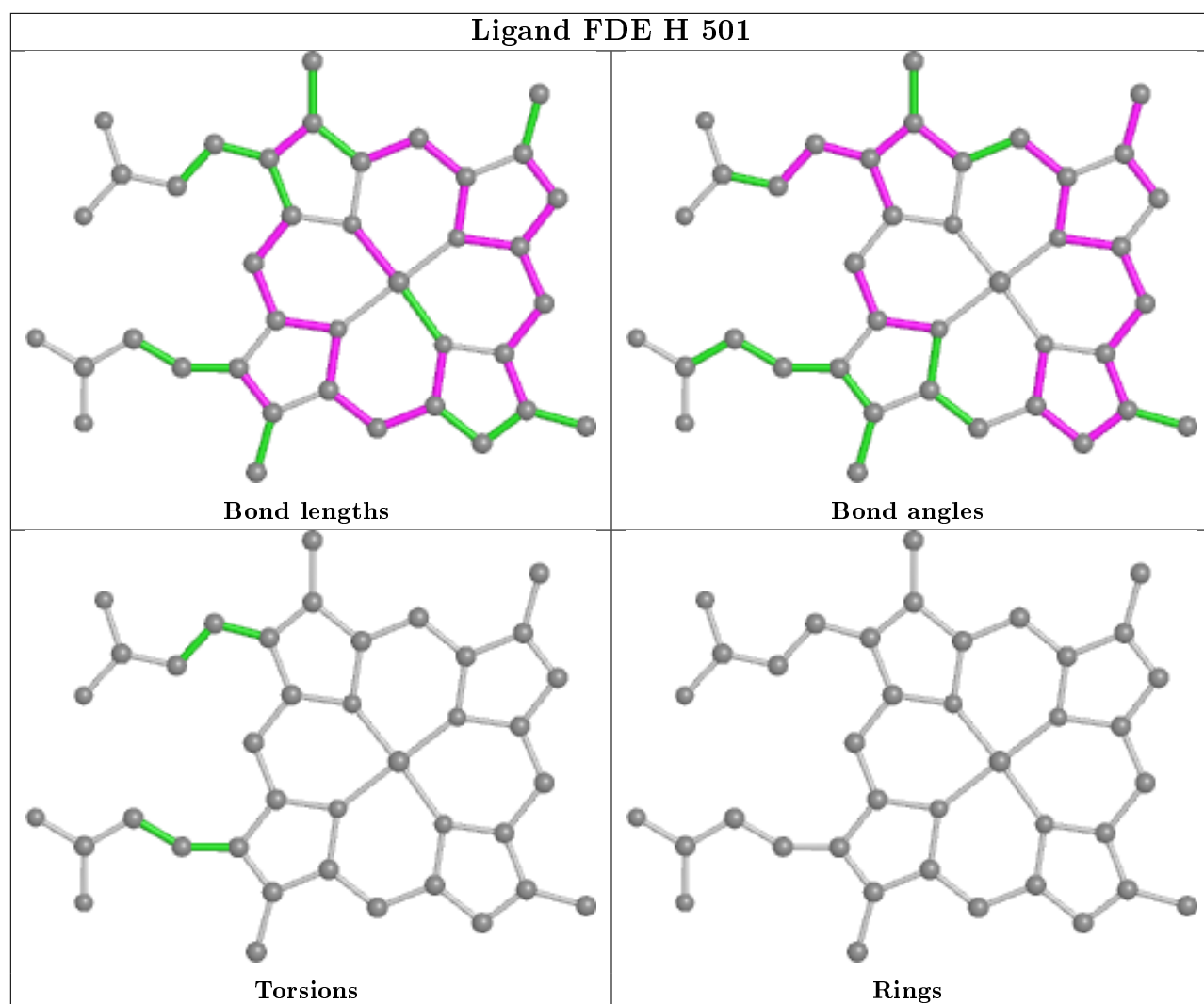
Mol	Chain	Res	Type	Atoms
2	E	501	FDE	C3A-C2A-CAA-CBA
2	D	501	FDE	C1A-C2A-CAA-CBA
2	B	501	FDE	C2A-CAA-CBA-CGA
2	D	501	FDE	C3A-C2A-CAA-CBA

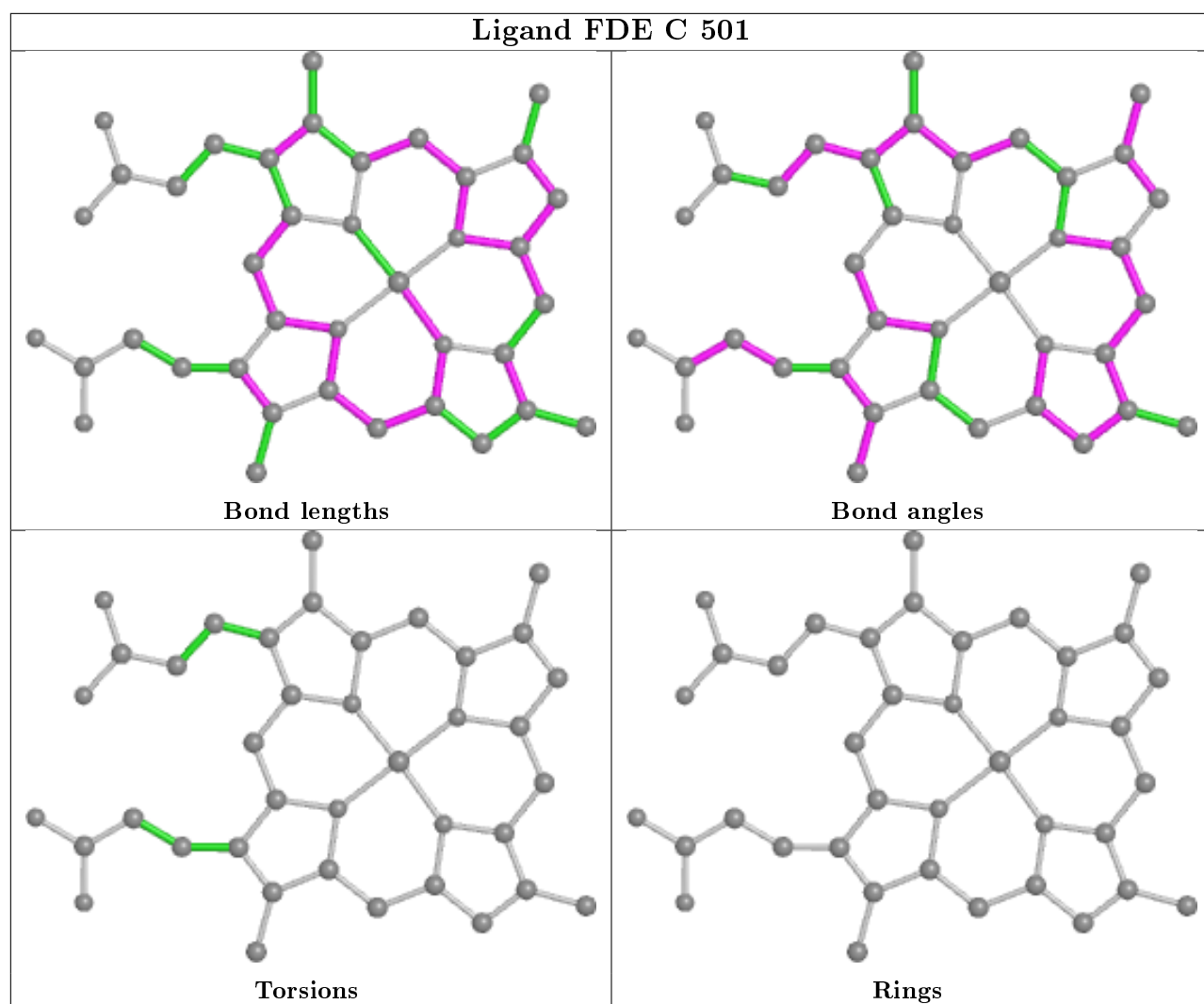
There are no ring outliers.

8 monomers are involved in 19 short contacts:

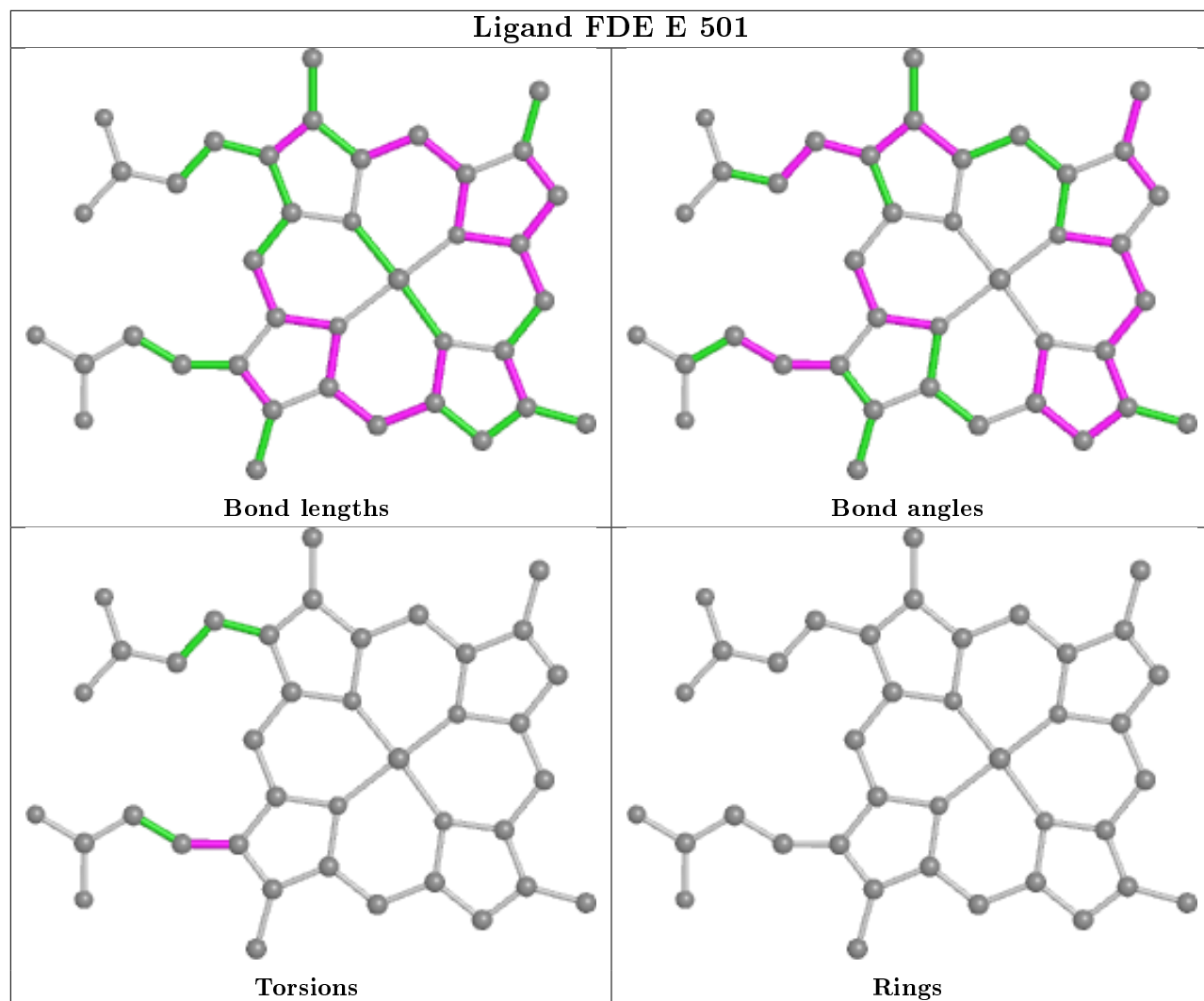
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	FDE	3	0
2	C	501	FDE	2	0
2	E	501	FDE	3	0
2	A	501	FDE	2	0
2	G	501	FDE	4	0
2	D	501	FDE	2	0
2	F	501	FDE	1	0
2	B	501	FDE	2	0

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.

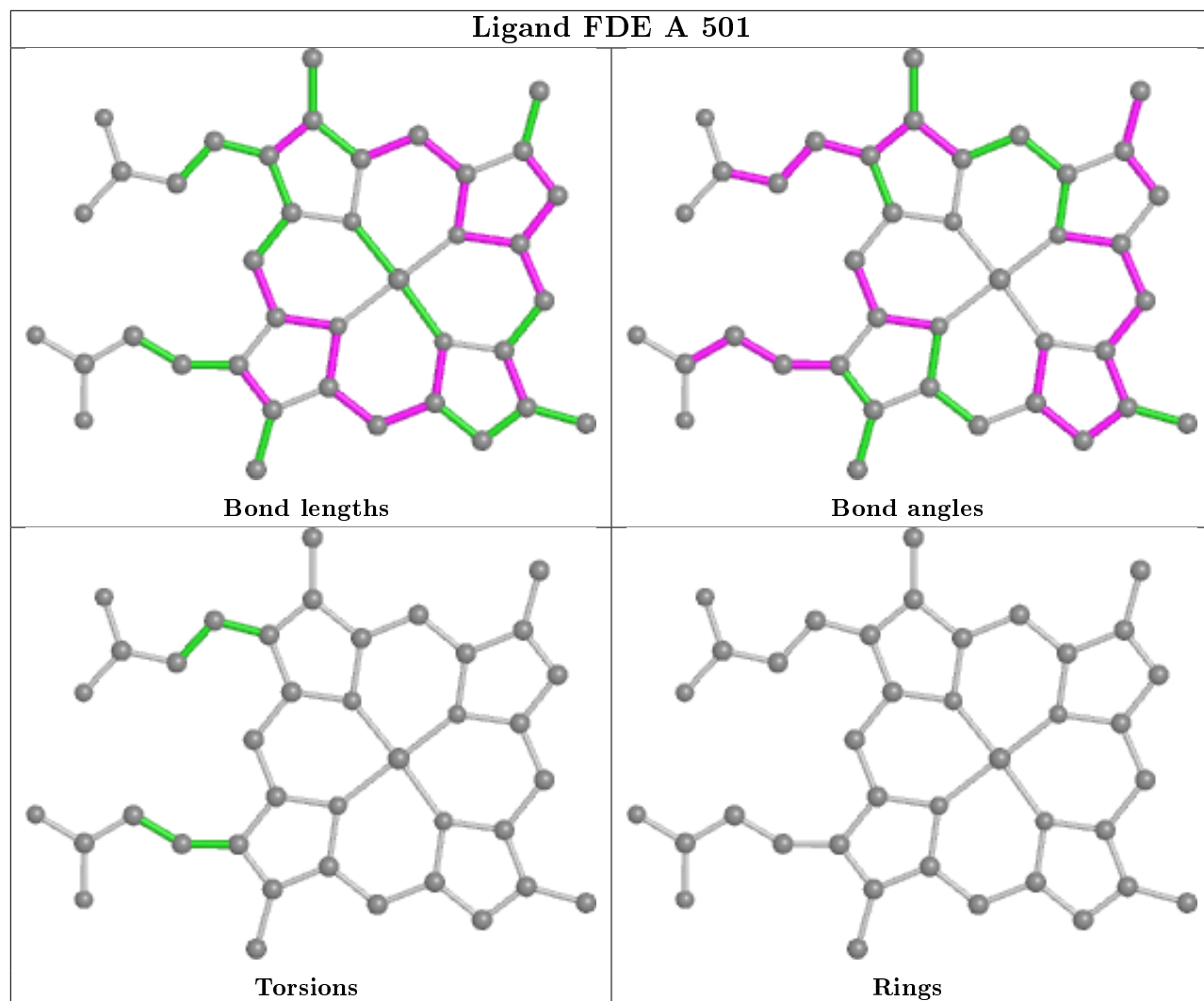


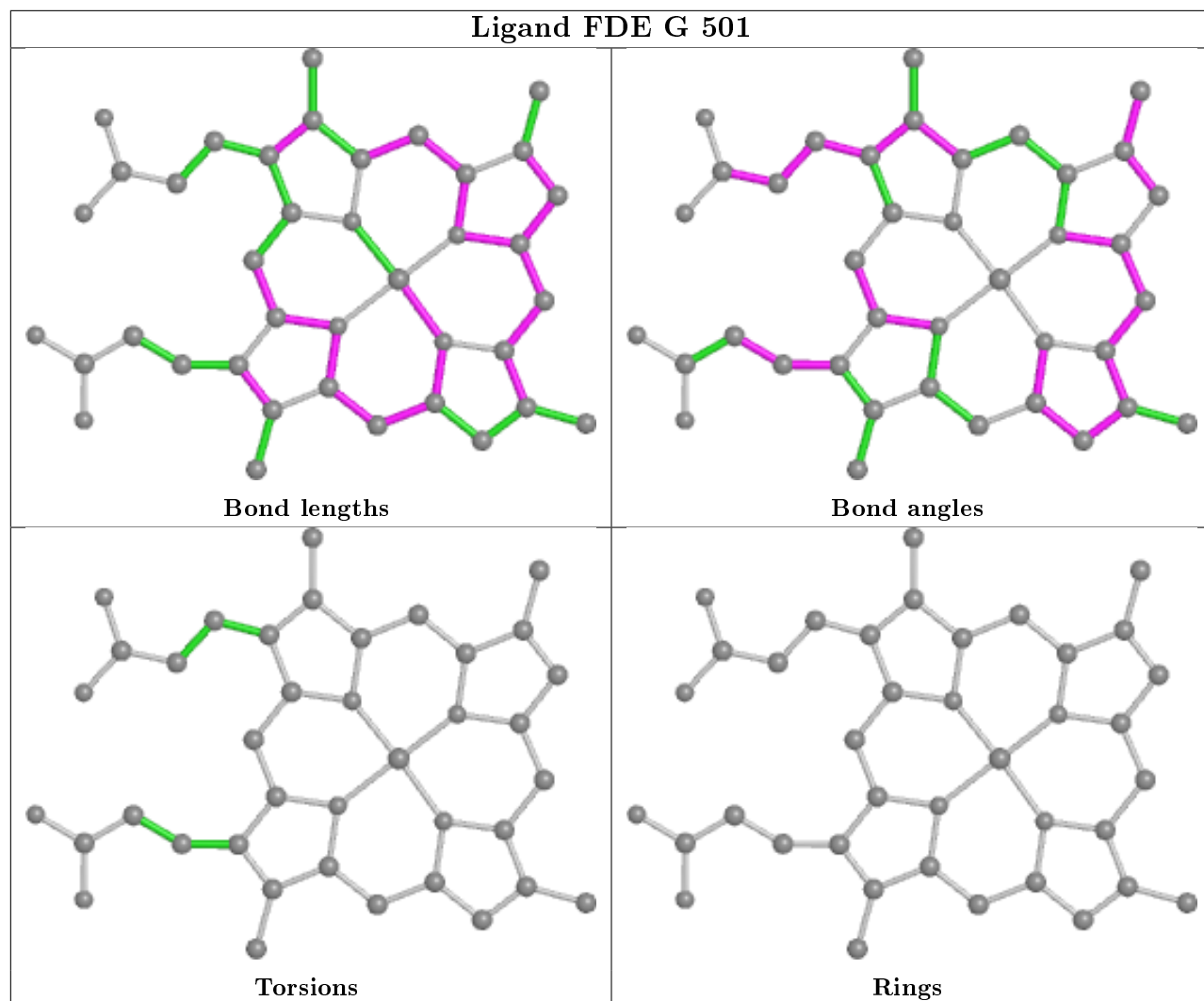


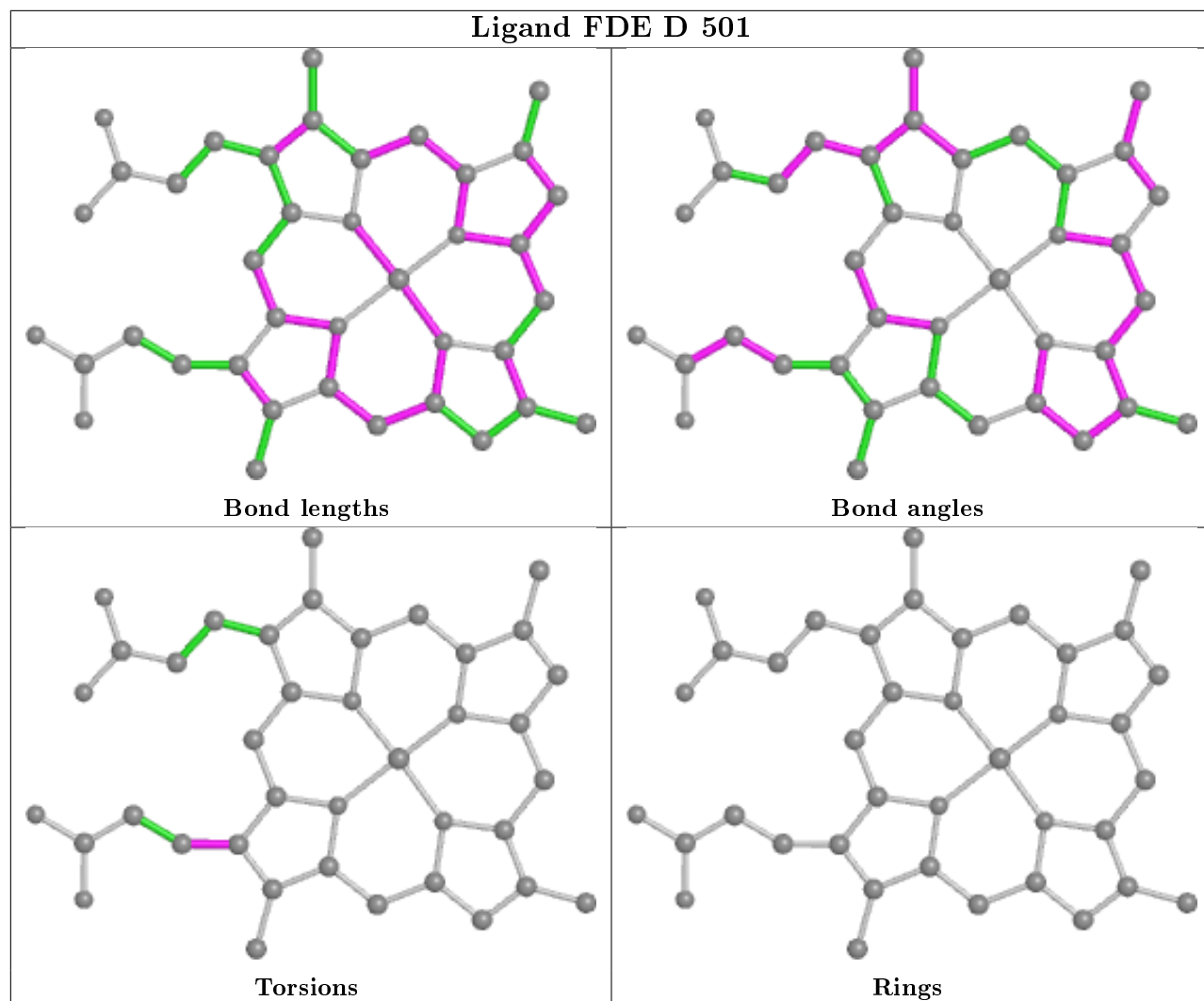
Ligand FDE E 501



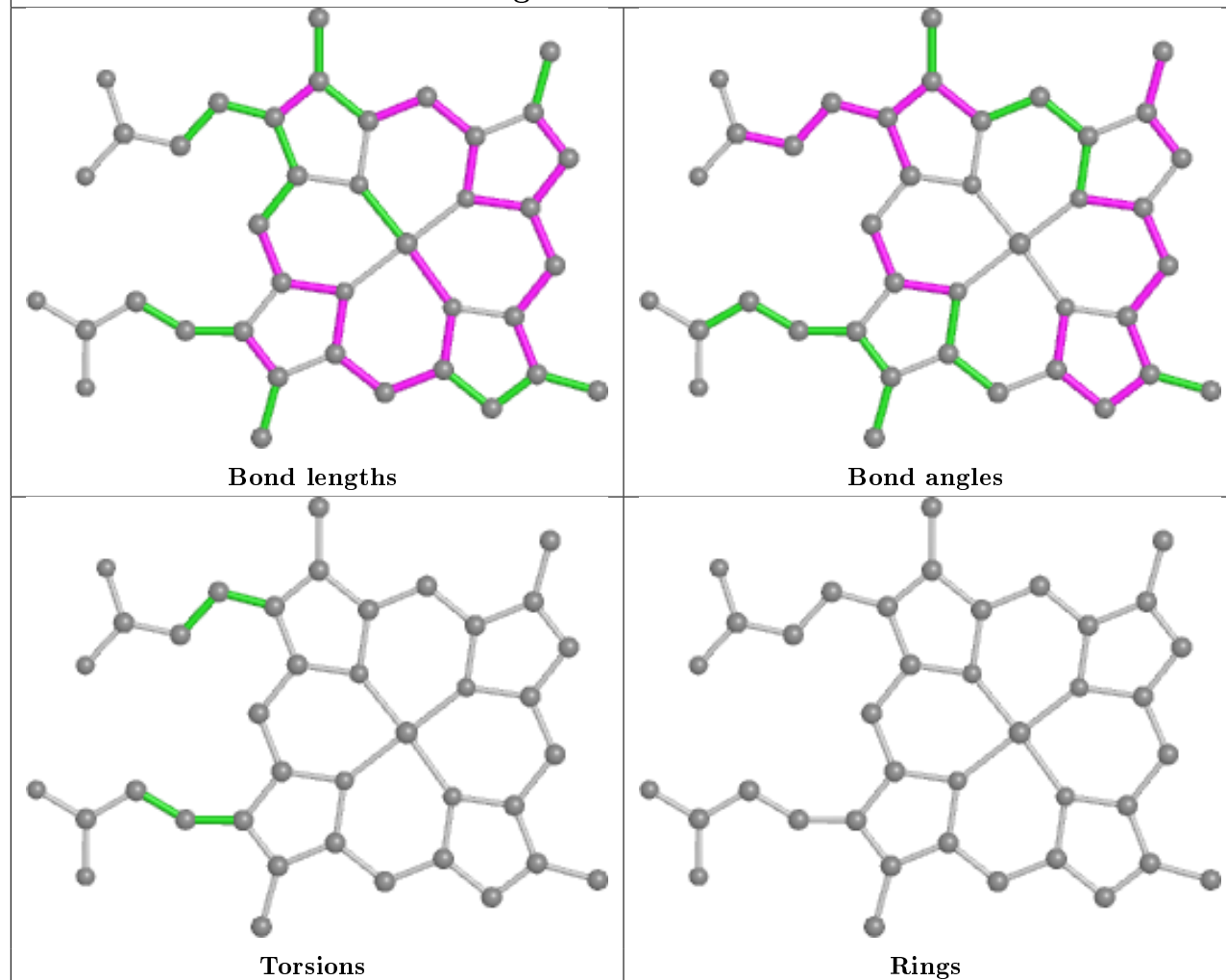
Ligand FDE A 501

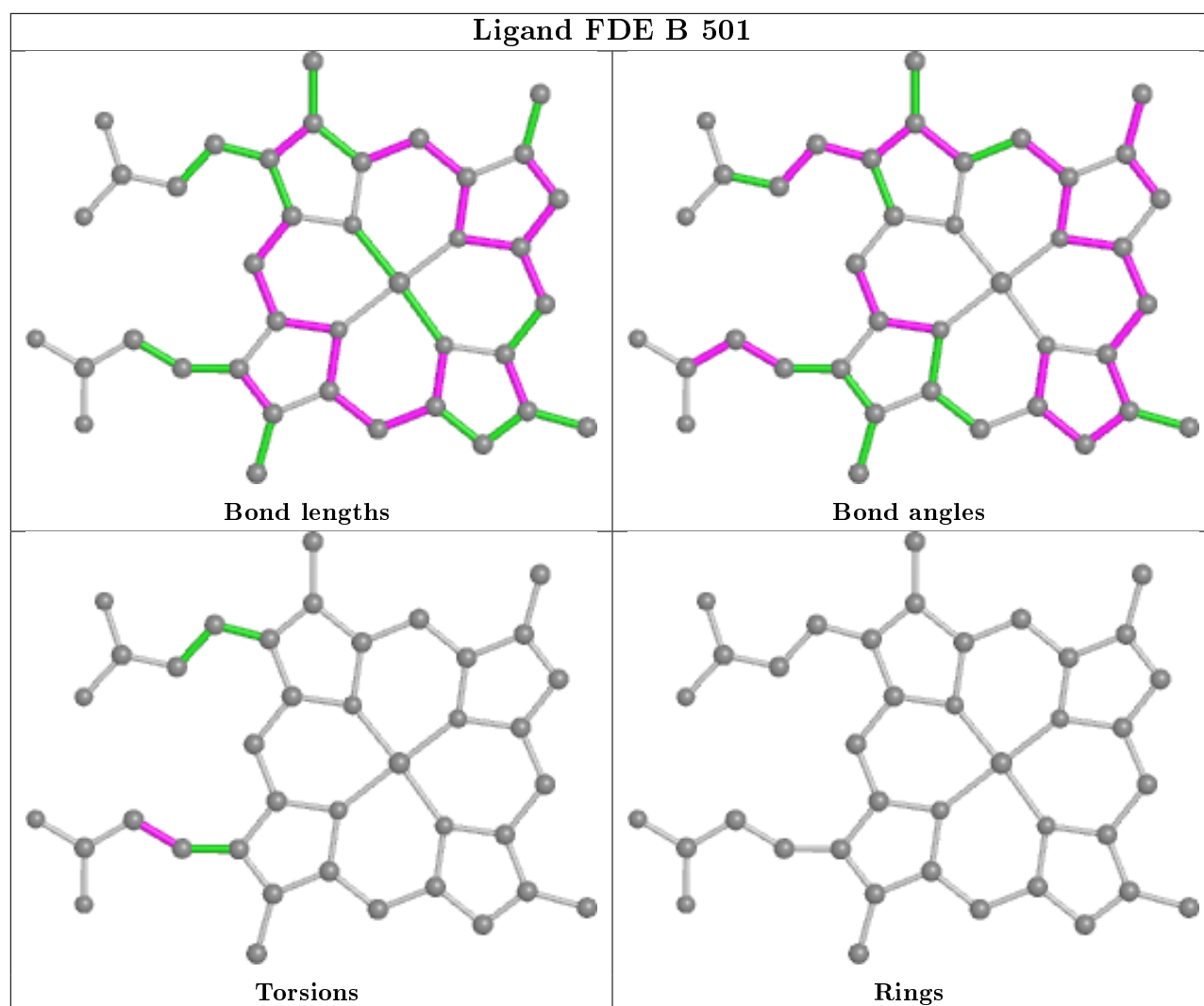






Ligand FDE F 501





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	452/471 (95%)	0.14	5 (1%) 80 85	4, 15, 28, 35	0
1	B	453/471 (96%)	0.01	0 100 100	2, 10, 25, 36	0
1	C	453/471 (96%)	0.03	5 (1%) 80 85	2, 11, 25, 37	0
1	D	454/471 (96%)	0.30	12 (2%) 56 64	10, 21, 33, 42	0
1	E	451/471 (95%)	0.06	4 (0%) 84 88	4, 12, 26, 37	0
1	F	455/471 (96%)	0.20	8 (1%) 68 75	7, 19, 32, 38	0
1	G	451/471 (95%)	0.10	6 (1%) 77 82	4, 16, 32, 42	0
1	H	450/471 (95%)	0.10	4 (0%) 84 88	3, 13, 26, 36	0
All	All	3619/3768 (96%)	0.12	44 (1%) 79 83	2, 15, 29, 42	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	6.5
1	F	191	ALA	4.6
1	G	379	PHE	3.8
1	D	173	PHE	3.7
1	G	11	PHE	3.7
1	D	150	LEU	3.2
1	F	136	ASP	3.1
1	C	229	GLN	3.0
1	G	369	ASP	3.0
1	G	225	ALA	3.0
1	F	269	VAL	2.8
1	D	245	THR	2.5
1	D	263	ILE	2.5
1	H	385	ILE	2.5
1	A	383	SER	2.5
1	D	261	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	148	LEU	2.5
1	A	295	ALA	2.4
1	F	347	LEU	2.4
1	C	410	ALA	2.4
1	D	265	PHE	2.3
1	F	248	PRO	2.3
1	C	153	ILE	2.3
1	D	357	ILE	2.3
1	A	298	LEU	2.2
1	D	414	LEU	2.2
1	D	350	GLY	2.2
1	C	407	LEU	2.2
1	F	314	VAL	2.2
1	F	388	HIS	2.2
1	H	366	ILE	2.2
1	E	369	ASP	2.2
1	A	263	ILE	2.1
1	F	268	THR	2.1
1	G	298	LEU	2.1
1	D	152	THR	2.1
1	E	318	LEU	2.1
1	E	385	ILE	2.0
1	H	413	VAL	2.0
1	C	369	ASP	2.0
1	G	231	ASP	2.0
1	D	299	VAL	2.0
1	E	413	VAL	2.0
1	H	74	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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,

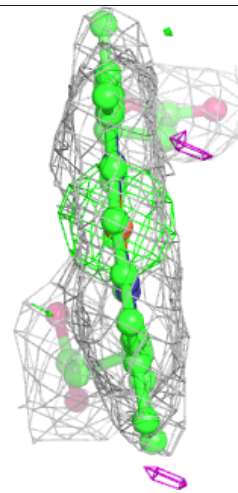
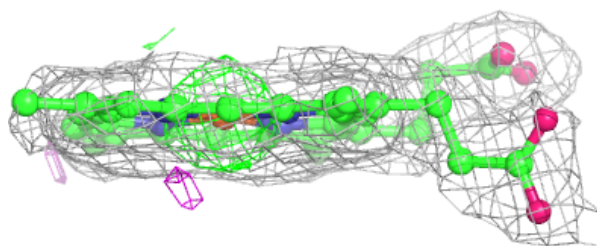
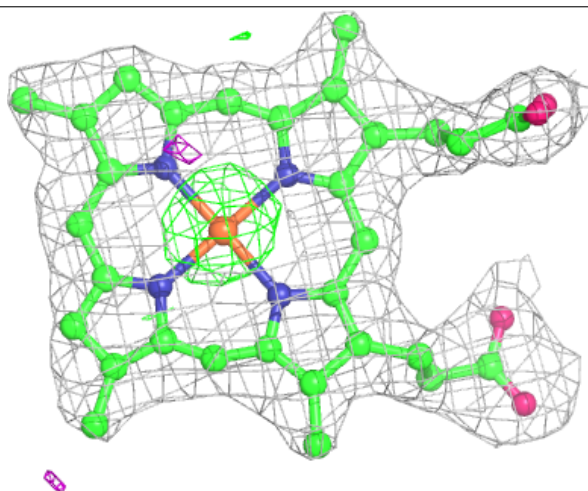
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FDE	A	501	39/39	0.82	0.19	5,10,16,127	0
2	FDE	C	501	39/39	0.93	0.19	2,2,7,10	0
2	FDE	H	501	39/39	0.94	0.18	2,2,7,7	0
2	FDE	G	501	39/39	0.94	0.17	3,6,11,16	0
2	FDE	D	501	39/39	0.94	0.18	5,10,15,17	0
2	FDE	F	501	39/39	0.94	0.15	4,8,18,25	0
2	FDE	E	501	39/39	0.95	0.17	2,4,18,24	0
2	FDE	B	501	39/39	0.95	0.18	2,3,11,16	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.

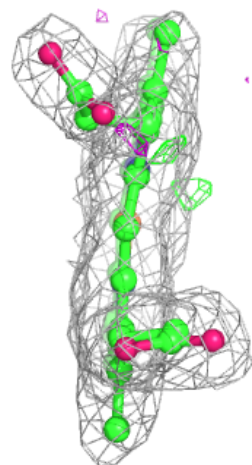
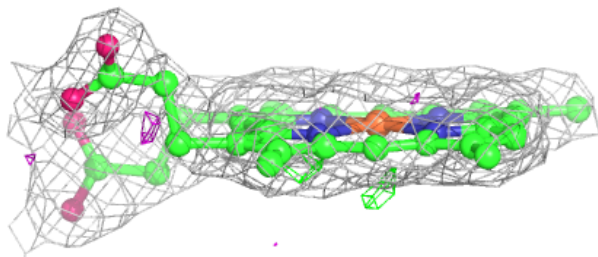
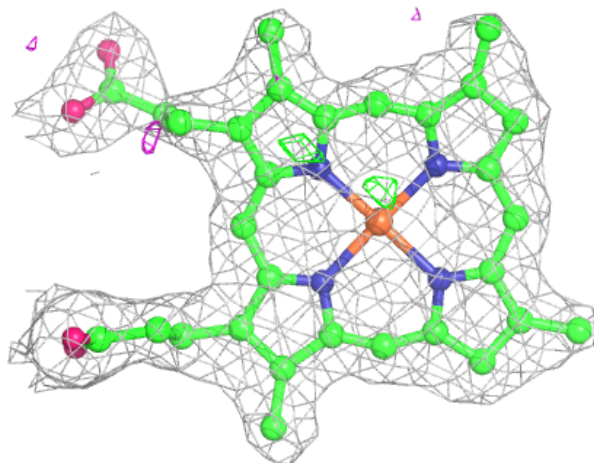
Electron density around FDE A 501:

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



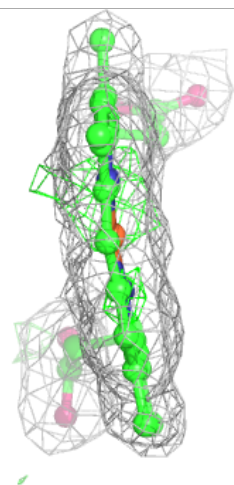
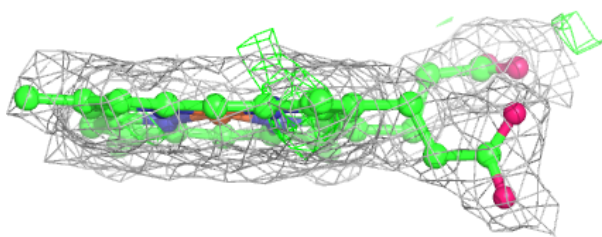
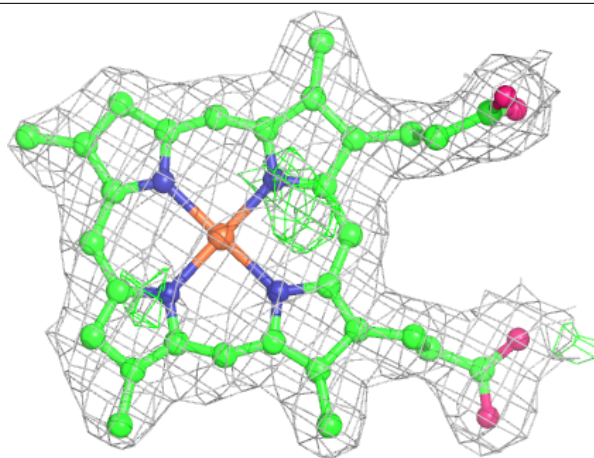
Electron density around FDE C 501:

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



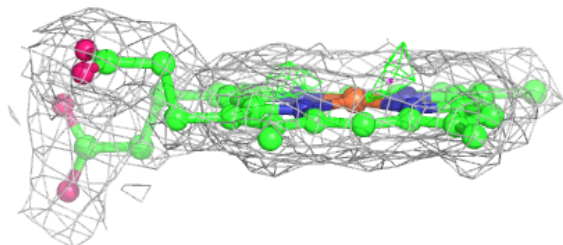
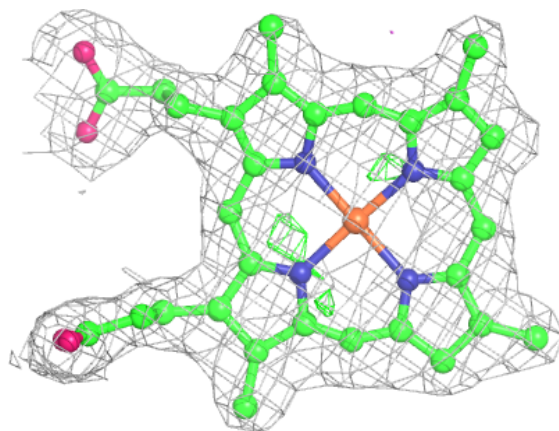
Electron density around FDE H 501:

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



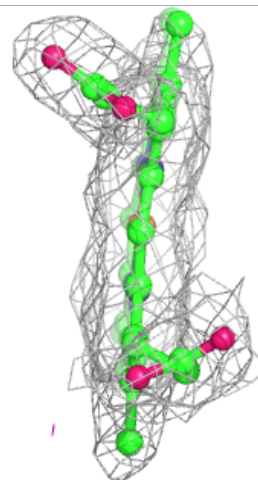
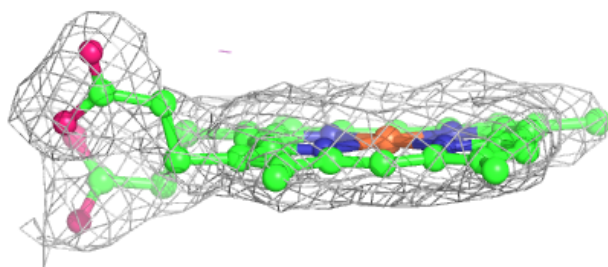
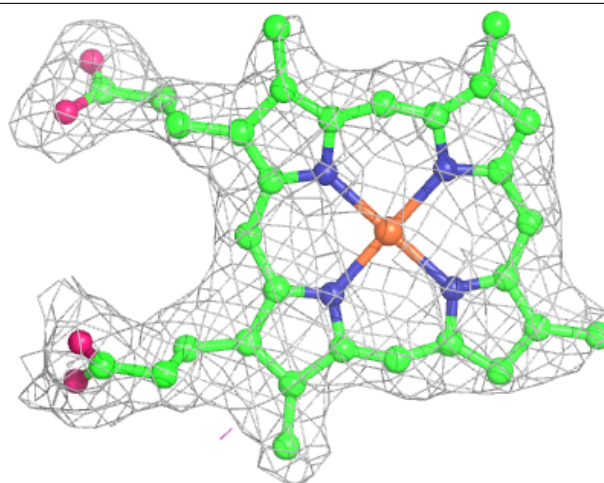
Electron density around FDE G 501:

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



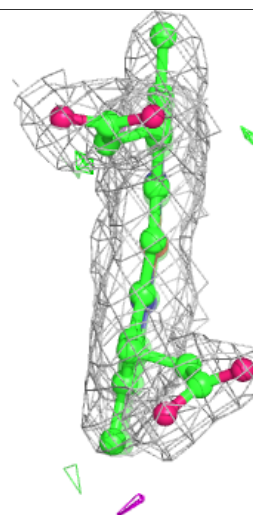
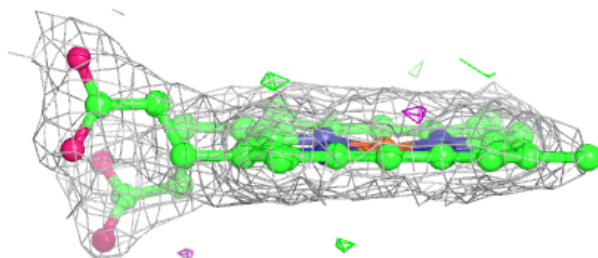
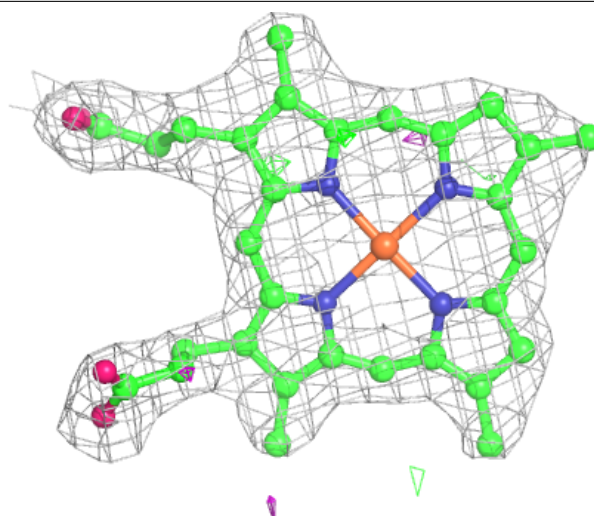
Electron density around FDE D 501:

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



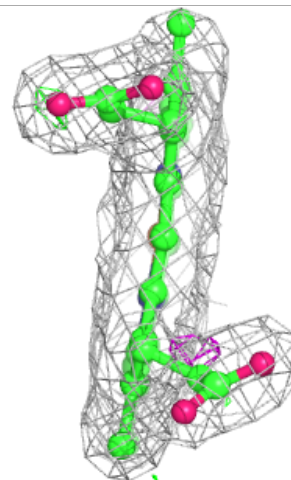
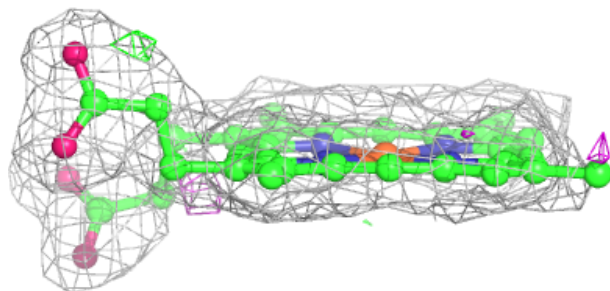
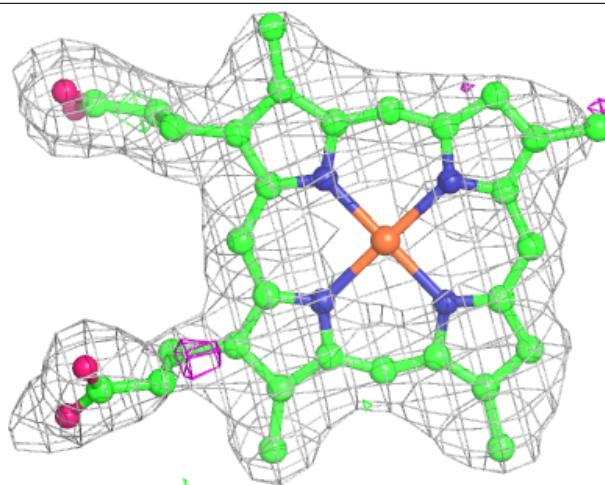
Electron density around FDE F 501:

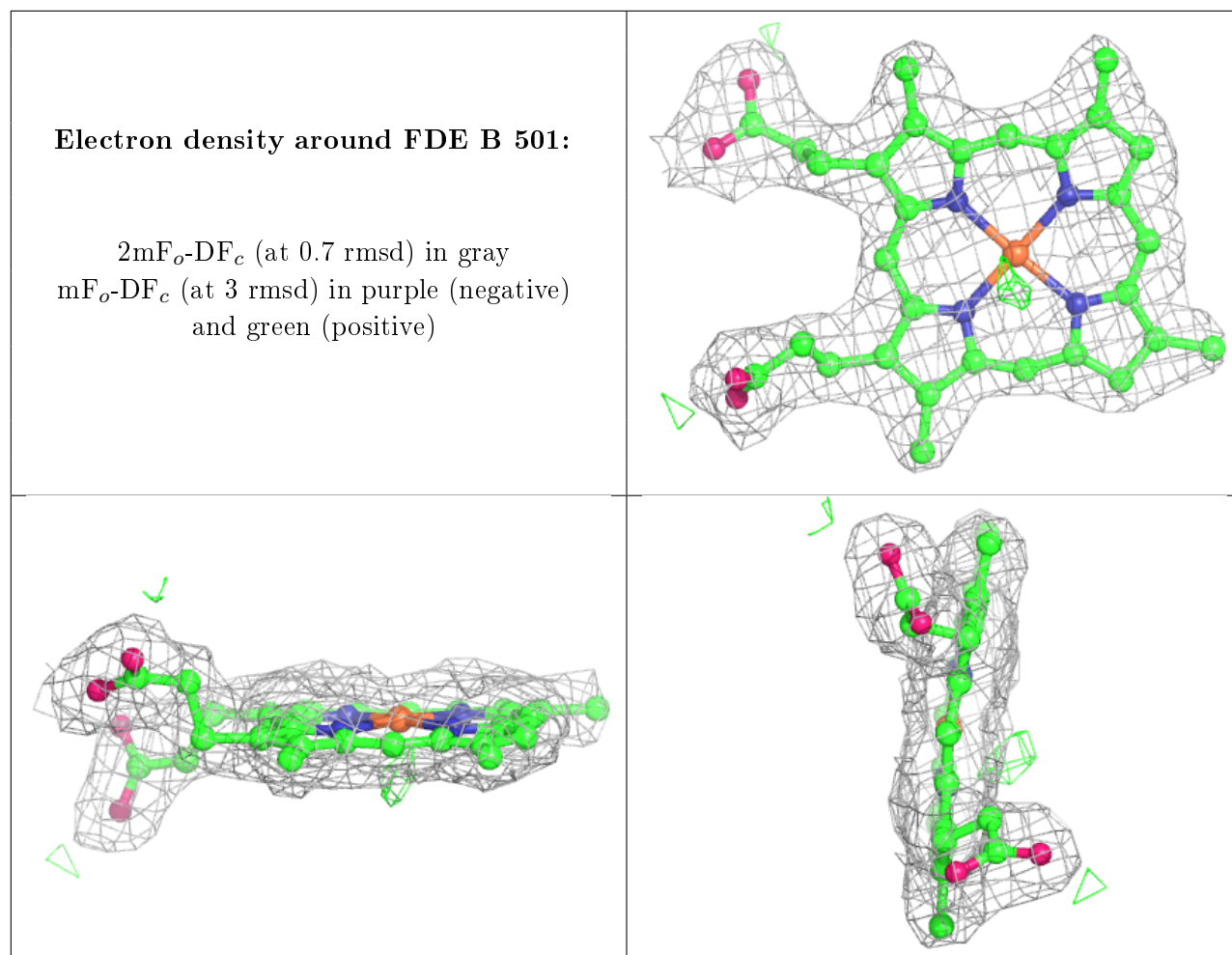
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FDE E 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.