



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:10 am BST

PDB ID : 3NHQ
Title : The dark Pfr structure of the photosensory core module of *P. aeruginosa* Bacteriophytochrome
Authors : Yang, X.; Ren, Z.; Kuk, J.; Moffat, K.
Deposited on : 2010-06-14
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

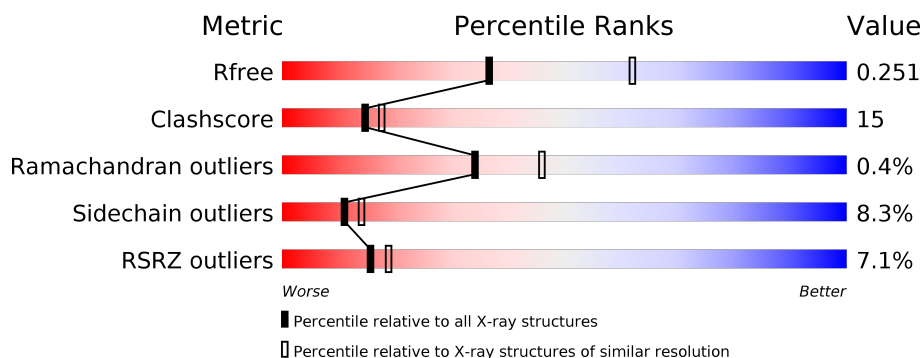
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	505	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>5%</div> </div> </div>
1	B	505	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>7%</div> </div> </div>
1	C	505	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>5%</div> </div> </div>
1	D	505	<div> <div>9%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>5%</div> </div> </div>
1	E	505	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>5%</div> </div> </div>
1	F	505	<div> <div>11%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>5%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	505	<div><div>%</div><div><div></div><div>65%</div><div>26%</div><div>• 5%</div></div></div>
1	H	505	<div><div>14%</div><div><div></div><div>64%</div><div>28%</div><div>• 5%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30788 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3790	2386	682	703	19			
1	B	470	Total	C	N	O	S	0	0	0
			3709	2332	665	693	19			
1	C	482	Total	C	N	O	S	0	0	0
			3812	2398	688	707	19			
1	D	480	Total	C	N	O	S	0	0	0
			3801	2391	686	705	19			
1	E	479	Total	C	N	O	S	0	0	0
			3790	2386	683	702	19			
1	F	471	Total	C	N	O	S	0	0	0
			3717	2338	666	694	19			
1	G	482	Total	C	N	O	S	0	1	0
			3816	2401	688	708	19			
1	H	481	Total	C	N	O	S	0	0	0
			3808	2396	687	706	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
A	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
A	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
B	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
B	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3

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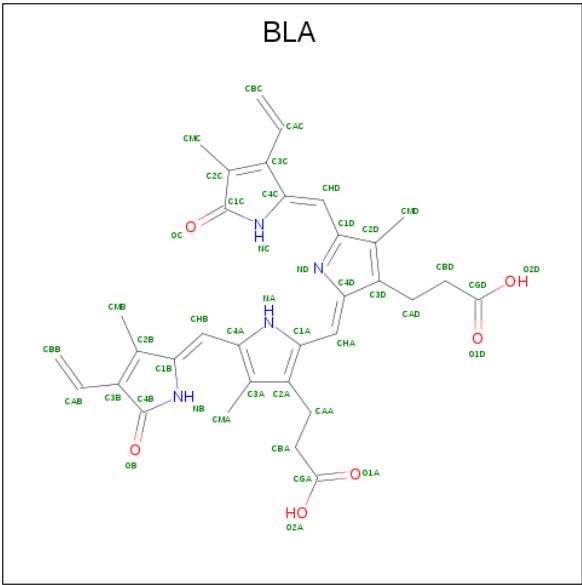
Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
C	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
C	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
D	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
D	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
E	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
E	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
F	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
F	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
G	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
G	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
H	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
H	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		
2	E	1	Total	C	N	O	0	0
			43	33	4	6		
2	F	1	Total	C	N	O	0	0
			43	33	4	6		
2	G	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			43	33	4	6		

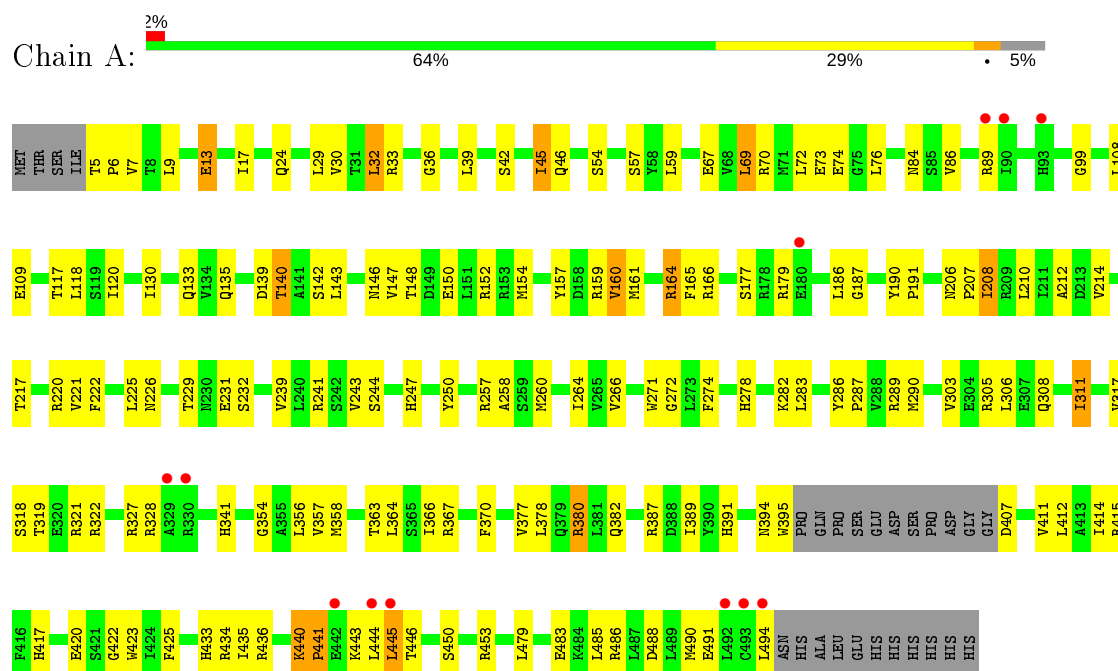
- Molecule 3 is water.

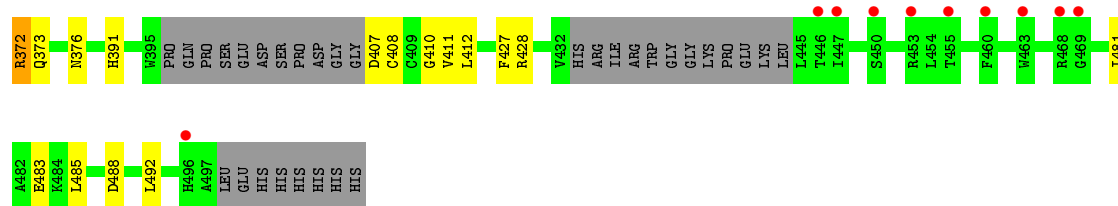
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	16	Total	O	0	0
			16	16		
3	C	44	Total	O	0	0
			44	44		
3	D	14	Total	O	0	0
			14	14		
3	E	15	Total	O	0	0
			15	15		
3	F	7	Total	O	0	0
			7	7		
3	G	37	Total	O	0	0
			37	37		
3	H	7	Total	O	0	0
			7	7		

3 Residue-property plots

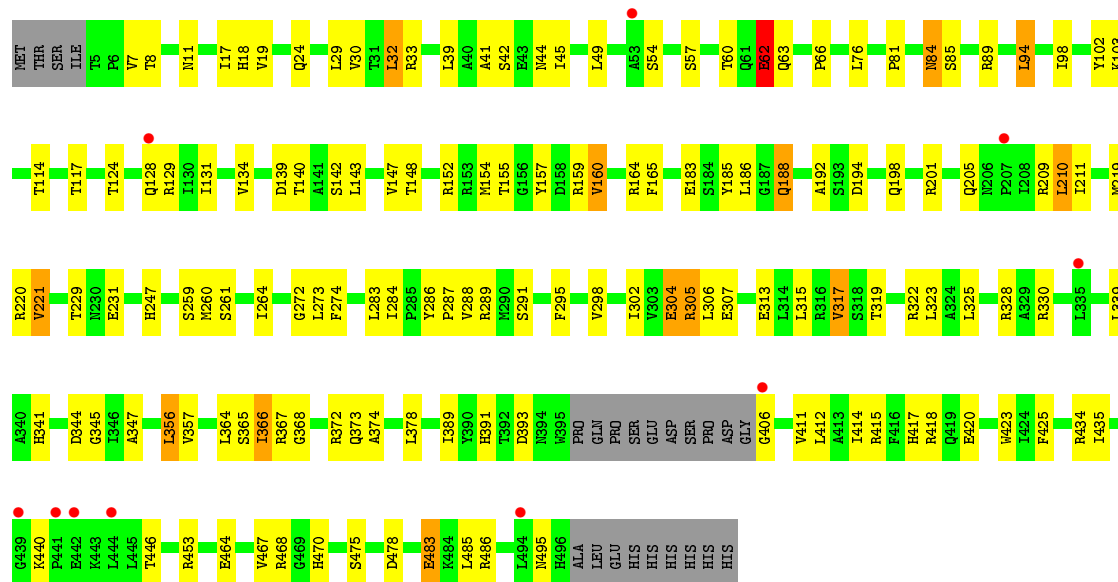
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Bacteriophytochrome

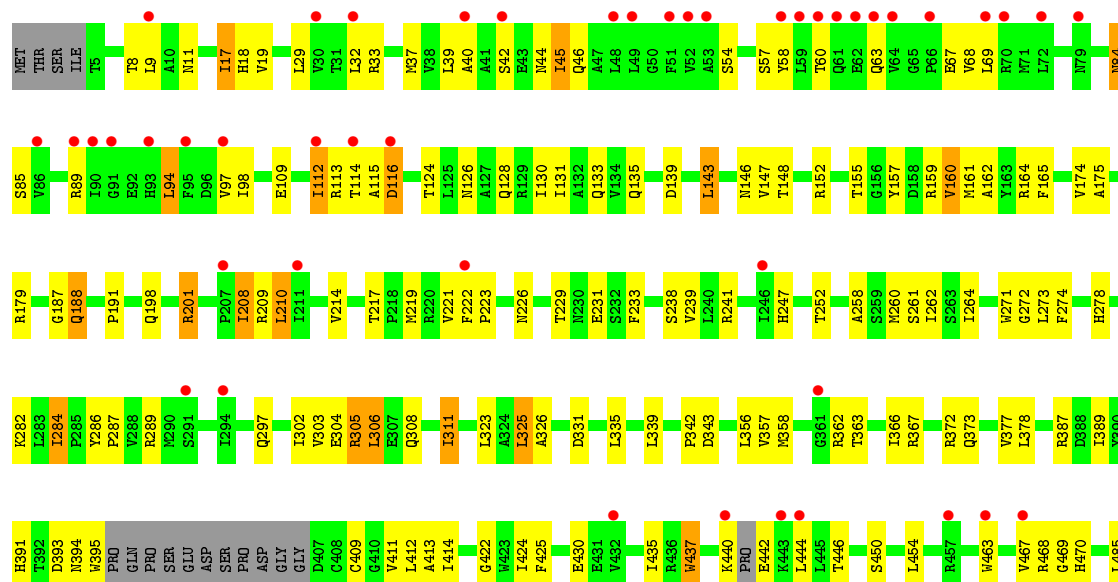


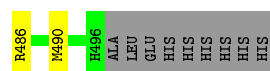


• Molecule 1: Bacteriophytochrome

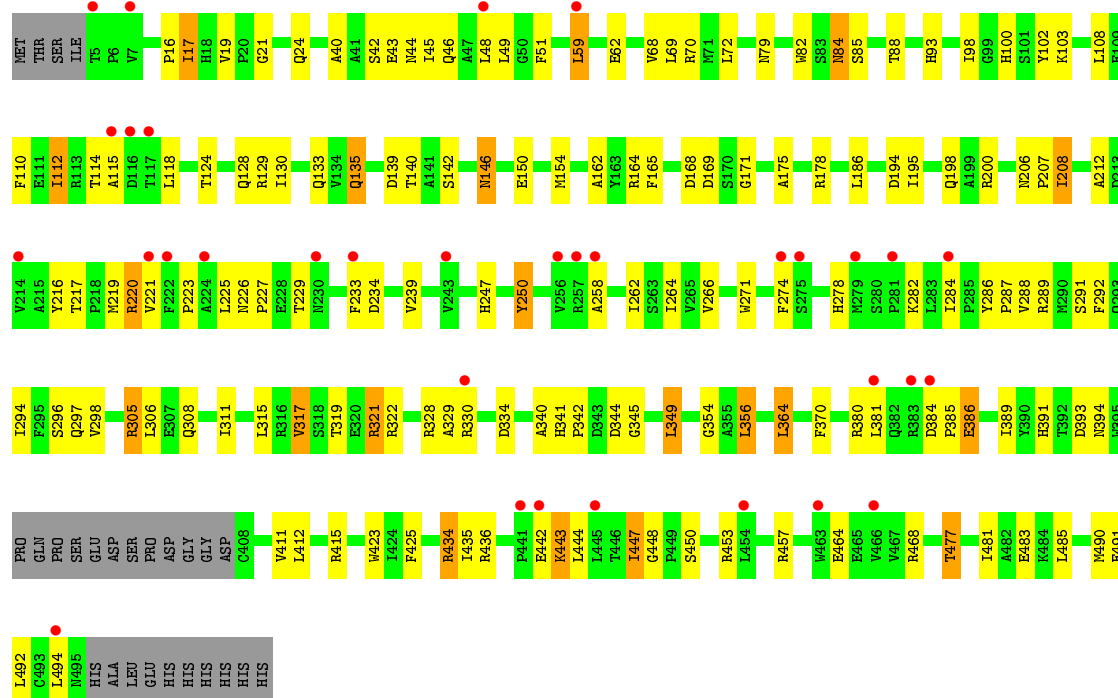


• Molecule 1: Bacteriophytochrome

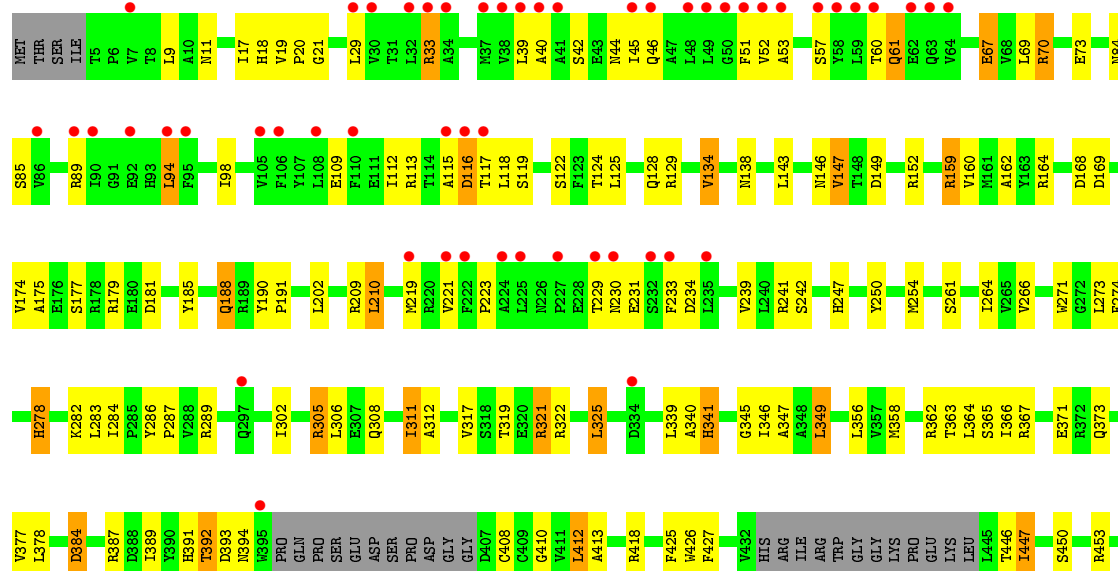


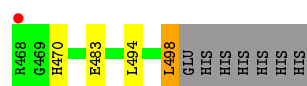


• Molecule 1: Bacteriophytochrome

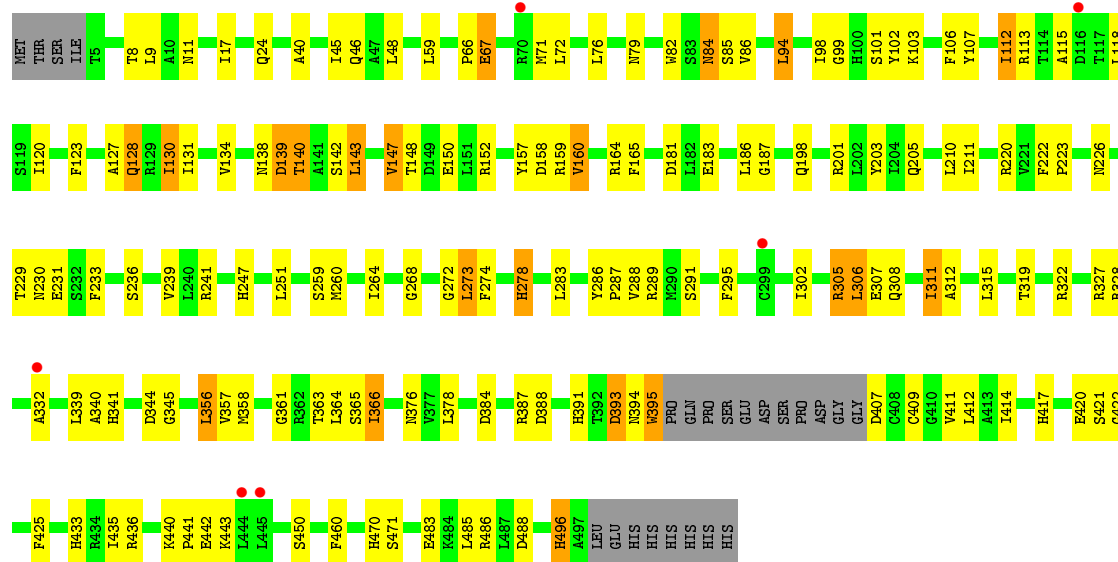


• Molecule 1: Bacteriophytochrome

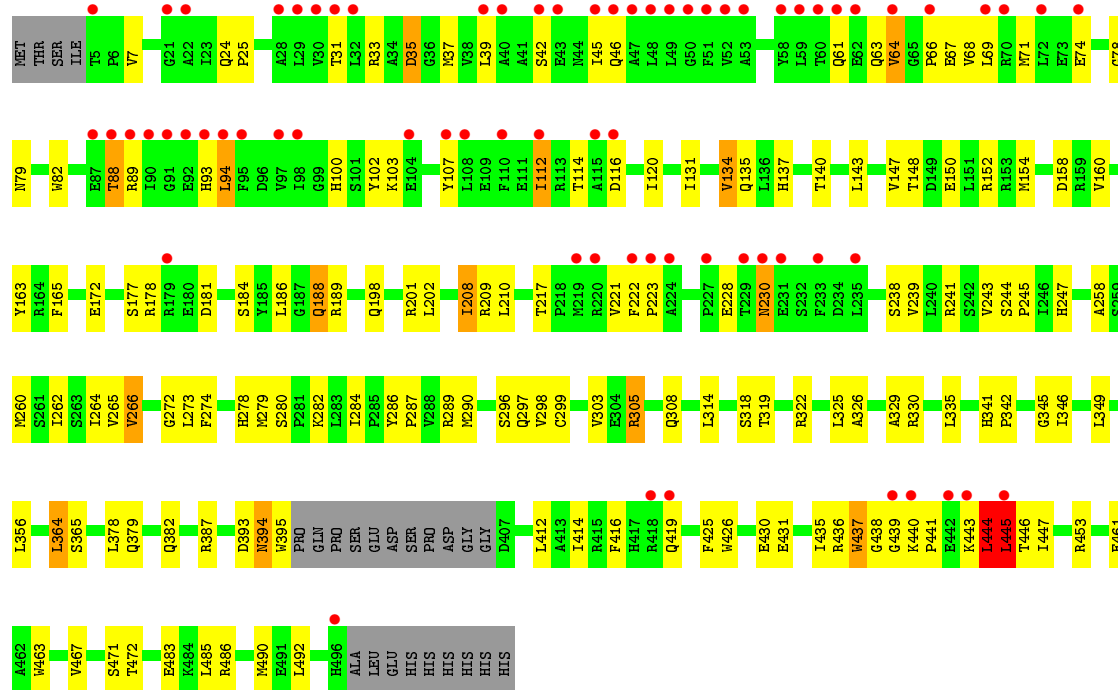




• Molecule 1: Bacteriophytochrome



• Molecule 1: Bacteriophytochrome



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.38 Å 162.98 Å 436.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.55 49.49 – 2.53	Depositor EDS
% Data completeness (in resolution range)	82.9 (48.48-2.55) 81.3 (49.49-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.215 , 0.258 0.209 , 0.251	Depositor DCC
R_{free} test set	7437 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLA

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	0.26	0/3874	0.48	0/5258
1	B	0.24	0/3789	0.45	0/5144
1	C	0.25	0/3897	0.46	0/5289
1	D	0.24	0/3884	0.45	0/5269
1	E	0.23	0/3874	0.45	0/5258
1	F	0.23	0/3797	0.45	0/5155
1	G	0.25	0/3904	0.47	0/5299
1	H	0.24	0/3893	0.44	0/5284
All	All	0.24	0/30912	0.46	0/41956

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	B	0	1
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ASP	Peptide
1	A	441	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	92	GLU	Peptide
1	C	62	GLU	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	3790	0	3734	104	0
1	B	3709	0	3641	119	0
1	C	3812	0	3750	108	0
1	D	3801	0	3739	122	0
1	E	3790	0	3736	124	0
1	F	3717	0	3652	125	0
1	G	3816	0	3757	116	0
1	H	3808	0	3747	115	0
2	A	43	0	30	4	0
2	B	43	0	31	8	0
2	C	43	0	31	14	0
2	D	43	0	31	5	0
2	E	43	0	30	7	0
2	F	43	0	31	9	0
2	G	43	0	30	5	0
2	H	43	0	31	6	0
3	A	61	0	0	4	0
3	B	16	0	0	1	0
3	C	44	0	0	4	0
3	D	14	0	0	6	0
3	E	15	0	0	4	0
3	F	7	0	0	1	0
3	G	37	0	0	0	0
3	H	7	0	0	0	0
All	All	30788	0	30001	925	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (925) 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:F:70:ARG:HG3	1:F:70:ARG:HH11	1.00	1.10
1:H:444:LEU:HD23	1:H:444:LEU:H	1.26	0.96
1:F:70:ARG:HG3	1:F:70:ARG:NH1	1.76	0.93
1:G:84:ASN:HD22	1:G:85:SER:H	1.02	0.92
1:D:112:ILE:HD13	1:D:112:ILE:H	1.36	0.91
1:A:364:LEU:HD21	1:G:435:ILE:HB	1.53	0.90
1:G:319:THR:HG22	1:G:322:ARG:HH21	1.36	0.89
1:C:41:ALA:HB1	1:C:45:ILE:HD12	1.53	0.89
1:E:447:ILE:HG12	1:E:448:GLY:N	1.87	0.88
1:C:17:ILE:HD11	3:C:909:HOH:O	1.75	0.87
1:A:140:THR:HG22	1:A:306:LEU:HB3	1.56	0.86
1:D:201:ARG:HG3	1:D:201:ARG:HH11	1.41	0.85
1:C:84:ASN:HD22	1:C:85:SER:H	1.24	0.85
1:A:319:THR:HG22	1:A:322:ARG:HH21	1.41	0.84
1:B:7:VAL:HG21	1:B:245:PRO:HG2	1.57	0.84
1:G:394:ASN:HD21	1:G:470:HIS:CD2	1.95	0.84
2:C:900:BLA:HBC1	2:C:900:BLA:HMC1	1.58	0.84
1:G:198:GLN:HE22	1:G:201:ARG:NH1	1.75	0.83
1:G:84:ASN:HD22	1:G:85:SER:N	1.77	0.82
1:H:441:PRO:HB3	1:H:443:LYS:HE2	1.61	0.82
1:B:210:LEU:HD12	1:B:289:ARG:HD3	1.61	0.81
1:D:394:ASN:O	1:D:395:TRP:HB2	1.80	0.81
1:D:201:ARG:CG	1:D:201:ARG:HH11	1.93	0.81
1:D:139:ASP:HB3	3:D:910:HOH:O	1.81	0.81
1:E:17:ILE:HG22	3:E:909:HOH:O	1.80	0.81
1:G:120:ILE:HA	1:H:120:ILE:HD11	1.63	0.81
1:D:124:THR:HG22	3:D:909:HOH:O	1.80	0.80
1:H:33:ARG:HG2	1:H:37:MET:HB3	1.64	0.80
1:H:440:LYS:N	1:H:441:PRO:HD2	1.96	0.80
1:D:37:MET:HB2	1:D:58:TYR:CZ	2.19	0.78
1:F:210:LEU:HD12	1:F:289:ARG:HD3	1.65	0.78
1:E:305:ARG:HA	1:E:308:GLN:HG2	1.63	0.78
1:H:198:GLN:HE22	1:H:201:ARG:HH11	1.32	0.76
1:F:70:ARG:CG	1:F:70:ARG:HH11	1.91	0.76
1:A:479:LEU:O	1:A:483:GLU:HG3	1.86	0.75
1:H:198:GLN:NE2	1:H:201:ARG:HH11	1.83	0.75
1:C:414:ILE:HD12	1:C:486:ARG:HB2	1.69	0.75
1:F:356:LEU:HD23	1:F:365:SER:HB3	1.69	0.75
1:H:258:ALA:HB3	1:H:278:HIS:HB3	1.68	0.74
1:G:378:LEU:HD11	1:G:425:PHE:HZ	1.52	0.74
1:A:143:LEU:O	1:A:147:VAL:HG12	1.87	0.74
1:D:188:GLN:NE2	2:D:900:BLA:HBB1	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:VAL:HG12	1:H:266:VAL:O	1.89	0.73
1:C:41:ALA:HB1	1:C:45:ILE:CD1	2.17	0.73
1:B:139:ASP:HB2	1:B:142:SER:HB2	1.70	0.73
1:B:356:LEU:HD23	1:B:365:SER:HB3	1.71	0.73
1:A:117:THR:HG22	1:A:118:LEU:H	1.54	0.73
1:G:210:LEU:HD23	1:G:260:MET:HG2	1.70	0.72
1:B:258:ALA:HB3	1:B:278:HIS:HB3	1.72	0.72
1:B:214:VAL:HB	1:B:257:ARG:HA	1.69	0.72
1:G:139:ASP:HB2	1:G:142:SER:HB2	1.70	0.72
1:H:230:ASN:HD22	1:H:230:ASN:N	1.88	0.72
1:C:475:SER:HB2	1:C:478:ASP:H	1.55	0.71
1:D:89:ARG:HA	1:D:94:LEU:HA	1.71	0.71
1:E:434:ARG:HD2	1:E:435:ILE:HG23	1.70	0.71
1:F:447:ILE:H	1:F:447:ILE:HD13	1.55	0.71
1:H:346:ILE:O	1:H:426:TRP:HZ3	1.74	0.71
1:B:305:ARG:HA	1:B:308:GLN:HG2	1.73	0.71
1:D:210:LEU:HD12	1:D:289:ARG:HD3	1.73	0.70
1:E:84:ASN:HD22	1:E:85:SER:H	1.39	0.70
1:H:305:ARG:HD2	1:H:305:ARG:N	2.06	0.70
1:E:194:ASP:HB3	2:E:900:BLA:HHB	1.73	0.70
1:A:440:LYS:HD2	1:G:361:GLY:HA3	1.74	0.69
1:B:410:GLY:O	1:B:427:PHE:HA	1.92	0.69
1:A:264:ILE:HD11	1:A:274:PHE:CE1	2.27	0.69
1:E:140:THR:HG22	1:E:306:LEU:HB3	1.75	0.69
1:H:444:LEU:HD23	1:H:444:LEU:N	2.05	0.69
1:H:112:ILE:H	1:H:112:ILE:HD13	1.56	0.69
1:B:220:ARG:HE	1:B:222:PHE:HZ	1.41	0.69
1:B:208:ILE:HD11	1:B:293:GLN:N	2.06	0.69
1:C:94:LEU:H	1:C:94:LEU:HD22	1.58	0.69
1:E:88:THR:HG21	3:E:908:HOH:O	1.93	0.69
1:G:128:GLN:HA	1:H:297:GLN:HE22	1.55	0.69
1:E:317:VAL:O	1:E:321:ARG:HG2	1.93	0.69
1:F:305:ARG:HH11	1:F:305:ARG:HG2	1.58	0.69
1:G:127:ALA:O	1:G:131:ILE:HG23	1.93	0.69
1:E:305:ARG:HH21	1:E:308:GLN:HE22	1.41	0.68
1:G:131:ILE:HD11	1:H:297:GLN:HB3	1.75	0.68
1:H:286:TYR:HB3	1:H:287:PRO:HD3	1.75	0.68
1:E:328:ARG:HH12	1:E:344:ASP:HB2	1.57	0.68
1:E:297:GLN:HE22	1:F:128:GLN:HA	1.58	0.68
1:F:45:ILE:HD12	1:F:46:GLN:H	1.59	0.68
1:D:157:TYR:OH	1:D:284:ILE:HD11	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:HH21	1:B:376:ASN:HD21	1.42	0.67
1:C:84:ASN:ND2	1:C:85:SER:H	1.92	0.67
1:E:162:ALA:HB3	1:E:175:ALA:HB3	1.76	0.67
1:D:372:ARG:HB2	3:D:904:HOH:O	1.94	0.67
1:F:168:ASP:O	1:F:169:ASP:HB2	1.95	0.67
1:B:205:GLN:HE22	1:H:419:GLN:HG2	1.59	0.67
1:H:45:ILE:HD12	1:H:46:GLN:N	2.09	0.67
1:C:129:ARG:HE	1:C:154:MET:HG2	1.60	0.66
1:C:435:ILE:HD11	1:E:340:ALA:HB1	1.77	0.66
1:H:64:VAL:HG12	1:H:68:VAL:HG11	1.77	0.66
1:A:444:LEU:HD22	1:A:444:LEU:H	1.60	0.66
1:C:319:THR:HG22	1:C:322:ARG:HH21	1.58	0.66
1:C:17:ILE:HG12	3:C:930:HOH:O	1.94	0.66
1:G:157:TYR:HA	1:G:278:HIS:HD2	1.59	0.66
1:B:64:VAL:HG12	1:B:68:VAL:HB	1.78	0.66
1:F:239:VAL:HG11	1:F:289:ARG:HH21	1.60	0.66
1:D:356:LEU:HD21	1:D:363:THR:HG23	1.77	0.66
1:B:45:ILE:HD12	1:B:46:GLN:H	1.60	0.66
1:D:8:THR:H	1:D:11:ASN:HB3	1.60	0.65
1:E:442:GLU:HG3	1:E:443:LYS:H	1.62	0.65
1:E:464:GLU:O	1:E:468:ARG:HG2	1.97	0.65
1:A:9:LEU:HD21	1:A:450:SER:HB3	1.78	0.65
1:A:45:ILE:HD12	1:A:46:GLN:H	1.61	0.65
1:C:328:ARG:HH12	1:C:344:ASP:HB2	1.61	0.65
1:H:89:ARG:HA	1:H:94:LEU:HA	1.79	0.65
1:D:45:ILE:HD12	1:D:46:GLN:H	1.61	0.65
1:E:321:ARG:HH11	1:E:321:ARG:CG	2.09	0.65
1:C:148:THR:HG23	1:C:160:VAL:HG22	1.79	0.65
1:D:286:TYR:HB3	1:D:287:PRO:HD3	1.78	0.64
1:F:45:ILE:HD12	1:F:46:GLN:N	2.12	0.64
1:G:159:ARG:NH1	1:G:183:GLU:O	2.29	0.64
1:D:54:SER:OG	1:D:57:SER:HB3	1.97	0.64
1:E:381:LEU:O	1:E:381:LEU:HD13	1.97	0.64
1:B:9:LEU:HD22	1:B:9:LEU:H	1.62	0.64
1:F:346:ILE:HB	1:F:426:TRP:CH2	2.32	0.64
1:G:143:LEU:O	1:G:147:VAL:HG13	1.98	0.64
1:B:201:ARG:HH21	1:B:236:SER:HB3	1.62	0.64
1:G:157:TYR:HA	1:G:278:HIS:CD2	2.33	0.64
1:E:447:ILE:HG12	1:E:448:GLY:H	1.63	0.64
1:D:435:ILE:HB	1:H:364:LEU:HD13	1.80	0.63
1:H:346:ILE:O	1:H:426:TRP:CZ3	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ALA:HB1	1:E:492:LEU:HD21	1.79	0.63
1:F:179:ARG:NH1	1:F:181:ASP:HB3	2.14	0.63
1:F:319:THR:HG22	1:F:322:ARG:HH21	1.64	0.63
1:A:13:GLU:HG2	3:A:925:HOH:O	1.98	0.63
1:G:198:GLN:HE22	1:G:201:ARG:HH11	1.46	0.63
2:C:900:BLA:O2A	2:C:900:BLA:HMA2	1.99	0.62
1:A:226:ASN:HB3	1:A:229:THR:HG22	1.81	0.62
1:B:308:GLN:O	1:B:311:ILE:HD13	1.99	0.62
1:C:198:GLN:HE22	1:C:201:ARG:HE	1.46	0.62
1:F:317:VAL:O	1:F:321:ARG:HG2	1.99	0.62
1:G:198:GLN:NE2	1:G:201:ARG:NH1	2.47	0.62
1:H:178:ARG:HE	1:H:184:SER:HB2	1.64	0.62
1:F:46:GLN:HB2	1:F:52:VAL:HG22	1.80	0.62
1:G:220:ARG:HE	1:G:222:PHE:HZ	1.47	0.62
1:F:143:LEU:O	1:F:147:VAL:HG13	2.00	0.62
1:G:378:LEU:HD11	1:G:425:PHE:CZ	2.33	0.62
1:A:208:ILE:H	1:A:208:ILE:HD13	1.65	0.62
1:B:213:ASP:O	1:B:216:TYR:HB3	1.99	0.62
1:C:209:ARG:HD2	3:C:939:HOH:O	1.99	0.62
1:H:445:LEU:HD12	1:H:447:ILE:HG23	1.82	0.62
1:E:21:GLY:HA2	1:E:233:PHE:CE1	2.34	0.62
1:A:444:LEU:N	1:A:444:LEU:HD22	2.16	0.61
1:C:209:ARG:HH12	2:C:900:BLA:CGD	2.13	0.61
1:A:356:LEU:HD21	1:A:363:THR:HG23	1.83	0.61
1:C:165:PHE:CD1	1:C:272:GLY:HA2	2.36	0.61
1:G:140:THR:HG21	1:G:307:GLU:OE2	2.01	0.61
1:B:42:SER:O	1:B:45:ILE:HG13	2.00	0.61
1:F:152:ARG:HB2	1:F:160:VAL:HG11	1.83	0.61
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.64	0.61
1:A:229:THR:HG23	1:A:231:GLU:H	1.65	0.61
1:C:209:ARG:HH11	1:C:209:ARG:HG2	1.66	0.61
1:F:89:ARG:HG2	1:F:94:LEU:HB3	1.81	0.61
1:B:139:ASP:HB2	1:B:142:SER:CB	2.31	0.61
1:C:229:THR:HG23	1:C:231:GLU:H	1.64	0.60
1:D:229:THR:HG23	1:D:231:GLU:H	1.66	0.60
1:D:258:ALA:HB3	1:D:278:HIS:HB3	1.83	0.60
1:H:319:THR:HG22	1:H:322:ARG:HH21	1.66	0.60
1:G:327:ARG:HG2	1:H:330:ARG:NH2	2.16	0.60
1:B:130:ILE:HG23	1:B:154:MET:SD	2.42	0.60
1:G:143:LEU:C	1:G:143:LEU:HD12	2.22	0.60
1:B:51:PHE:HB2	1:B:63:GLN:OE1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:H	1:A:59:LEU:HD22	1.66	0.60
1:F:286:TYR:N	1:F:287:PRO:HD2	2.17	0.60
1:A:266:VAL:HG22	1:A:271:TRP:HB2	1.83	0.60
1:B:98:ILE:HG21	1:B:286:TYR:CD1	2.37	0.60
1:D:148:THR:HG23	1:D:160:VAL:HG22	1.83	0.60
1:A:54:SER:O	1:A:57:SER:HB3	2.02	0.59
1:D:201:ARG:CG	1:D:201:ARG:NH1	2.60	0.59
1:B:294:ILE:O	1:B:298:VAL:HG23	2.02	0.59
1:C:30:VAL:HG22	1:C:45:ILE:CD1	2.32	0.59
1:D:94:LEU:O	1:D:94:LEU:HD13	2.01	0.59
1:E:17:ILE:CD1	1:E:198:GLN:HB3	2.31	0.59
1:C:434:ARG:NH2	1:E:340:ALA:O	2.35	0.59
1:E:59:LEU:HD13	1:E:69:LEU:HD22	1.84	0.59
1:D:29:LEU:HD13	1:D:109:GLU:HG2	1.85	0.59
1:G:328:ARG:HH12	1:G:344:ASP:HB2	1.67	0.59
1:A:486:ARG:O	1:A:490:MET:HG3	2.02	0.59
1:B:349:LEU:HD12	1:B:481:ILE:HG21	1.84	0.59
1:C:84:ASN:HD22	1:C:85:SER:N	1.95	0.59
1:C:315:LEU:O	1:C:319:THR:HG23	2.02	0.59
2:C:900:BLA:HMB3	2:C:900:BLA:CMA	2.32	0.59
1:G:358:MET:O	1:G:422:GLY:HA2	2.02	0.59
1:E:84:ASN:ND2	1:E:85:SER:H	2.01	0.59
1:C:417:HIS:HD2	1:C:420:GLU:H	1.51	0.58
1:F:113:ARG:HH22	1:F:119:SER:HA	1.68	0.58
1:G:440:LYS:HG3	1:G:440:LYS:O	2.04	0.58
2:A:900:BLA:HMB3	2:A:900:BLA:CMA	2.33	0.58
1:F:188:GLN:NE2	2:F:900:BLA:OB	2.37	0.58
1:F:266:VAL:HG22	1:F:271:TRP:HB2	1.84	0.58
1:D:409:CYS:SG	1:D:430:GLU:HG3	2.43	0.58
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.01	0.58
1:E:24:GLN:HE22	1:E:212:ALA:H	1.51	0.58
1:G:98:ILE:HG21	1:G:286:TYR:CE1	2.38	0.58
1:C:134:VAL:HG12	1:C:302:ILE:HG12	1.84	0.58
1:H:158:ASP:OD2	1:H:279:MET:HG2	2.03	0.58
1:G:322:ARG:HD2	1:G:488:ASP:OD2	2.03	0.58
1:B:139:ASP:HB3	1:B:142:SER:H	1.68	0.58
1:F:373:GLN:O	1:F:377:VAL:HG23	2.04	0.58
1:A:366:ILE:O	1:A:367:ARG:HB2	2.04	0.57
1:C:198:GLN:NE2	1:C:201:ARG:HE	2.01	0.57
1:F:264:ILE:HD11	1:F:274:PHE:CE1	2.39	0.57
1:F:346:ILE:O	1:F:426:TRP:HZ3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:NH2	1:G:340:ALA:O	2.37	0.57
1:B:140:THR:HA	1:B:306:LEU:HD23	1.84	0.57
1:B:8:THR:HG23	1:B:11:ASN:HB3	1.85	0.57
1:C:210:LEU:HD12	1:C:289:ARG:HD3	1.87	0.57
1:A:354:GLY:HA3	1:A:370:PHE:CE1	2.39	0.57
2:B:900:BLA:HMB3	2:B:900:BLA:CMA	2.34	0.57
1:G:134:VAL:HG13	1:G:302:ILE:HG21	1.85	0.57
1:A:148:THR:HG23	1:A:160:VAL:HG22	1.84	0.57
1:E:21:GLY:HA2	1:E:233:PHE:CZ	2.39	0.57
1:G:123:PHE:CD2	1:H:120:ILE:HD12	2.39	0.57
1:H:230:ASN:HD22	1:H:230:ASN:H	1.53	0.57
1:B:7:VAL:HG21	1:B:245:PRO:CG	2.33	0.57
1:B:112:ILE:HD13	1:B:112:ILE:H	1.67	0.57
1:H:444:LEU:CD2	1:H:444:LEU:H	2.05	0.57
1:F:152:ARG:HB2	1:F:160:VAL:CG1	2.35	0.57
1:G:264:ILE:HD11	1:G:274:PHE:CE1	2.39	0.57
1:G:72:LEU:O	1:G:76:LEU:HD13	2.05	0.57
1:B:137:HIS:NE2	1:B:146:ASN:ND2	2.52	0.57
1:C:366:ILE:O	1:C:367:ARG:HB2	2.05	0.57
1:G:139:ASP:HB2	1:G:142:SER:CB	2.35	0.57
1:D:187:GLY:HA3	1:D:435:ILE:HD11	1.87	0.57
1:E:239:VAL:HG11	1:E:289:ARG:NH2	2.19	0.57
1:E:45:ILE:HD12	1:E:46:GLN:N	2.19	0.57
1:H:45:ILE:HD12	1:H:46:GLN:H	1.69	0.57
1:A:130:ILE:HD11	1:A:150:GLU:HG2	1.87	0.56
1:B:102:TYR:CE2	1:B:103:LYS:HE2	2.41	0.56
1:F:113:ARG:HH21	1:F:287:PRO:HG3	1.70	0.56
1:H:114:THR:HG22	1:H:116:ASP:H	1.70	0.56
1:B:410:GLY:HA3	1:B:428:ARG:HB2	1.88	0.56
1:B:179:ARG:HD2	1:B:181:ASP:OD2	2.06	0.56
1:C:30:VAL:HG22	1:C:45:ILE:HD13	1.87	0.56
1:D:40:ALA:CB	1:D:223:PRO:HD2	2.34	0.56
1:F:308:GLN:HA	1:F:311:ILE:HD13	1.87	0.56
1:A:444:LEU:CD2	1:A:444:LEU:H	2.19	0.56
1:A:322:ARG:HD2	1:A:488:ASP:OD1	2.04	0.56
1:D:128:GLN:HB2	3:D:909:HOH:O	2.05	0.56
1:H:414:ILE:HD12	1:H:486:ARG:HB2	1.88	0.56
1:D:67:GLU:H	1:D:67:GLU:CD	2.08	0.56
1:E:319:THR:HG22	1:E:322:ARG:HH21	1.71	0.56
1:F:278:HIS:CD2	1:F:282:LYS:HD2	2.41	0.56
1:H:152:ARG:HB2	1:H:160:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:900:BLA:O2A	2:E:900:BLA:HMA2	2.06	0.56
1:B:122:SER:HB3	1:B:125:LEU:HB2	1.87	0.55
1:B:408:CYS:SG	1:B:428:ARG:O	2.64	0.55
1:E:258:ALA:HB2	1:E:282:LYS:H	1.71	0.55
1:C:194:ASP:OD2	1:C:453:ARG:NH2	2.38	0.55
1:D:40:ALA:HB2	1:D:223:PRO:HD2	1.88	0.55
1:F:340:ALA:HB2	1:F:364:LEU:HD21	1.89	0.55
1:F:384:ASP:OD2	1:F:387:ARG:HG3	2.06	0.55
1:A:319:THR:HG22	1:A:322:ARG:NH2	2.17	0.55
1:G:8:THR:H	1:G:11:ASN:HB2	1.71	0.55
1:E:297:GLN:NE2	1:F:128:GLN:HA	2.21	0.55
1:B:373:GLN:HE22	1:B:408:CYS:N	2.05	0.55
2:C:900:BLA:CBC	2:C:900:BLA:HMC1	2.34	0.55
1:D:84:ASN:HD22	1:D:85:SER:H	1.55	0.55
1:F:311:ILE:HG12	1:F:312:ALA:N	2.21	0.55
1:H:439:GLY:C	1:H:441:PRO:HD2	2.26	0.55
1:A:356:LEU:HD13	1:A:357:VAL:N	2.22	0.55
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.42	0.55
1:E:250:TYR:HD2	2:E:900:BLA:OC	1.90	0.55
1:F:9:LEU:HD21	1:F:450:SER:HB2	1.88	0.55
1:E:164:ARG:O	1:E:171:GLY:HA2	2.07	0.55
1:B:51:PHE:HB2	1:B:63:GLN:CD	2.27	0.54
1:D:394:ASN:O	1:D:395:TRP:CB	2.54	0.54
1:B:137:HIS:CE1	1:B:146:ASN:HD22	2.25	0.54
1:F:188:GLN:HE21	2:F:900:BLA:HBB1	1.73	0.54
1:B:21:GLY:O	1:B:221:VAL:HG22	2.07	0.54
1:F:356:LEU:HB3	1:F:425:PHE:HB2	1.90	0.54
1:A:435:ILE:HB	1:G:364:LEU:HD11	1.88	0.54
1:A:305:ARG:HD2	1:B:306:LEU:HD13	1.88	0.54
1:F:418:ARG:N	1:F:418:ARG:HD2	2.22	0.54
1:G:339:LEU:HD12	1:G:357:VAL:HG11	1.90	0.54
1:A:210:LEU:HD13	1:A:289:ARG:HD3	1.90	0.54
2:B:900:BLA:O2A	2:B:900:BLA:HMA2	2.07	0.54
1:B:16:PRO:O	1:B:20:PRO:HD3	2.08	0.54
1:B:340:ALA:HB2	1:B:364:LEU:HD21	1.89	0.54
1:C:185:TYR:O	1:C:188:GLN:HB2	2.08	0.54
1:F:346:ILE:HG13	1:F:347:ALA:N	2.23	0.54
1:F:247:HIS:CD2	2:F:900:BLA:HBD1	2.43	0.54
1:D:162:ALA:HB3	1:D:175:ALA:HB3	1.90	0.54
2:H:900:BLA:CMA	2:H:900:BLA:HMB3	2.38	0.54
1:F:44:ASN:HB3	1:F:219:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:THR:HG23	1:F:231:GLU:H	1.73	0.54
1:D:114:THR:HG22	1:D:115:ALA:H	1.72	0.54
1:C:54:SER:O	1:C:57:SER:HB3	2.08	0.53
1:D:305:ARG:HE	1:D:308:GLN:NE2	2.07	0.53
1:H:356:LEU:HB3	1:H:425:PHE:HB2	1.90	0.53
1:H:379:GLN:O	1:H:382:GLN:HB2	2.09	0.53
1:B:19:VAL:N	1:B:20:PRO:CD	2.71	0.53
1:D:208:ILE:H	1:D:208:ILE:HD13	1.73	0.53
1:D:32:LEU:N	1:D:32:LEU:HD12	2.23	0.53
1:C:435:ILE:HG23	1:E:364:LEU:HD21	1.89	0.53
1:H:209:ARG:HH12	2:H:900:BLA:CGD	2.21	0.53
1:D:486:ARG:O	1:D:490:MET:HG3	2.08	0.53
1:E:45:ILE:O	1:E:49:LEU:HB2	2.08	0.53
1:G:341:HIS:O	1:G:345:GLY:HA3	2.08	0.53
1:G:376:ASN:HB3	1:G:395:TRP:HH2	1.74	0.53
1:A:164:ARG:HD2	3:A:952:HOH:O	2.08	0.53
1:B:152:ARG:HD2	1:B:177:SER:OG	2.09	0.53
1:B:134:VAL:CG1	1:B:302:ILE:HG12	2.39	0.53
1:F:321:ARG:HD3	1:F:349:LEU:HD22	1.91	0.53
1:D:271:TRP:CE2	1:D:303:VAL:HG11	2.44	0.53
1:F:51:PHE:N	1:F:51:PHE:CD2	2.75	0.53
1:A:42:SER:O	1:A:45:ILE:HG13	2.09	0.53
1:A:434:ARG:HG2	1:A:435:ILE:HG23	1.90	0.53
1:D:450:SER:CB	1:D:454:LEU:HD22	2.39	0.53
1:E:391:HIS:HA	1:E:411:VAL:O	2.09	0.53
1:E:415:ARG:HD3	1:E:423:TRP:CZ2	2.43	0.53
1:C:33:ARG:HB3	1:C:39:LEU:HD11	1.90	0.52
1:D:126:ASN:O	1:D:130:ILE:HG23	2.09	0.52
1:G:273:LEU:C	1:G:273:LEU:HD12	2.30	0.52
1:G:67:GLU:H	1:G:67:GLU:CD	2.11	0.52
1:B:205:GLN:NE2	1:H:419:GLN:HG2	2.21	0.52
1:D:356:LEU:HB3	1:D:425:PHE:HB2	1.90	0.52
1:E:385:PRO:O	1:E:386:GLU:HB2	2.09	0.52
1:A:305:ARG:HA	1:A:308:GLN:HG2	1.91	0.52
1:B:356:LEU:HD21	1:B:363:THR:OG1	2.09	0.52
1:H:152:ARG:HD3	1:H:177:SER:O	2.09	0.52
1:A:165:PHE:CD1	1:A:272:GLY:HA2	2.44	0.52
1:B:328:ARG:HB3	1:B:338:ALA:HB2	1.92	0.52
1:B:38:VAL:O	1:B:55:PRO:HA	2.10	0.52
1:E:321:ARG:NH1	1:E:321:ARG:HG3	2.24	0.52
1:F:356:LEU:HD21	1:F:363:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:CYS:SG	1:F:427:PHE:HB3	2.49	0.52
1:G:305:ARG:HA	1:G:308:GLN:HG2	1.92	0.52
1:F:33:ARG:HB3	1:F:39:LEU:HD11	1.90	0.52
1:H:286:TYR:O	1:H:290:MET:HG2	2.09	0.52
1:F:273:LEU:C	1:F:273:LEU:HD12	2.29	0.52
1:G:328:ARG:O	1:G:332:ALA:HB3	2.10	0.52
1:A:258:ALA:HB3	1:A:278:HIS:HB3	1.92	0.52
1:B:87:GLU:OE2	1:B:113:ARG:HG2	2.10	0.52
1:G:67:GLU:HB2	1:G:86:VAL:HG11	1.92	0.52
1:B:98:ILE:HG21	1:B:286:TYR:CE1	2.45	0.51
1:B:134:VAL:HG13	1:B:302:ILE:HG12	1.92	0.51
1:E:46:GLN:HA	1:E:49:LEU:O	2.10	0.51
1:F:61:GLN:HG2	1:F:69:LEU:CD1	2.40	0.51
1:B:152:ARG:HB2	1:B:160:VAL:CG1	2.40	0.51
1:D:325:LEU:HD12	1:D:326:ALA:N	2.25	0.51
2:H:900:BLA:HMA2	2:H:900:BLA:O2A	2.10	0.51
1:C:347:ALA:CB	1:C:366:ILE:HD11	2.40	0.51
1:F:29:LEU:HD13	1:F:109:GLU:HG2	1.92	0.51
1:G:229:THR:HG23	1:G:231:GLU:H	1.75	0.51
1:H:209:ARG:HH11	1:H:209:ARG:HG2	1.76	0.51
1:D:113:ARG:HG3	1:D:114:THR:O	2.10	0.51
1:E:48:LEU:HD11	1:E:93:HIS:CD2	2.45	0.51
1:B:286:TYR:N	1:B:287:PRO:HD2	2.26	0.51
1:C:464:GLU:O	1:C:468:ARG:HG2	2.10	0.51
1:E:43:GLU:OE1	1:E:220:ARG:HG3	2.10	0.51
1:E:354:GLY:HA3	1:E:370:PHE:CE1	2.45	0.51
1:F:134:VAL:HG22	1:F:302:ILE:HG21	1.92	0.51
1:F:98:ILE:HG21	1:F:286:TYR:CE1	2.46	0.51
1:G:152:ARG:HB2	1:G:160:VAL:CG1	2.40	0.51
1:H:208:ILE:H	1:H:208:ILE:HD13	1.76	0.51
1:F:19:VAL:N	1:F:20:PRO:HD3	2.24	0.51
1:A:317:VAL:O	1:A:321:ARG:HB2	2.10	0.51
1:B:46:GLN:HB2	1:B:52:VAL:HG22	1.93	0.51
1:C:45:ILE:HG23	1:C:49:LEU:HD12	1.92	0.51
1:D:44:ASN:HB2	1:D:219:MET:HG2	1.92	0.51
1:F:209:ARG:NH1	2:F:900:BLA:O1D	2.43	0.51
1:H:258:ALA:HB2	1:H:282:LYS:H	1.76	0.51
1:A:414:ILE:HG13	1:A:414:ILE:O	2.09	0.51
1:F:366:ILE:O	1:F:367:ARG:HB2	2.11	0.51
1:C:24:GLN:HE22	1:C:211:ILE:HA	1.75	0.51
1:G:113:ARG:CZ	1:G:115:ALA:HB3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:LEU:HD13	1:H:241:ARG:NH1	2.26	0.51
1:H:31:THR:HG22	1:H:107:TYR:CD1	2.46	0.51
1:D:435:ILE:HB	1:H:364:LEU:CD1	2.40	0.51
1:E:42:SER:HA	1:E:221:VAL:HG12	1.93	0.51
1:E:68:VAL:HG23	3:E:908:HOH:O	2.10	0.51
1:H:325:LEU:O	1:H:325:LEU:HD13	2.11	0.51
1:A:364:LEU:HA	1:G:436:ARG:O	2.11	0.50
1:H:463:TRP:CZ2	1:H:467:VAL:HG11	2.47	0.50
1:C:313:GLU:O	1:C:317:VAL:HG13	2.11	0.50
1:F:250:TYR:O	1:F:254:MET:HG3	2.10	0.50
1:F:61:GLN:HG2	1:F:69:LEU:HD11	1.93	0.50
1:A:9:LEU:CD2	1:A:450:SER:HB3	2.42	0.50
1:B:32:LEU:HD12	1:B:32:LEU:N	2.26	0.50
1:H:445:LEU:HG	1:H:445:LEU:O	2.11	0.50
1:B:208:ILE:HD12	1:B:293:GLN:HB2	1.92	0.50
1:C:304:GLU:HG2	1:D:135:GLN:HE22	1.76	0.50
1:F:389:ILE:HD11	1:F:483:GLU:OE2	2.11	0.50
1:B:21:GLY:O	1:B:221:VAL:HG13	2.12	0.50
1:F:17:ILE:O	1:F:241:ARG:HD2	2.11	0.50
1:F:188:GLN:NE2	2:F:900:BLA:HBB1	2.25	0.50
1:B:273:LEU:C	1:B:273:LEU:HD12	2.31	0.50
1:E:305:ARG:HH22	1:F:138:ASN:HD22	1.58	0.50
1:G:319:THR:HG22	1:G:322:ARG:NH2	2.16	0.50
1:A:436:ARG:HH11	1:A:436:ARG:HG3	1.77	0.50
1:B:133:GLN:OE1	1:B:137:HIS:HE1	1.95	0.50
1:B:201:ARG:CG	1:B:201:ARG:HH11	2.25	0.50
1:C:124:THR:O	1:C:128:GLN:HG3	2.12	0.50
1:C:155:THR:OG1	1:C:157:TYR:HD1	1.95	0.50
1:E:305:ARG:HA	1:E:308:GLN:CG	2.40	0.50
1:B:314:LEU:O	1:B:317:VAL:HG22	2.11	0.50
1:D:325:LEU:HD12	1:D:325:LEU:C	2.32	0.50
1:F:284:ILE:HG22	1:F:289:ARG:HG2	1.93	0.50
1:B:201:ARG:HH21	1:B:236:SER:CB	2.24	0.50
1:E:321:ARG:HH11	1:E:321:ARG:HG3	1.76	0.50
1:E:490:MET:O	1:E:494:LEU:HD23	2.12	0.50
1:A:308:GLN:O	1:A:311:ILE:HD13	2.11	0.49
1:B:391:HIS:HA	1:B:411:VAL:O	2.12	0.49
1:D:155:THR:HB	1:D:157:TYR:HD1	1.76	0.49
1:D:414:ILE:HD12	1:D:486:ARG:HB2	1.92	0.49
1:F:308:GLN:HA	1:F:311:ILE:CD1	2.41	0.49
1:H:230:ASN:ND2	1:H:230:ASN:N	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:H	1:B:112:ILE:CD1	2.25	0.49
1:B:54:SER:O	1:B:57:SER:HB3	2.12	0.49
1:D:305:ARG:N	1:D:305:ARG:HD2	2.27	0.49
1:G:148:THR:HG23	1:G:160:VAL:HG22	1.94	0.49
1:H:440:LYS:N	1:H:441:PRO:CD	2.71	0.49
1:D:19:VAL:HG12	1:D:233:PHE:O	2.12	0.49
1:D:366:ILE:O	1:D:367:ARG:HB2	2.13	0.49
1:E:262:ILE:CG2	1:E:296:SER:HB2	2.41	0.49
1:E:330:ARG:HG2	1:E:492:LEU:HD11	1.94	0.49
1:F:164:ARG:HD2	1:F:174:VAL:HG11	1.94	0.49
1:F:239:VAL:HG11	1:F:289:ARG:NH2	2.26	0.49
1:H:172:GLU:HB2	1:H:189:ARG:HD3	1.94	0.49
1:A:32:LEU:HD11	1:A:59:LEU:HD21	1.94	0.49
1:G:340:ALA:HB2	1:G:364:LEU:HD21	1.95	0.49
1:B:112:ILE:HD13	1:B:112:ILE:N	2.27	0.49
1:B:88:THR:HG23	1:B:89:ARG:N	2.27	0.49
1:F:53:ALA:HB2	1:F:60:THR:HG21	1.93	0.49
1:G:247:HIS:NE2	1:G:251:LEU:HD11	2.27	0.49
1:H:222:PHE:HA	1:H:223:PRO:C	2.33	0.49
1:H:71:MET:O	1:H:74:GLU:HG3	2.12	0.49
1:E:140:THR:CG2	1:E:306:LEU:HB3	2.42	0.49
1:H:150:GLU:O	1:H:154:MET:HG3	2.13	0.49
1:C:418:ARG:HD2	1:G:205:GLN:HE22	1.78	0.49
1:D:152:ARG:HH21	1:D:179:ARG:CG	2.26	0.49
1:A:17:ILE:O	1:A:241:ARG:HD2	2.13	0.49
2:F:900:BLA:HMC1	2:F:900:BLA:CBC	2.42	0.49
1:G:118:LEU:H	1:G:118:LEU:HD23	1.78	0.49
1:B:24:GLN:HE22	1:B:211:ILE:HA	1.77	0.49
1:D:373:GLN:O	1:D:377:VAL:HG23	2.13	0.49
1:E:114:THR:HG22	1:E:115:ALA:N	2.27	0.49
1:D:33:ARG:HB3	1:D:39:LEU:CG	2.43	0.48
1:D:435:ILE:HA	1:H:365:SER:O	2.13	0.48
2:D:900:BLA:HBB1	2:D:900:BLA:OB	2.12	0.48
1:F:149:ASP:OD1	1:F:177:SER:HB3	2.13	0.48
1:H:394:ASN:O	1:H:395:TRP:HB2	2.13	0.48
2:C:900:BLA:HBC1	2:C:900:BLA:CMC	2.38	0.48
2:G:900:BLA:CMA	2:G:900:BLA:HMB3	2.43	0.48
1:A:187:GLY:O	1:A:433:HIS:HE1	1.95	0.48
1:H:33:ARG:HB3	1:H:39:LEU:HD21	1.95	0.48
1:C:139:ASP:HB3	1:C:142:SER:OG	2.14	0.48
1:F:391:HIS:O	1:F:392:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:SER:HA	1:H:221:VAL:HA	1.95	0.48
1:C:286:TYR:N	1:C:287:PRO:HD2	2.28	0.48
1:G:45:ILE:HD12	1:G:46:GLN:N	2.29	0.48
1:H:147:VAL:HG21	1:H:274:PHE:CZ	2.48	0.48
1:B:328:ARG:HH12	1:B:344:ASP:HB2	1.78	0.48
1:F:185:TYR:O	1:F:188:GLN:HB2	2.14	0.48
1:G:59:LEU:H	1:G:59:LEU:HD22	1.78	0.48
1:E:195:ILE:HG22	1:E:200:ARG:HB2	1.94	0.48
1:D:116:ASP:N	1:D:116:ASP:OD2	2.43	0.48
1:E:59:LEU:CD1	1:E:69:LEU:HD22	2.43	0.48
1:B:209:ARG:HH11	1:B:209:ARG:HG2	1.79	0.48
1:C:365:SER:HB3	1:C:368:GLY:O	2.13	0.48
1:D:98:ILE:HD12	1:D:239:VAL:HG21	1.95	0.48
1:F:116:ASP:N	1:F:117:THR:HB	2.29	0.48
1:H:35:ASP:OD1	1:H:37:MET:HE3	2.13	0.48
1:A:286:TYR:N	1:A:287:PRO:HD2	2.29	0.48
1:A:414:ILE:HD12	1:A:486:ARG:HB2	1.95	0.48
1:D:18:HIS:ND1	1:D:198:GLN:HG2	2.29	0.48
1:H:341:HIS:CG	1:H:342:PRO:HD2	2.48	0.48
1:D:247:HIS:CD2	2:D:900:BLA:HBD1	2.49	0.47
1:F:325:LEU:C	1:F:325:LEU:HD12	2.34	0.47
2:F:900:BLA:HBC1	2:F:900:BLA:HMC1	1.95	0.47
1:G:134:VAL:CG1	1:G:302:ILE:HG12	2.44	0.47
1:G:128:GLN:CA	1:H:297:GLN:HE22	2.25	0.47
1:C:284:ILE:HG22	1:C:289:ARG:HG2	1.96	0.47
1:C:323:LEU:HA	1:D:323:LEU:HD13	1.96	0.47
1:D:155:THR:HB	1:D:157:TYR:CD1	2.49	0.47
1:G:388:ASP:HB3	1:G:486:ARG:HE	1.78	0.47
1:A:42:SER:HA	1:A:221:VAL:HA	1.96	0.47
1:E:258:ALA:HB3	1:E:278:HIS:HB3	1.96	0.47
1:F:134:VAL:HG23	1:F:143:LEU:HD11	1.96	0.47
1:F:283:LEU:C	1:F:284:ILE:HD12	2.34	0.47
1:G:286:TYR:N	1:G:287:PRO:HD2	2.29	0.47
1:D:84:ASN:ND2	1:D:85:SER:H	2.12	0.47
1:E:48:LEU:HD23	1:E:112:ILE:HD12	1.95	0.47
1:F:358:MET:SD	1:F:378:LEU:HD11	2.54	0.47
1:H:238:SER:HB3	1:H:241:ARG:HB3	1.96	0.47
1:A:140:THR:CG2	1:A:306:LEU:HB3	2.36	0.47
1:D:143:LEU:O	1:D:147:VAL:HG12	2.14	0.47
2:F:900:BLA:HMB3	2:F:900:BLA:CMA	2.45	0.47
1:H:364:LEU:HD12	1:H:364:LEU:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:HD11	1:B:292:PHE:C	2.35	0.47
1:C:140:THR:HG21	1:C:307:GLU:OE2	2.14	0.47
1:E:266:VAL:HG22	1:E:271:TRP:HB2	1.97	0.47
1:F:410:GLY:O	1:F:427:PHE:HA	2.15	0.47
1:G:158:ASP:H	1:G:278:HIS:CD2	2.33	0.47
1:H:94:LEU:HD13	1:H:94:LEU:O	2.15	0.47
1:E:286:TYR:HB3	1:E:287:PRO:HD3	1.96	0.47
1:F:19:VAL:HG12	1:F:234:ASP:HA	1.97	0.47
1:G:150:GLU:OE1	1:G:150:GLU:HA	2.14	0.47
1:B:299:CYS:O	1:B:303:VAL:HG23	2.14	0.47
1:E:139:ASP:OD1	1:E:142:SER:HB2	2.14	0.47
2:G:900:BLA:HBB1	2:G:900:BLA:OB	2.15	0.47
1:A:70:ARG:O	1:A:74:GLU:HG2	2.15	0.47
1:B:95:PHE:CE2	1:B:112:ILE:HG22	2.50	0.47
1:B:130:ILE:O	1:B:133:GLN:HB2	2.14	0.47
1:E:44:ASN:HB3	1:E:219:MET:SD	2.55	0.47
1:H:188:GLN:HE21	1:H:188:GLN:HB3	1.59	0.47
1:B:188:GLN:HG2	2:B:900:BLA:HBB1	1.97	0.47
1:C:134:VAL:HG12	1:C:134:VAL:O	2.15	0.47
2:D:900:BLA:HMB3	2:D:900:BLA:CMA	2.45	0.47
1:D:45:ILE:CD1	1:D:46:GLN:H	2.27	0.46
1:E:84:ASN:HD22	1:E:85:SER:N	2.08	0.46
1:A:143:LEU:HD23	1:A:303:VAL:HG23	1.97	0.46
1:D:339:LEU:HD13	1:D:357:VAL:HG21	1.96	0.46
1:E:42:SER:CA	1:E:221:VAL:HG12	2.44	0.46
1:F:418:ARG:HD2	1:F:418:ARG:H	1.79	0.46
1:A:30:VAL:HG12	1:A:32:LEU:CD1	2.45	0.46
1:B:168:ASP:O	1:B:169:ASP:HB2	2.14	0.46
1:B:147:VAL:HG21	1:B:274:PHE:CZ	2.50	0.46
1:C:60:THR:H	1:C:63:GLN:HE21	1.63	0.46
1:G:288:VAL:O	1:G:291:SER:HB3	2.15	0.46
1:H:314:LEU:O	1:H:318:SER:HB2	2.15	0.46
1:A:417:HIS:CD2	1:A:420:GLU:H	2.33	0.46
1:C:94:LEU:HD13	1:C:94:LEU:N	2.31	0.46
1:F:363:THR:HG21	1:F:371:GLU:CD	2.36	0.46
1:F:394:ASN:HD21	1:F:470:HIS:CE1	2.33	0.46
1:G:356:LEU:HD13	1:G:357:VAL:N	2.31	0.46
1:C:391:HIS:HA	1:C:411:VAL:O	2.15	0.46
1:E:250:TYR:CD2	2:E:900:BLA:OC	2.68	0.46
1:B:19:VAL:H	1:B:20:PRO:CD	2.29	0.46
1:B:209:ARG:NH1	2:B:900:BLA:O1D	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ARG:HB2	1:E:380:ARG:NH1	2.31	0.46
1:F:42:SER:HA	1:F:221:VAL:HA	1.98	0.46
1:H:165:PHE:CE1	1:H:272:GLY:HA2	2.51	0.46
1:A:159:ARG:HD3	1:A:161:MET:SD	2.56	0.46
1:A:278:HIS:CD2	1:A:282:LYS:HB2	2.51	0.46
1:C:152:ARG:HB2	1:C:160:VAL:CG1	2.46	0.46
2:C:900:BLA:HBB1	2:C:900:BLA:OB	2.16	0.46
1:C:17:ILE:CD1	2:C:900:BLA:HMD1	2.45	0.46
1:D:209:ARG:O	1:D:260:MET:HA	2.16	0.46
1:E:258:ALA:HB2	1:E:282:LYS:N	2.31	0.46
1:F:115:ALA:C	1:F:117:THR:HB	2.36	0.46
1:F:261:SER:HA	1:F:274:PHE:O	2.16	0.46
2:G:900:BLA:HMA2	2:G:900:BLA:HBA2	1.97	0.46
1:A:33:ARG:HB3	1:A:39:LEU:HG	1.98	0.46
2:B:900:BLA:HMB3	2:B:900:BLA:HMA1	1.98	0.46
1:D:152:ARG:HH21	1:D:179:ARG:HG3	1.81	0.46
1:F:190:TYR:HB2	1:F:191:PRO:HD2	1.97	0.46
1:G:302:ILE:HA	1:G:305:ARG:HG2	1.98	0.46
1:H:134:VAL:CG2	1:H:143:LEU:HD13	2.46	0.46
1:H:186:LEU:HB2	1:H:437:TRP:HZ3	1.81	0.46
1:B:71:MET:O	1:B:74:GLU:HG2	2.15	0.45
1:C:165:PHE:HD1	1:C:272:GLY:HA2	1.80	0.45
1:G:496:HIS:ND1	1:G:496:HIS:C	2.69	0.45
1:A:290:MET:CE	1:B:128:GLN:HE22	2.30	0.45
1:B:31:THR:HG22	1:B:107:TYR:HD1	1.81	0.45
1:B:373:GLN:NE2	1:B:407:ASP:HA	2.31	0.45
1:H:239:VAL:CG1	1:H:289:ARG:HH22	2.29	0.45
1:C:264:ILE:HD11	1:C:274:PHE:CE1	2.52	0.45
1:D:389:ILE:HG23	1:D:414:ILE:HG22	1.98	0.45
1:D:33:ARG:HB3	1:D:39:LEU:HG	1.98	0.45
1:D:42:SER:O	1:D:45:ILE:HG13	2.17	0.45
1:E:221:VAL:HG23	1:E:233:PHE:CZ	2.51	0.45
1:E:315:LEU:O	1:E:319:THR:HG23	2.17	0.45
1:F:51:PHE:HD2	1:F:51:PHE:N	2.14	0.45
1:G:417:HIS:CD2	1:G:420:GLU:H	2.34	0.45
1:G:48:LEU:HD11	1:G:112:ILE:HD11	1.97	0.45
1:H:445:LEU:CD1	1:H:447:ILE:HG23	2.45	0.45
1:A:354:GLY:HA3	1:A:370:PHE:CZ	2.52	0.45
1:B:266:VAL:HG23	1:B:266:VAL:O	2.16	0.45
1:C:284:ILE:HG22	1:C:289:ARG:CG	2.46	0.45
1:D:161:MET:O	1:D:274:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:PHE:CD1	1:D:272:GLY:HA2	2.51	0.45
1:G:24:GLN:HE22	1:G:211:ILE:HA	1.81	0.45
1:H:148:THR:HG23	1:H:160:VAL:HG13	1.98	0.45
1:C:264:ILE:HB	1:C:272:GLY:O	2.16	0.45
1:D:98:ILE:HG21	1:D:286:TYR:CD1	2.51	0.45
1:F:21:GLY:O	1:F:221:VAL:HG22	2.16	0.45
1:G:138:ASN:HA	1:H:305:ARG:HH22	1.82	0.45
1:G:414:ILE:HD12	1:G:486:ARG:HB2	1.98	0.45
1:H:416:PHE:O	1:H:490:MET:HG2	2.16	0.45
2:H:900:BLA:HBB1	2:H:900:BLA:OB	2.17	0.45
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.52	0.45
1:C:283:LEU:C	1:C:284:ILE:HD12	2.36	0.45
1:C:415:ARG:HD3	1:C:423:TRP:CZ2	2.51	0.45
2:D:900:BLA:HMA2	2:D:900:BLA:O2A	2.16	0.45
1:E:59:LEU:HD22	1:E:72:LEU:CD2	2.47	0.45
1:F:159:ARG:HD2	3:F:509:HOH:O	2.16	0.45
1:F:284:ILE:HG22	1:F:289:ARG:CG	2.47	0.45
1:G:203:TYR:OH	2:G:900:BLA:HAA1	2.16	0.45
1:A:363:THR:HG22	3:A:954:HOH:O	2.17	0.45
1:B:257:ARG:HG3	1:B:279:MET:O	2.17	0.45
1:C:440:LYS:HA	1:C:440:LYS:HD3	1.80	0.45
1:D:133:GLN:HG3	1:D:146:ASN:HD21	1.81	0.45
1:D:302:ILE:HG22	1:D:306:LEU:HD22	1.98	0.45
1:E:264:ILE:HD11	1:E:274:PHE:CZ	2.52	0.45
2:E:900:BLA:HBB1	2:E:900:BLA:OB	2.17	0.45
1:E:85:SER:HB2	1:E:98:ILE:HG22	1.98	0.45
1:B:18:HIS:CD2	1:B:19:VAL:HG13	2.51	0.45
1:B:71:MET:SD	1:B:86:VAL:HG23	2.56	0.45
1:D:217:THR:HG23	1:D:217:THR:O	2.17	0.45
1:E:59:LEU:HD22	1:E:72:LEU:HD23	1.98	0.45
1:F:339:LEU:HD22	1:F:346:ILE:HG23	1.99	0.45
1:G:187:GLY:O	1:G:433:HIS:HE1	2.00	0.45
1:G:94:LEU:HD22	1:G:113:ARG:HB3	1.99	0.45
1:H:443:LYS:O	1:H:444:LEU:O	2.33	0.45
1:A:378:LEU:O	1:A:382:GLN:HG2	2.16	0.45
1:A:440:LYS:H	1:A:440:LYS:HG3	1.56	0.45
1:D:308:GLN:O	1:D:311:ILE:HD13	2.16	0.45
1:D:467:VAL:O	1:D:470:HIS:HB2	2.17	0.45
1:C:435:ILE:CD1	1:E:340:ALA:HB1	2.46	0.45
1:E:45:ILE:HD12	1:E:46:GLN:H	1.81	0.45
1:G:308:GLN:O	1:G:311:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:417:HIS:O	1:G:421:SER:HA	2.17	0.45
1:H:305:ARG:HE	1:H:308:GLN:NE2	2.14	0.45
1:A:24:GLN:HE22	1:A:212:ALA:H	1.63	0.45
1:A:220:ARG:HE	1:A:222:PHE:HZ	1.64	0.45
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.81	0.45
1:C:273:LEU:HD12	1:C:273:LEU:C	2.37	0.45
1:D:342:PRO:O	1:D:343:ASP:HB2	2.16	0.45
1:E:321:ARG:NH1	1:E:321:ARG:CG	2.72	0.45
1:E:442:GLU:OE2	1:E:457:ARG:HD2	2.17	0.45
1:G:226:ASN:HB2	1:G:233:PHE:CE1	2.52	0.45
1:G:417:HIS:HD2	1:G:420:GLU:H	1.65	0.45
1:H:7:VAL:HG21	1:H:245:PRO:HG2	1.99	0.45
1:F:494:LEU:O	1:F:498:LEU:HD12	2.16	0.44
1:H:326:ALA:HB1	1:H:330:ARG:HH12	1.82	0.44
1:A:17:ILE:HB	3:A:939:HOH:O	2.16	0.44
1:A:190:TYR:HB2	1:A:191:PRO:HD2	1.99	0.44
2:A:900:BLA:HMB3	2:A:900:BLA:HMA2	1.99	0.44
1:C:356:LEU:HB3	1:C:425:PHE:HB2	1.99	0.44
1:C:372:ARG:HH12	1:C:406:GLY:HA2	1.81	0.44
1:D:264:ILE:HD11	1:D:274:PHE:CZ	2.52	0.44
1:C:495:ASN:HD21	1:D:331:ASP:CG	2.21	0.44
1:D:33:ARG:HB3	1:D:39:LEU:HD11	1.98	0.44
1:E:294:ILE:O	1:E:298:VAL:HG23	2.17	0.44
1:F:118:LEU:HB2	1:F:122:SER:HB2	1.99	0.44
1:G:76:LEU:HD12	1:G:106:PHE:CE2	2.53	0.44
1:A:394:ASN:O	1:A:395:TRP:HB2	2.17	0.44
1:C:372:ARG:NH1	1:C:406:GLY:HA2	2.33	0.44
1:H:435:ILE:O	1:H:435:ILE:HG13	2.17	0.44
1:C:102:TYR:O	1:C:103:LYS:HB2	2.18	0.44
1:C:209:ARG:NH1	2:C:900:BLA:CGD	2.81	0.44
1:E:305:ARG:HB3	1:E:305:ARG:HE	1.54	0.44
1:E:305:ARG:HE	1:E:308:GLN:NE2	2.14	0.44
1:A:5:THR:HB	1:A:6:PRO:HD2	1.99	0.44
1:B:326:ALA:HB1	1:B:330:ARG:NH1	2.32	0.44
1:C:159:ARG:NH1	1:C:183:GLU:O	2.49	0.44
1:D:164:ARG:HG3	1:D:174:VAL:HG11	1.99	0.44
1:D:222:PHE:HA	1:D:223:PRO:C	2.38	0.44
1:D:391:HIS:HA	1:D:411:VAL:O	2.17	0.44
1:A:435:ILE:HG22	1:G:366:ILE:HB	1.98	0.44
1:A:84:ASN:HB2	1:A:99:GLY:O	2.18	0.44
1:C:347:ALA:HB2	1:C:366:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:PHE:HA	1:E:171:GLY:HA2	2.00	0.44
1:E:356:LEU:HB3	1:E:425:PHE:HB2	1.99	0.44
1:G:82:TRP:H	1:G:101:SER:HB3	1.83	0.44
1:G:131:ILE:HD11	1:H:297:GLN:CB	2.47	0.44
1:G:201:ARG:NH2	1:G:236:SER:OG	2.51	0.44
1:G:165:PHE:CD1	1:G:272:GLY:HA2	2.53	0.44
1:B:237:TYR:HB2	3:B:513:HOH:O	2.18	0.44
1:B:59:LEU:N	1:B:59:LEU:HD22	2.33	0.44
1:C:417:HIS:CD2	1:C:420:GLU:H	2.32	0.44
1:E:82:TRP:O	1:E:100:HIS:HA	2.18	0.44
1:G:356:LEU:HD22	1:G:365:SER:HB2	1.99	0.44
1:G:358:MET:HG3	1:G:363:THR:HG22	2.00	0.44
1:C:30:VAL:HG22	1:C:45:ILE:HD11	2.00	0.44
2:G:900:BLA:CMA	2:G:900:BLA:HBA2	2.48	0.44
1:H:112:ILE:N	1:H:112:ILE:HD13	2.29	0.44
1:H:172:GLU:HG3	1:H:189:ARG:HD3	2.00	0.44
1:H:131:ILE:HG21	1:H:298:VAL:HG21	2.00	0.44
1:H:326:ALA:HB1	1:H:330:ARG:NH1	2.33	0.44
1:D:162:ALA:O	1:D:174:VAL:HG22	2.17	0.43
1:F:366:ILE:HG22	1:F:367:ARG:HG3	1.99	0.43
2:F:900:BLA:OB	2:F:900:BLA:HBB1	2.17	0.43
1:A:214:VAL:HB	1:A:257:ARG:HA	2.00	0.43
1:E:169:ASP:HB3	1:E:200:ARG:CZ	2.48	0.43
1:E:262:ILE:HG22	1:E:296:SER:HB2	2.00	0.43
1:E:311:ILE:HG23	1:E:477:THR:CG2	2.48	0.43
1:F:278:HIS:HD2	1:F:282:LYS:HB2	1.82	0.43
1:F:425:PHE:HB3	1:F:427:PHE:CE1	2.53	0.43
1:G:393:ASP:C	1:G:394:ASN:HD22	2.21	0.43
1:A:328:ARG:NH1	1:A:341:HIS:CD2	2.86	0.43
1:D:130:ILE:HG13	1:D:131:ILE:N	2.34	0.43
1:D:238:SER:HB3	1:D:241:ARG:HB2	1.99	0.43
1:E:208:ILE:HD13	1:E:208:ILE:H	1.82	0.43
1:F:67:GLU:CD	1:F:67:GLU:H	2.22	0.43
1:G:384:ASP:CG	1:G:387:ARG:HG3	2.39	0.43
1:H:262:ILE:HG22	1:H:296:SER:HB3	2.00	0.43
1:H:341:HIS:ND1	1:H:342:PRO:HD2	2.34	0.43
1:A:356:LEU:HD13	1:A:356:LEU:C	2.38	0.43
1:A:377:VAL:HG22	1:A:395:TRP:CH2	2.54	0.43
1:B:201:ARG:CG	1:B:201:ARG:NH1	2.81	0.43
1:B:31:THR:HG22	1:B:107:TYR:CD1	2.54	0.43
1:B:8:THR:CG2	1:B:11:ASN:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASN:CG	1:C:219:MET:HG2	2.39	0.43
1:D:284:ILE:HB	1:D:289:ARG:HG3	2.00	0.43
1:E:49:LEU:HB3	1:E:51:PHE:CE2	2.53	0.43
1:F:284:ILE:CG2	1:F:289:ARG:HG2	2.48	0.43
1:H:264:ILE:HD11	1:H:274:PHE:CZ	2.53	0.43
1:B:323:LEU:C	1:B:323:LEU:HD23	2.39	0.43
1:C:84:ASN:ND2	1:C:85:SER:N	2.62	0.43
1:H:356:LEU:HD13	1:H:356:LEU:C	2.38	0.43
1:C:467:VAL:O	1:C:470:HIS:HB2	2.17	0.43
1:C:17:ILE:HD12	2:C:900:BLA:HMD1	1.99	0.43
1:E:217:THR:O	1:E:217:THR:HG23	2.18	0.43
1:G:40:ALA:HB2	1:G:223:PRO:HD2	2.01	0.43
2:B:900:BLA:OB	2:B:900:BLA:HBB1	2.18	0.43
1:C:17:ILE:HD12	2:C:900:BLA:CMD	2.48	0.43
1:D:387:ARG:HB3	3:D:913:HOH:O	2.17	0.43
1:D:437:TRP:HA	1:D:437:TRP:CE3	2.54	0.43
1:E:341:HIS:O	1:E:345:GLY:HA3	2.19	0.43
1:F:447:ILE:H	1:F:447:ILE:CD1	2.29	0.43
1:F:45:ILE:H	1:F:45:ILE:HG13	1.60	0.43
1:G:356:LEU:HB3	1:G:425:PHE:HB2	2.00	0.43
1:H:430:GLU:HA	1:H:471:SER:HA	2.00	0.43
1:A:72:LEU:HD13	1:A:76:LEU:HD13	2.01	0.43
1:B:206:ASN:HA	1:B:207:PRO:HD2	1.87	0.43
1:B:229:THR:HG23	1:B:231:GLU:H	1.82	0.43
1:B:188:GLN:HG2	2:B:900:BLA:CBB	2.49	0.43
1:C:209:ARG:NH1	2:C:900:BLA:O1D	2.45	0.43
1:D:191:PRO:HD3	1:D:463:TRP:HB2	2.00	0.43
1:E:17:ILE:HD12	1:E:198:GLN:HB3	2.01	0.43
1:F:305:ARG:CG	1:F:305:ARG:HH11	2.28	0.43
1:H:165:PHE:CD1	1:H:272:GLY:HA2	2.53	0.43
1:B:261:SER:HA	1:B:274:PHE:O	2.19	0.43
1:D:467:VAL:HG23	1:D:468:ARG:N	2.34	0.43
1:H:102:TYR:CZ	1:H:103:LYS:HE3	2.54	0.43
1:H:260:MET:HE2	1:H:284:ILE:HD13	2.01	0.43
1:A:157:TYR:CD2	1:A:278:HIS:HB2	2.53	0.43
1:A:358:MET:O	1:A:422:GLY:HA2	2.19	0.43
1:A:247:HIS:CD2	2:A:900:BLA:HBD1	2.53	0.43
1:B:341:HIS:O	1:B:345:GLY:HA3	2.19	0.43
1:B:373:GLN:HE22	1:B:408:CYS:H	1.66	0.43
1:B:51:PHE:CD2	1:B:51:PHE:N	2.87	0.43
1:E:384:ASP:N	1:E:385:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:ILE:HD11	1:E:483:GLU:OE2	2.19	0.43
1:E:48:LEU:HD12	1:E:48:LEU:HA	1.76	0.43
1:H:184:SER:HB3	1:H:437:TRP:CH2	2.54	0.43
1:C:192:ALA:HA	3:C:938:HOH:O	2.17	0.42
1:D:273:LEU:HD12	1:D:273:LEU:C	2.39	0.42
1:D:9:LEU:HD22	1:D:9:LEU:H	1.83	0.42
1:E:135:GLN:OE1	1:F:305:ARG:NH1	2.51	0.42
1:F:117:THR:HG23	1:F:117:THR:O	2.19	0.42
1:G:84:ASN:ND2	1:G:85:SER:H	1.87	0.42
1:H:152:ARG:HB2	1:H:160:VAL:CG1	2.48	0.42
3:D:906:HOH:O	1:H:436:ARG:HG3	2.19	0.42
1:H:78:GLY:HA2	1:H:79:ASN:HA	1.69	0.42
1:A:391:HIS:HA	1:A:411:VAL:O	2.19	0.42
1:B:356:LEU:HD13	1:B:357:VAL:N	2.34	0.42
1:G:306:LEU:HD11	1:H:305:ARG:NH2	2.34	0.42
1:H:247:HIS:CD2	2:H:900:BLA:HBD1	2.54	0.42
1:A:206:ASN:HA	1:A:207:PRO:HD2	1.80	0.42
1:A:389:ILE:HD13	1:A:483:GLU:HG2	2.01	0.42
1:B:13:GLU:H	1:B:13:GLU:HG3	1.70	0.42
1:C:295:PHE:HA	1:C:298:VAL:HG12	2.01	0.42
1:C:389:ILE:HD11	1:C:483:GLU:HG2	2.01	0.42
1:G:130:ILE:HG23	1:G:295:PHE:CD1	2.54	0.42
1:G:17:ILE:O	1:G:241:ARG:HD2	2.18	0.42
1:G:66:PRO:HG2	1:G:67:GLU:OE1	2.19	0.42
1:A:29:LEU:HD13	1:A:109:GLU:HG2	2.02	0.42
1:C:305:ARG:HD2	1:C:305:ARG:HA	1.92	0.42
1:D:261:SER:HA	1:D:274:PHE:O	2.19	0.42
1:D:393:ASP:N	1:D:393:ASP:OD2	2.53	0.42
1:D:39:LEU:HD13	1:D:226:ASN:OD1	2.19	0.42
1:D:468:ARG:HG3	1:D:469:GLY:H	1.85	0.42
1:D:98:ILE:HG13	1:D:98:ILE:O	2.19	0.42
1:E:16:PRO:HB2	1:E:19:VAL:HG22	2.01	0.42
1:F:19:VAL:HG12	1:F:233:PHE:O	2.20	0.42
1:A:30:VAL:HG12	1:A:32:LEU:HD13	2.02	0.42
1:C:339:LEU:HD12	1:C:357:VAL:HG11	2.01	0.42
1:D:60:THR:OG1	1:D:63:GLN:HG3	2.19	0.42
1:E:108:LEU:HB3	1:E:110:PHE:CE1	2.55	0.42
1:H:299:CYS:O	1:H:303:VAL:HB	2.19	0.42
1:B:318:SER:O	1:B:322:ARG:HB2	2.19	0.42
1:C:247:HIS:CD2	2:C:900:BLA:HBD1	2.54	0.42
1:D:165:PHE:CE1	1:D:272:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:TYR:O	1:E:103:LYS:HB2	2.19	0.42
1:G:99:GLY:HA2	1:G:107:TYR:O	2.20	0.42
1:H:24:GLN:HA	1:H:25:PRO:HD3	1.89	0.42
1:A:133:GLN:OE1	1:A:146:ASN:HB3	2.19	0.42
1:A:210:LEU:HD12	1:A:260:MET:HG2	2.01	0.42
1:D:358:MET:CE	1:D:378:LEU:HD11	2.50	0.42
1:E:381:LEU:C	1:E:381:LEU:HD13	2.40	0.42
1:F:384:ASP:CG	1:F:387:ARG:HG3	2.40	0.42
1:F:412:LEU:HB3	1:F:426:TRP:CD1	2.55	0.42
1:G:384:ASP:OD2	1:G:387:ARG:HG3	2.19	0.42
1:H:243:VAL:HG12	1:H:244:SER:N	2.35	0.42
1:B:247:HIS:CD2	2:B:900:BLA:HBD1	2.55	0.42
1:E:284:ILE:HD12	1:E:284:ILE:N	2.35	0.42
1:E:436:ARG:HG3	3:E:914:HOH:O	2.18	0.42
1:G:394:ASN:ND2	1:G:470:HIS:CD2	2.75	0.42
1:C:201:ARG:O	1:C:205:GLN:HG2	2.20	0.42
1:D:155:THR:O	1:D:282:LYS:HE2	2.20	0.42
1:C:131:ILE:HD11	1:D:297:GLN:HB2	2.02	0.42
1:D:363:THR:HB	1:H:438:GLY:O	2.20	0.42
1:E:42:SER:C	1:E:44:ASN:H	2.23	0.42
1:F:162:ALA:HB3	1:F:175:ALA:HB3	2.01	0.42
1:F:44:ASN:OD1	1:F:219:MET:HG2	2.19	0.42
1:F:85:SER:HB3	1:F:98:ILE:HG22	2.02	0.42
1:G:440:LYS:O	1:G:442:GLU:N	2.53	0.42
1:B:152:ARG:HB2	1:B:160:VAL:HG11	2.01	0.42
1:B:45:ILE:HG13	1:B:45:ILE:H	1.63	0.42
1:C:152:ARG:HB2	1:C:160:VAL:HG13	2.02	0.42
1:C:30:VAL:HG12	1:C:32:LEU:CD1	2.50	0.42
1:H:278:HIS:HD2	1:H:280:SER:O	2.03	0.42
1:A:147:VAL:HG13	1:A:274:PHE:HE2	1.85	0.41
1:A:356:LEU:HB3	1:A:425:PHE:HB2	2.01	0.41
1:A:36:GLY:HA2	1:A:76:LEU:HD21	2.01	0.41
1:D:358:MET:O	1:D:422:GLY:HA2	2.20	0.41
1:D:42:SER:HA	1:D:221:VAL:HA	2.02	0.41
1:F:413:ALA:HB2	1:F:425:PHE:CE2	2.55	0.41
1:A:318:SER:O	1:A:322:ARG:HG3	2.20	0.41
1:D:304:GLU:O	1:D:308:GLN:HG2	2.20	0.41
1:F:40:ALA:HB2	1:F:223:PRO:HD2	2.01	0.41
1:G:409:CYS:HB2	1:G:471:SER:HB3	2.01	0.41
1:H:258:ALA:HB2	1:H:282:LYS:N	2.35	0.41
1:B:408:CYS:SG	1:B:428:ARG:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:HH21	1:G:268:GLY:HA2	1.85	0.41
1:D:214:VAL:HG11	1:D:252:THR:HG23	2.01	0.41
1:D:17:ILE:O	1:D:241:ARG:HD2	2.20	0.41
1:D:358:MET:HE2	1:D:358:MET:HB3	1.75	0.41
1:E:19:VAL:HG12	1:E:234:ASP:HA	2.02	0.41
1:F:358:MET:CE	1:F:378:LEU:HD11	2.51	0.41
1:F:89:ARG:HA	1:F:94:LEU:HA	2.01	0.41
1:G:211:ILE:HB	1:G:259:SER:HB3	2.03	0.41
1:A:444:LEU:C	1:A:445:LEU:O	2.58	0.41
1:C:341:HIS:O	1:C:345:GLY:HA3	2.19	0.41
2:C:900:BLA:HMA2	2:C:900:BLA:HMB3	2.02	0.41
1:D:284:ILE:HD12	1:D:284:ILE:N	2.35	0.41
1:F:152:ARG:HH21	1:F:179:ARG:HB3	1.85	0.41
1:G:443:LYS:HD2	1:G:443:LYS:H	1.85	0.41
1:H:186:LEU:HB2	1:H:437:TRP:CZ3	2.55	0.41
1:H:68:VAL:CG2	1:H:88:THR:HG21	2.50	0.41
1:A:139:ASP:HB2	1:A:142:SER:OG	2.21	0.41
1:D:440:LYS:O	1:D:442:GLU:N	2.54	0.41
1:G:102:TYR:O	1:G:103:LYS:HB2	2.20	0.41
1:G:394:ASN:HD22	1:G:394:ASN:N	2.19	0.41
1:A:491:GLU:HA	1:A:494:LEU:HD12	2.02	0.41
1:B:64:VAL:O	1:B:64:VAL:HG12	2.21	0.41
1:C:446:THR:HG23	1:C:446:THR:O	2.20	0.41
1:E:112:ILE:N	1:E:112:ILE:HD13	2.35	0.41
1:E:341:HIS:HA	1:E:342:PRO:HD3	1.84	0.41
1:G:239:VAL:HG11	1:G:289:ARG:NH2	2.35	0.41
1:B:139:ASP:CB	1:B:142:SER:H	2.33	0.41
1:B:329:ALA:HB3	1:B:492:LEU:HD21	2.03	0.41
1:B:45:ILE:HD12	1:B:46:GLN:N	2.32	0.41
1:E:284:ILE:O	1:E:289:ARG:HD3	2.21	0.41
1:F:18:HIS:CD2	1:F:19:VAL:HG13	2.56	0.41
1:F:341:HIS:O	1:F:345:GLY:HA3	2.21	0.41
1:F:346:ILE:O	1:F:426:TRP:CZ3	2.70	0.41
1:H:61:GLN:HA	1:H:69:LEU:HD11	2.02	0.41
1:H:82:TRP:O	1:H:100:HIS:HA	2.20	0.41
2:A:900:BLA:HMA2	2:A:900:BLA:O2A	2.21	0.41
1:B:349:LEU:HD12	1:B:481:ILE:CG2	2.50	0.41
1:C:147:VAL:HG21	1:C:274:PHE:CZ	2.56	0.41
1:C:374:ALA:O	1:C:378:LEU:HB2	2.21	0.41
1:C:8:THR:H	1:C:11:ASN:HB2	1.86	0.41
1:F:164:ARG:HB2	1:F:174:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:384:ASP:O	1:F:384:ASP:CG	2.59	0.41
1:A:152:ARG:NH2	1:A:179:ARG:HB3	2.36	0.41
1:B:208:ILE:HG12	1:B:262:ILE:CD1	2.51	0.41
1:C:42:SER:HA	1:C:221:VAL:HA	2.03	0.41
1:C:7:VAL:O	1:C:7:VAL:HG23	2.21	0.41
1:D:413:ALA:HA	1:D:424:ILE:O	2.21	0.41
1:E:130:ILE:HD11	1:E:150:GLU:HB2	2.02	0.41
1:G:315:LEU:O	1:G:319:THR:HG23	2.21	0.41
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.89	0.41
1:C:261:SER:HA	1:C:274:PHE:O	2.20	0.41
1:C:288:VAL:O	1:C:291:SER:HB2	2.20	0.41
1:F:202:LEU:HD13	1:F:241:ARG:CZ	2.50	0.41
1:F:147:VAL:CG2	1:F:274:PHE:CE2	3.04	0.41
1:A:69:LEU:O	1:A:73:GLU:HG3	2.20	0.41
2:E:900:BLA:HMB3	2:E:900:BLA:CMA	2.51	0.41
1:F:446:THR:HG23	1:F:446:THR:O	2.21	0.41
1:G:9:LEU:HD21	1:G:450:SER:HB3	2.03	0.41
1:A:150:GLU:O	1:A:154:MET:HG3	2.20	0.40
1:C:295:PHE:O	1:C:298:VAL:HG12	2.21	0.40
1:C:41:ALA:CB	1:C:45:ILE:HD12	2.38	0.40
1:E:311:ILE:HG23	1:E:477:THR:HG21	2.02	0.40
1:E:45:ILE:HG13	1:E:45:ILE:H	1.70	0.40
1:G:391:HIS:HA	1:G:411:VAL:O	2.20	0.40
1:G:433:HIS:CD2	1:G:460:PHE:CZ	3.09	0.40
1:H:42:SER:O	1:H:45:ILE:HG13	2.21	0.40
1:A:243:VAL:HG12	1:A:244:SER:N	2.37	0.40
1:A:67:GLU:HB3	1:A:86:VAL:HG11	2.02	0.40
1:C:435:ILE:HG23	1:E:364:LEU:CD2	2.51	0.40
1:D:68:VAL:HG13	1:D:97:VAL:HG11	2.02	0.40
1:F:339:LEU:HD22	1:F:346:ILE:CG2	2.50	0.40
1:F:9:LEU:HD22	1:F:9:LEU:H	1.86	0.40
1:A:157:TYR:OH	1:A:260:MET:HB2	2.22	0.40
1:B:112:ILE:O	1:B:112:ILE:HG12	2.22	0.40
1:B:226:ASN:O	1:B:230:ASN:N	2.55	0.40
1:C:19:VAL:O	1:C:19:VAL:HG23	2.21	0.40
1:E:129:ARG:O	1:E:133:GLN:HG2	2.21	0.40
1:E:142:SER:O	1:E:146:ASN:HB2	2.21	0.40
1:E:291:SER:O	1:E:294:ILE:HB	2.21	0.40
1:E:294:ILE:HD11	1:F:124:THR:HA	2.03	0.40
1:F:305:ARG:HG2	1:F:305:ARG:NH1	2.31	0.40
1:A:33:ARG:HB3	1:A:39:LEU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:ARG:HH12	1:H:178:ARG:NH2	2.19	0.40
1:D:467:VAL:HG23	1:D:468:ARG:H	1.87	0.40
1:E:118:LEU:HA	1:E:118:LEU:HD23	1.88	0.40
1:E:168:ASP:O	1:E:169:ASP:HB2	2.21	0.40
1:E:206:ASN:HA	1:E:207:PRO:HD2	1.80	0.40
1:E:226:ASN:HA	1:E:227:PRO:HD3	1.94	0.40
1:E:305:ARG:HB3	1:E:308:GLN:HE21	1.86	0.40
1:E:349:LEU:HD22	1:E:481:ILE:HG21	2.04	0.40
1:E:247:HIS:CE1	2:E:900:BLA:CHA	3.04	0.40
1:G:414:ILE:HG13	1:G:414:ILE:O	2.20	0.40
1:G:71:MET:SD	1:G:86:VAL:HG23	2.62	0.40
1:C:475:SER:HB2	1:C:478:ASP:CG	2.42	0.40
1:D:159:ARG:HD3	1:D:161:MET:HG3	2.04	0.40
1:D:356:LEU:C	1:D:356:LEU:HD13	2.41	0.40
1:E:118:LEU:HD12	1:E:288:VAL:HG13	2.03	0.40
1:E:288:VAL:HG12	1:E:292:PHE:CE2	2.57	0.40
1:E:40:ALA:HB2	1:E:223:PRO:HD2	2.04	0.40
1:F:89:ARG:HG2	1:F:94:LEU:CB	2.49	0.40
1:G:152:ARG:HB2	1:G:160:VAL:HG13	2.03	0.40
1:G:311:ILE:HD13	1:G:312:ALA:N	2.36	0.40
1:H:329:ALA:HB1	1:H:492:LEU:HD21	2.02	0.40
2:H:900:BLA:HMA1	2:H:900:BLA:HMB3	2.03	0.40

There are no symmetry-related clashes.

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	475/505 (94%)	442 (93%)	30 (6%)	3 (1%)	25	34
1	B	464/505 (92%)	436 (94%)	28 (6%)	0	100	100
1	C	478/505 (95%)	455 (95%)	20 (4%)	3 (1%)	25	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	474/505 (94%)	451 (95%)	23 (5%)	0	100	100
1	E	475/505 (94%)	452 (95%)	22 (5%)	1 (0%)	47	60
1	F	465/505 (92%)	436 (94%)	27 (6%)	2 (0%)	34	46
1	G	479/505 (95%)	460 (96%)	18 (4%)	1 (0%)	47	60
1	H	477/505 (94%)	444 (93%)	28 (6%)	5 (1%)	15	22
All	All	3787/4040 (94%)	3576 (94%)	196 (5%)	15 (0%)	34	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	LEU
1	H	444	LEU
1	H	445	LEU
1	E	443	LYS
1	A	441	PRO
1	A	446	THR
1	C	62	GLU
1	C	81	PRO
1	H	345	GLY
1	F	242	SER
1	G	441	PRO
1	F	57	SER
1	C	66	PRO
1	H	66	PRO
1	H	266	VAL

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	408/431 (95%)	377 (92%)	31 (8%)	13	17
1	B	400/431 (93%)	365 (91%)	35 (9%)	10	12
1	C	410/431 (95%)	376 (92%)	34 (8%)	11	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	409/431 (95%)	384 (94%)	25 (6%)	18	24
1	E	408/431 (95%)	369 (90%)	39 (10%)	8	9
1	F	401/431 (93%)	366 (91%)	35 (9%)	10	12
1	G	411/431 (95%)	380 (92%)	31 (8%)	13	17
1	H	410/431 (95%)	370 (90%)	40 (10%)	8	9
All	All	3257/3448 (94%)	2987 (92%)	270 (8%)	11	14

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	GLU
1	A	32	LEU
1	A	45	ILE
1	A	69	LEU
1	A	89	ARG
1	A	108	LEU
1	A	120	ILE
1	A	135	GLN
1	A	140	THR
1	A	160	VAL
1	A	164	ARG
1	A	166	ARG
1	A	177	SER
1	A	186	LEU
1	A	208	ILE
1	A	217	THR
1	A	225	LEU
1	A	232	SER
1	A	239	VAL
1	A	250	TYR
1	A	283	LEU
1	A	311	ILE
1	A	327	ARG
1	A	380	ARG
1	A	387	ARG
1	A	412	LEU
1	A	440	LYS
1	A	443	LYS
1	A	453	ARG

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Mol	Chain	Res	Type
1	A	485	LEU
1	B	8	THR
1	B	11	ASN
1	B	13	GLU
1	B	32	LEU
1	B	45	ILE
1	B	61	GLN
1	B	70	ARG
1	B	76	LEU
1	B	88	THR
1	B	93	HIS
1	B	94	LEU
1	B	112	ILE
1	B	125	LEU
1	B	130	ILE
1	B	140	THR
1	B	178	ARG
1	B	180	GLU
1	B	181	ASP
1	B	198	GLN
1	B	201	ARG
1	B	210	LEU
1	B	250	TYR
1	B	257	ARG
1	B	273	LEU
1	B	291	SER
1	B	305	ARG
1	B	311	ILE
1	B	325	LEU
1	B	349	LEU
1	B	362	ARG
1	B	372	ARG
1	B	412	LEU
1	B	483	GLU
1	B	485	LEU
1	B	488	ASP
1	C	18	HIS
1	C	29	LEU
1	C	32	LEU
1	C	62	GLU
1	C	76	LEU
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	89	ARG
1	C	94	LEU
1	C	98	ILE
1	C	114	THR
1	C	117	THR
1	C	143	LEU
1	C	160	VAL
1	C	164	ARG
1	C	186	LEU
1	C	188	GLN
1	C	210	LEU
1	C	221	VAL
1	C	259	SER
1	C	260	MET
1	C	304	GLU
1	C	305	ARG
1	C	306	LEU
1	C	317	VAL
1	C	325	LEU
1	C	330	ARG
1	C	356	LEU
1	C	364	LEU
1	C	366	ILE
1	C	373	GLN
1	C	393	ASP
1	C	412	LEU
1	C	483	GLU
1	C	485	LEU
1	D	17	ILE
1	D	45	ILE
1	D	69	LEU
1	D	84	ASN
1	D	94	LEU
1	D	112	ILE
1	D	116	ASP
1	D	143	LEU
1	D	160	VAL
1	D	188	GLN
1	D	201	ARG
1	D	208	ILE
1	D	210	LEU
1	D	262	ILE

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Mol	Chain	Res	Type
1	D	284	ILE
1	D	305	ARG
1	D	306	LEU
1	D	311	ILE
1	D	325	LEU
1	D	335	LEU
1	D	412	LEU
1	D	437	TRP
1	D	444	LEU
1	D	446	THR
1	D	485	LEU
1	E	17	ILE
1	E	59	LEU
1	E	62	GLU
1	E	70	ARG
1	E	79	ASN
1	E	84	ASN
1	E	112	ILE
1	E	124	THR
1	E	128	GLN
1	E	135	GLN
1	E	146	ASN
1	E	154	MET
1	E	178	ARG
1	E	186	LEU
1	E	208	ILE
1	E	216	TYR
1	E	220	ARG
1	E	225	LEU
1	E	229	THR
1	E	250	TYR
1	E	305	ARG
1	E	317	VAL
1	E	321	ARG
1	E	334	ASP
1	E	349	LEU
1	E	356	LEU
1	E	364	LEU
1	E	386	GLU
1	E	393	ASP
1	E	394	ASN
1	E	412	LEU

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Mol	Chain	Res	Type
1	E	434	ARG
1	E	444	LEU
1	E	447	ILE
1	E	450	SER
1	E	453	ARG
1	E	477	THR
1	E	485	LEU
1	E	491	GLU
1	F	11	ASN
1	F	33	ARG
1	F	61	GLN
1	F	67	GLU
1	F	70	ARG
1	F	73	GLU
1	F	84	ASN
1	F	94	LEU
1	F	112	ILE
1	F	116	ASP
1	F	125	LEU
1	F	129	ARG
1	F	134	VAL
1	F	146	ASN
1	F	147	VAL
1	F	159	ARG
1	F	188	GLN
1	F	210	LEU
1	F	230	ASN
1	F	278	HIS
1	F	305	ARG
1	F	306	LEU
1	F	311	ILE
1	F	321	ARG
1	F	325	LEU
1	F	341	HIS
1	F	349	LEU
1	F	362	ARG
1	F	384	ASP
1	F	392	THR
1	F	393	ASP
1	F	412	LEU
1	F	447	ILE
1	F	453	ARG

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Mol	Chain	Res	Type
1	F	498	LEU
1	G	67	GLU
1	G	79	ASN
1	G	84	ASN
1	G	94	LEU
1	G	112	ILE
1	G	128	GLN
1	G	130	ILE
1	G	139	ASP
1	G	140	THR
1	G	143	LEU
1	G	147	VAL
1	G	160	VAL
1	G	164	ARG
1	G	181	ASP
1	G	186	LEU
1	G	230	ASN
1	G	273	LEU
1	G	278	HIS
1	G	283	LEU
1	G	305	ARG
1	G	306	LEU
1	G	311	ILE
1	G	356	LEU
1	G	366	ILE
1	G	393	ASP
1	G	395	TRP
1	G	407	ASP
1	G	412	LEU
1	G	483	GLU
1	G	485	LEU
1	G	496	HIS
1	H	35	ASP
1	H	63	GLN
1	H	64	VAL
1	H	67	GLU
1	H	88	THR
1	H	93	HIS
1	H	94	LEU
1	H	112	ILE
1	H	134	VAL
1	H	135	GLN

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Mol	Chain	Res	Type
1	H	137	HIS
1	H	140	THR
1	H	163	TYR
1	H	181	ASP
1	H	188	GLN
1	H	208	ILE
1	H	210	LEU
1	H	217	THR
1	H	228	GLU
1	H	230	ASN
1	H	273	LEU
1	H	305	ARG
1	H	335	LEU
1	H	349	LEU
1	H	364	LEU
1	H	378	LEU
1	H	387	ARG
1	H	393	ASP
1	H	394	ASN
1	H	412	LEU
1	H	431	GLU
1	H	437	TRP
1	H	444	LEU
1	H	445	LEU
1	H	446	THR
1	H	453	ARG
1	H	461	GLU
1	H	472	THR
1	H	483	GLU
1	H	485	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	128	GLN
1	A	198	GLN
1	A	230	ASN
1	A	293	GLN
1	A	391	HIS
1	A	394	ASN
1	A	417	HIS

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Mol	Chain	Res	Type
1	A	433	HIS
1	A	470	HIS
1	B	24	GLN
1	B	84	ASN
1	B	128	GLN
1	B	137	HIS
1	B	146	ASN
1	B	198	GLN
1	B	205	GLN
1	B	373	GLN
1	B	376	ASN
1	B	391	HIS
1	C	11	ASN
1	C	24	GLN
1	C	61	GLN
1	C	63	GLN
1	C	84	ASN
1	C	126	ASN
1	C	137	HIS
1	C	138	ASN
1	C	146	ASN
1	C	198	GLN
1	C	293	GLN
1	C	417	HIS
1	C	495	ASN
1	D	61	GLN
1	D	84	ASN
1	D	128	GLN
1	D	137	HIS
1	D	188	GLN
1	D	198	GLN
1	D	308	GLN
1	D	496	HIS
1	E	24	GLN
1	E	79	ASN
1	E	84	ASN
1	E	137	HIS
1	E	247	HIS
1	E	293	GLN
1	E	308	GLN
1	E	394	ASN
1	E	433	HIS

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Mol	Chain	Res	Type
1	F	24	GLN
1	F	26	HIS
1	F	84	ASN
1	F	128	GLN
1	F	133	GLN
1	F	138	ASN
1	F	198	GLN
1	F	247	HIS
1	F	293	GLN
1	F	394	ASN
1	F	417	HIS
1	G	24	GLN
1	G	84	ASN
1	G	128	GLN
1	G	146	ASN
1	G	198	GLN
1	G	205	GLN
1	G	278	HIS
1	G	293	GLN
1	G	394	ASN
1	G	417	HIS
1	G	419	GLN
1	G	433	HIS
1	G	470	HIS
1	H	24	GLN
1	H	46	GLN
1	H	93	HIS
1	H	126	ASN
1	H	133	GLN
1	H	188	GLN
1	H	198	GLN
1	H	230	ASN
1	H	247	HIS
1	H	297	GLN
1	H	308	GLN
1	H	373	GLN
1	H	433	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	BLA	G	900	1	36,46,46	3.00	17 (47%)	47,67,67	1.70	9 (19%)
2	BLA	H	900	1	36,46,46	2.97	15 (41%)	47,67,67	1.66	7 (14%)
2	BLA	C	900	1	36,46,46	2.96	18 (50%)	47,67,67	1.90	8 (17%)
2	BLA	D	900	1	36,46,46	3.00	16 (44%)	47,67,67	2.25	7 (14%)
2	BLA	E	900	1	36,46,46	3.04	17 (47%)	47,67,67	1.70	7 (14%)
2	BLA	F	900	1	36,46,46	2.94	17 (47%)	47,67,67	1.76	7 (14%)
2	BLA	A	900	1	36,46,46	2.94	18 (50%)	47,67,67	2.00	8 (17%)
2	BLA	B	900	1	36,46,46	3.03	17 (47%)	47,67,67	1.80	8 (17%)

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	BLA	G	900	1	-	10/22/74/74	0/4/4/4
2	BLA	H	900	1	-	6/22/74/74	0/4/4/4
2	BLA	C	900	1	-	6/22/74/74	0/4/4/4
2	BLA	D	900	1	-	4/22/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	E	900	1	-	10/22/74/74	0/4/4/4
2	BLA	F	900	1	-	6/22/74/74	0/4/4/4
2	BLA	A	900	1	-	7/22/74/74	0/4/4/4
2	BLA	B	900	1	-	7/22/74/74	0/4/4/4

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	BLA	CHB-C1B	8.86	1.52	1.34
2	G	900	BLA	CHB-C1B	8.82	1.52	1.34
2	H	900	BLA	CHB-C1B	8.81	1.52	1.34
2	B	900	BLA	CHB-C1B	8.81	1.52	1.34
2	A	900	BLA	CHB-C1B	8.66	1.52	1.34
2	F	900	BLA	CHB-C1B	8.64	1.52	1.34
2	D	900	BLA	CHB-C1B	8.63	1.52	1.34
2	C	900	BLA	CHB-C1B	8.44	1.52	1.34
2	B	900	BLA	CHD-C4C	6.49	1.53	1.38
2	E	900	BLA	CHD-C4C	6.45	1.53	1.38
2	F	900	BLA	CHD-C4C	6.35	1.53	1.38
2	D	900	BLA	CHD-C4C	6.29	1.53	1.38
2	G	900	BLA	CHD-C4C	6.29	1.53	1.38
2	H	900	BLA	CHD-C4C	6.13	1.52	1.38
2	C	900	BLA	CHD-C4C	6.04	1.52	1.38
2	A	900	BLA	CHD-C4C	5.87	1.52	1.38
2	E	900	BLA	CHA-C4D	5.87	1.40	1.35
2	E	900	BLA	CHD-C1D	5.66	1.53	1.40
2	F	900	BLA	CHD-C1D	5.63	1.53	1.40
2	B	900	BLA	CHA-C4D	5.63	1.39	1.35
2	D	900	BLA	CHD-C1D	5.61	1.53	1.40
2	G	900	BLA	CHD-C1D	5.61	1.53	1.40
2	G	900	BLA	CHA-C4D	5.60	1.39	1.35
2	B	900	BLA	CHD-C1D	5.59	1.53	1.40
2	H	900	BLA	CHA-C4D	5.41	1.39	1.35
2	A	900	BLA	CHA-C4D	5.39	1.39	1.35
2	C	900	BLA	CHA-C4D	5.31	1.39	1.35
2	D	900	BLA	CHA-C4D	5.28	1.39	1.35
2	A	900	BLA	CHD-C1D	5.20	1.52	1.40
2	H	900	BLA	CHD-C1D	5.16	1.52	1.40
2	C	900	BLA	CHD-C1D	5.14	1.52	1.40
2	F	900	BLA	CHA-C4D	4.91	1.39	1.35
2	D	900	BLA	CBC-CAC	4.74	1.53	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	900	BLA	CBC-CAC	4.71	1.53	1.30
2	G	900	BLA	CBC-CAC	4.71	1.53	1.30
2	A	900	BLA	CBC-CAC	4.70	1.53	1.30
2	B	900	BLA	CBC-CAC	4.69	1.53	1.30
2	E	900	BLA	CBC-CAC	4.69	1.53	1.30
2	F	900	BLA	CBC-CAC	4.67	1.53	1.30
2	C	900	BLA	CBC-CAC	4.64	1.53	1.30
2	B	900	BLA	C4D-C3D	-4.04	1.39	1.45
2	C	900	BLA	C4D-C3D	-3.94	1.39	1.45
2	G	900	BLA	C4D-C3D	-3.87	1.39	1.45
2	D	900	BLA	C4D-C3D	-3.87	1.39	1.45
2	H	900	BLA	C4D-C3D	-3.86	1.39	1.45
2	A	900	BLA	C4D-C3D	-3.84	1.39	1.45
2	E	900	BLA	C4D-C3D	-3.75	1.39	1.45
2	F	900	BLA	C4D-C3D	-3.70	1.39	1.45
2	C	900	BLA	C3C-C4C	-3.70	1.39	1.45
2	A	900	BLA	C1D-C2D	-3.58	1.38	1.45
2	C	900	BLA	C1D-C2D	-3.56	1.38	1.45
2	F	900	BLA	C1C-C2C	-3.55	1.38	1.47
2	H	900	BLA	C1D-C2D	-3.51	1.38	1.45
2	B	900	BLA	C1C-C2C	-3.50	1.38	1.47
2	F	900	BLA	C3C-C4C	-3.48	1.39	1.45
2	G	900	BLA	C1C-C2C	-3.47	1.38	1.47
2	A	900	BLA	C3C-C4C	-3.46	1.39	1.45
2	G	900	BLA	C1D-C2D	-3.45	1.38	1.45
2	D	900	BLA	C3C-C4C	-3.44	1.39	1.45
2	C	900	BLA	C1C-C2C	-3.44	1.38	1.47
2	H	900	BLA	C1C-C2C	-3.42	1.38	1.47
2	B	900	BLA	C3C-C4C	-3.39	1.39	1.45
2	H	900	BLA	C3C-C4C	-3.39	1.39	1.45
2	D	900	BLA	C3B-C4B	-3.36	1.37	1.47
2	D	900	BLA	C1C-C2C	-3.34	1.38	1.47
2	C	900	BLA	C1B-C2B	-3.34	1.39	1.45
2	E	900	BLA	C1C-C2C	-3.33	1.38	1.47
2	G	900	BLA	C3C-C4C	-3.33	1.40	1.45
2	D	900	BLA	C1D-C2D	-3.31	1.38	1.45
2	F	900	BLA	C1D-C2D	-3.30	1.38	1.45
2	B	900	BLA	C1D-C2D	-3.28	1.38	1.45
2	B	900	BLA	CAB-C3B	-3.25	1.38	1.47
2	E	900	BLA	C3B-C4B	-3.25	1.38	1.47
2	A	900	BLA	CAB-C3B	-3.24	1.38	1.47
2	E	900	BLA	CAB-C3B	-3.23	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	BLA	C3C-C4C	-3.18	1.40	1.45
2	A	900	BLA	C1C-C2C	-3.18	1.39	1.47
2	E	900	BLA	C1D-C2D	-3.16	1.39	1.45
2	D	900	BLA	CAB-C3B	-3.15	1.38	1.47
2	E	900	BLA	C4A-CHB	3.12	1.53	1.41
2	D	900	BLA	C1B-C2B	-3.10	1.39	1.45
2	H	900	BLA	C1B-C2B	-3.08	1.39	1.45
2	B	900	BLA	C1B-C2B	-3.07	1.39	1.45
2	F	900	BLA	CAB-C3B	-3.06	1.39	1.47
2	D	900	BLA	C4A-CHB	3.05	1.53	1.41
2	B	900	BLA	C4A-CHB	3.05	1.53	1.41
2	H	900	BLA	C3B-C4B	-3.03	1.38	1.47
2	G	900	BLA	C4A-CHB	3.03	1.52	1.41
2	H	900	BLA	C4A-CHB	3.03	1.52	1.41
2	A	900	BLA	C3B-C4B	-3.01	1.38	1.47
2	G	900	BLA	CAB-C3B	-3.01	1.39	1.47
2	H	900	BLA	CAB-C3B	-3.00	1.39	1.47
2	G	900	BLA	C1B-C2B	-2.99	1.39	1.45
2	E	900	BLA	C1B-C2B	-2.98	1.39	1.45
2	G	900	BLA	C3B-C4B	-2.98	1.38	1.47
2	C	900	BLA	CAB-C3B	-2.95	1.39	1.47
2	A	900	BLA	C1B-C2B	-2.94	1.39	1.45
2	B	900	BLA	C3B-C4B	-2.89	1.39	1.47
2	F	900	BLA	C1B-C2B	-2.88	1.39	1.45
2	F	900	BLA	C4A-CHB	2.88	1.52	1.41
2	C	900	BLA	C3B-C4B	-2.87	1.39	1.47
2	A	900	BLA	C4A-CHB	2.85	1.52	1.41
2	C	900	BLA	C4A-CHB	2.76	1.51	1.41
2	F	900	BLA	C3B-C4B	-2.57	1.40	1.47
2	C	900	BLA	CAC-C3C	2.50	1.54	1.47
2	D	900	BLA	CAC-C3C	2.50	1.54	1.47
2	E	900	BLA	CAC-C3C	2.33	1.53	1.47
2	C	900	BLA	C1C-NC	-2.27	1.33	1.38
2	A	900	BLA	CAC-C3C	2.27	1.53	1.47
2	H	900	BLA	CAC-C3C	2.26	1.53	1.47
2	B	900	BLA	CAC-C3C	2.24	1.53	1.47
2	G	900	BLA	CAC-C3C	2.21	1.53	1.47
2	F	900	BLA	CAC-C3C	2.21	1.53	1.47
2	E	900	BLA	C4C-NC	-2.19	1.34	1.37
2	A	900	BLA	C4C-NC	-2.19	1.34	1.37
2	G	900	BLA	C1C-NC	-2.15	1.33	1.38
2	A	900	BLA	C1C-NC	-2.14	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C1B-NB	-2.14	1.34	1.37
2	E	900	BLA	C1C-NC	-2.13	1.33	1.38
2	C	900	BLA	C4C-NC	-2.13	1.34	1.37
2	B	900	BLA	C1B-NB	-2.12	1.34	1.37
2	F	900	BLA	C1C-NC	-2.11	1.33	1.38
2	G	900	BLA	C4C-NC	-2.10	1.34	1.37
2	B	900	BLA	C1C-NC	-2.10	1.33	1.38
2	F	900	BLA	C4C-NC	-2.10	1.34	1.37
2	E	900	BLA	C1B-NB	-2.09	1.34	1.37
2	C	900	BLA	C1B-NB	-2.09	1.34	1.37
2	H	900	BLA	C1B-NB	-2.08	1.34	1.37
2	A	900	BLA	C4D-ND	-2.07	1.34	1.38
2	B	900	BLA	C4C-NC	-2.07	1.34	1.37
2	C	900	BLA	C4D-ND	-2.06	1.34	1.38
2	D	900	BLA	C1C-NC	-2.06	1.33	1.38
2	D	900	BLA	C4C-NC	-2.05	1.34	1.37
2	F	900	BLA	C1B-NB	-2.03	1.34	1.37
2	G	900	BLA	C1B-NB	-2.03	1.34	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	BLA	C1A-CHA-C4D	-11.32	115.29	128.81
2	A	900	BLA	C1A-CHA-C4D	-9.92	116.95	128.81
2	C	900	BLA	C1A-CHA-C4D	-8.97	118.09	128.81
2	F	900	BLA	C1A-CHA-C4D	-7.65	119.67	128.81
2	B	900	BLA	C1A-CHA-C4D	-6.74	120.76	128.81
2	G	900	BLA	C1A-CHA-C4D	-6.12	121.50	128.81
2	B	900	BLA	C4C-CHD-C1D	-5.81	113.88	128.08
2	H	900	BLA	C1A-CHA-C4D	-5.67	122.03	128.81
2	E	900	BLA	C4C-CHD-C1D	-5.65	114.28	128.08
2	E	900	BLA	C1A-CHA-C4D	-5.25	122.53	128.81
2	D	900	BLA	C4C-CHD-C1D	-5.10	115.61	128.08
2	H	900	BLA	C4C-CHD-C1D	-4.67	116.67	128.08
2	G	900	BLA	C4C-CHD-C1D	-4.53	117.02	128.08
2	C	900	BLA	C4C-CHD-C1D	-4.03	118.23	128.08
2	D	900	BLA	C3B-C4B-NB	3.74	110.41	106.19
2	F	900	BLA	C4C-CHD-C1D	-3.27	120.10	128.08
2	G	900	BLA	CBC-CAC-C3C	-3.25	111.45	127.62
2	B	900	BLA	CBC-CAC-C3C	-3.23	111.57	127.62
2	F	900	BLA	CBC-CAC-C3C	-3.19	111.76	127.62
2	H	900	BLA	CBC-CAC-C3C	-3.17	111.84	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	BLA	CBC-CAC-C3C	-3.13	112.07	127.62
2	A	900	BLA	CBC-CAC-C3C	-3.06	112.40	127.62
2	A	900	BLA	C3B-C4B-NB	2.97	109.55	106.19
2	E	900	BLA	CMB-C2B-C1B	2.90	127.78	124.17
2	H	900	BLA	C3B-C4B-NB	2.85	109.41	106.19
2	E	900	BLA	C3B-C4B-NB	2.79	109.34	106.19
2	C	900	BLA	CBC-CAC-C3C	-2.78	113.80	127.62
2	D	900	BLA	CBC-CAC-C3C	-2.76	113.90	127.62
2	C	900	BLA	C3B-C4B-NB	2.68	109.21	106.19
2	G	900	BLA	C3B-C4B-NB	2.62	109.14	106.19
2	F	900	BLA	C3B-C4B-NB	2.47	108.98	106.19
2	F	900	BLA	CAD-C3D-C4D	2.44	129.33	125.01
2	D	900	BLA	CHA-C4D-C3D	-2.44	119.68	125.32
2	B	900	BLA	CHA-C4D-ND	2.43	132.20	128.83
2	C	900	BLA	CHA-C4D-C3D	-2.43	119.70	125.32
2	B	900	BLA	CHA-C4D-C3D	-2.43	119.70	125.32
2	B	900	BLA	CMB-C2B-C1B	2.37	127.13	124.17
2	F	900	BLA	CHA-C4D-C3D	-2.37	119.84	125.32
2	H	900	BLA	CHA-C4D-C3D	-2.36	119.86	125.32
2	A	900	BLA	CMB-C2B-C1B	2.36	127.11	124.17
2	G	900	BLA	CHA-C4D-C3D	-2.34	119.92	125.32
2	B	900	BLA	C3B-C4B-NB	2.26	108.74	106.19
2	C	900	BLA	CHA-C4D-ND	2.26	131.96	128.83
2	D	900	BLA	CHA-C4D-ND	2.25	131.95	128.83
2	A	900	BLA	CMC-C2C-C1C	2.25	126.67	121.39
2	A	900	BLA	CHA-C4D-C3D	-2.23	120.16	125.32
2	H	900	BLA	CHA-C4D-ND	2.23	131.92	128.83
2	E	900	BLA	C4D-ND-C1D	2.23	110.70	106.51
2	G	900	BLA	CMB-C2B-C1B	2.21	126.92	124.17
2	C	900	BLA	C3C-C4C-NC	2.20	110.24	106.80
2	G	900	BLA	C1D-C2D-C3D	2.18	109.02	106.51
2	H	900	BLA	CMB-C2B-C1B	2.18	126.89	124.17
2	B	900	BLA	C4D-ND-C1D	2.17	110.59	106.51
2	G	900	BLA	CHA-C4D-ND	2.15	131.80	128.83
2	D	900	BLA	CMB-C2B-C1B	2.14	126.84	124.17
2	G	900	BLA	C4D-ND-C1D	2.11	110.48	106.51
2	A	900	BLA	CAD-C3D-C4D	2.09	128.70	125.01
2	F	900	BLA	CHA-C4D-ND	2.07	131.70	128.83
2	C	900	BLA	C4C-NC-C1C	-2.07	108.03	110.67
2	A	900	BLA	C3C-C4C-NC	2.04	110.00	106.80
2	E	900	BLA	CHA-C4D-C3D	-2.04	120.61	125.32

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	900	BLA	NA-C1A-CHA-C4D
2	G	900	BLA	C2A-C1A-CHA-C4D
2	G	900	BLA	C1A-C2A-CAA-CBA
2	G	900	BLA	C3A-C2A-CAA-CBA
2	G	900	BLA	NA-C4A-CHB-C1B
2	G	900	BLA	NB-C1B-CHB-C4A
2	G	900	BLA	C2B-C1B-CHB-C4A
2	H	900	BLA	NA-C4A-CHB-C1B
2	H	900	BLA	C3A-C4A-CHB-C1B
2	H	900	BLA	NB-C1B-CHB-C4A
2	H	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	NA-C1A-CHA-C4D
2	C	900	BLA	C2A-C1A-CHA-C4D
2	C	900	BLA	NA-C4A-CHB-C1B
2	C	900	BLA	C3A-C4A-CHB-C1B
2	C	900	BLA	NB-C1B-CHB-C4A
2	C	900	BLA	C2B-C1B-CHB-C4A
2	D	900	BLA	NA-C4A-CHB-C1B
2	D	900	BLA	C3A-C4A-CHB-C1B
2	D	900	BLA	NB-C1B-CHB-C4A
2	D	900	BLA	C2B-C1B-CHB-C4A
2	E	900	BLA	NA-C4A-CHB-C1B
2	E	900	BLA	C3A-C4A-CHB-C1B
2	E	900	BLA	NB-C1B-CHB-C4A
2	E	900	BLA	C2B-C1B-CHB-C4A
2	F	900	BLA	NA-C4A-CHB-C1B
2	F	900	BLA	C3A-C4A-CHB-C1B
2	F	900	BLA	NB-C1B-CHB-C4A
2	F	900	BLA	C2B-C1B-CHB-C4A
2	A	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	A	900	BLA	NB-C1B-CHB-C4A
2	A	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	C2B-C1B-CHB-C4A
2	G	900	BLA	C2C-C3C-CAC-CBC
2	G	900	BLA	C4C-C3C-CAC-CBC
2	E	900	BLA	C2D-C1D-CHD-C4C
2	E	900	BLA	NC-C4C-CHD-C1D
2	E	900	BLA	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
2	H	900	BLA	C2C-C3C-CAC-CBC
2	E	900	BLA	C2C-C3C-CAC-CBC
2	B	900	BLA	C2C-C3C-CAC-CBC
2	F	900	BLA	NC-C4C-CHD-C1D
2	B	900	BLA	C4C-C3C-CAC-CBC
2	B	900	BLA	NC-C4C-CHD-C1D
2	E	900	BLA	C3C-C4C-CHD-C1D
2	G	900	BLA	NC-C4C-CHD-C1D
2	A	900	BLA	NC-C4C-CHD-C1D
2	A	900	BLA	C2C-C3C-CAC-CBC
2	H	900	BLA	C4C-C3C-CAC-CBC
2	E	900	BLA	C4C-C3C-CAC-CBC
2	A	900	BLA	C4C-C3C-CAC-CBC
2	F	900	BLA	C3C-C4C-CHD-C1D

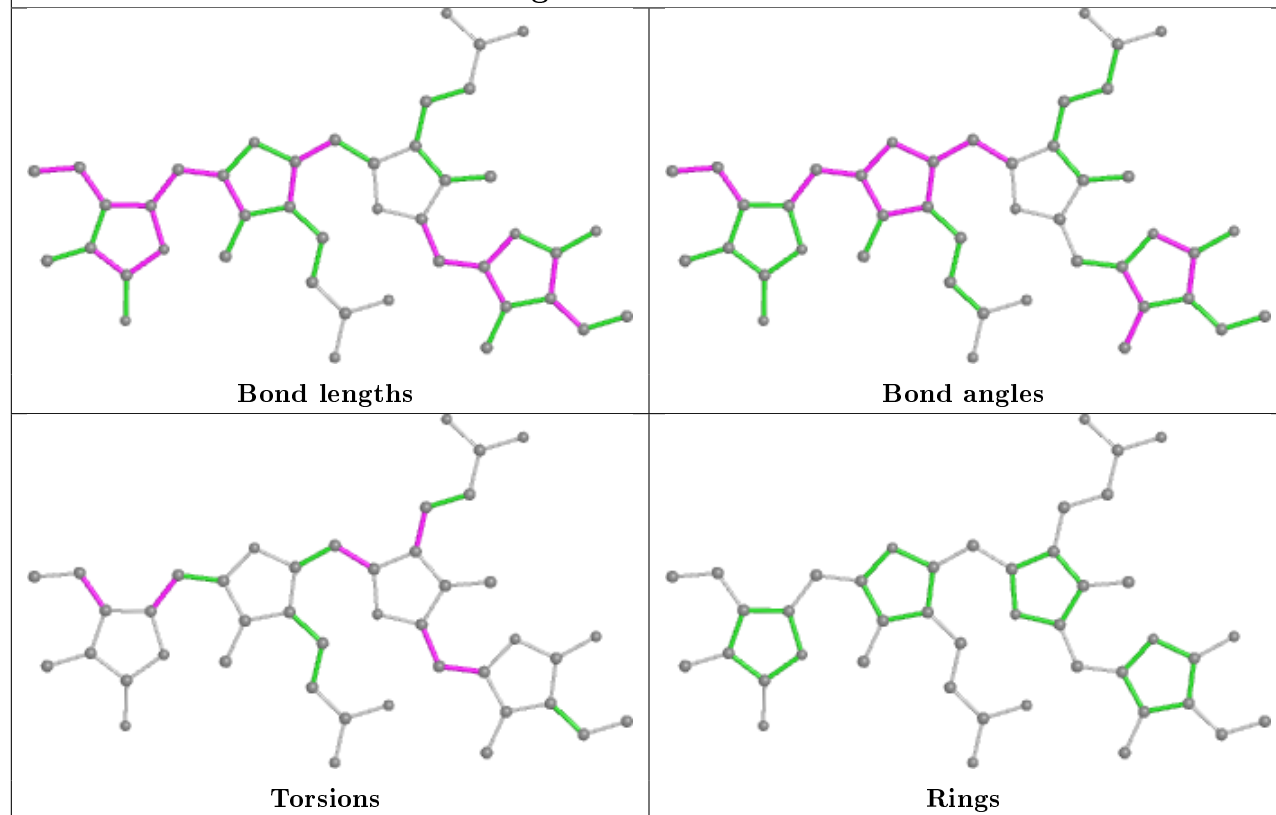
There are no ring outliers.

8 monomers are involved in 58 short contacts:

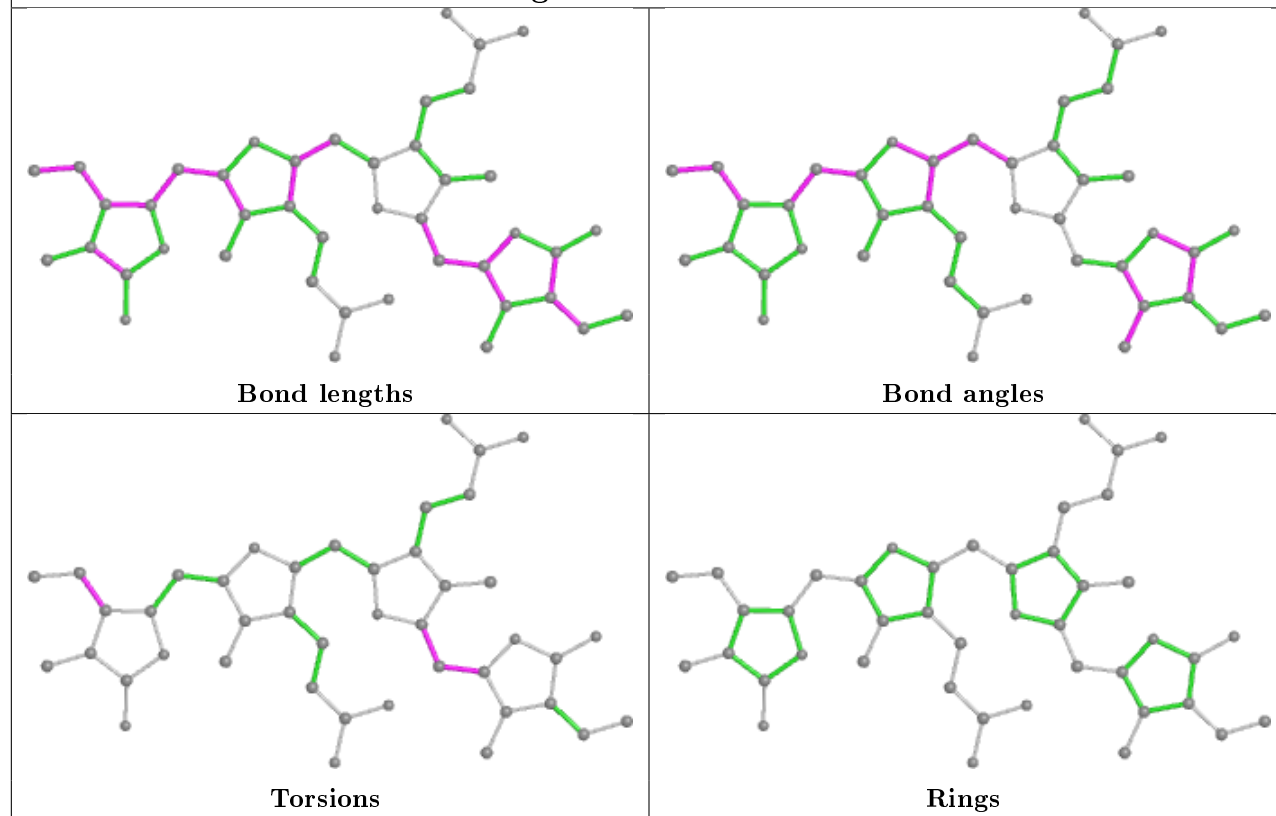
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	900	BLA	5	0
2	H	900	BLA	6	0
2	C	900	BLA	14	0
2	D	900	BLA	5	0
2	E	900	BLA	7	0
2	F	900	BLA	9	0
2	A	900	BLA	4	0
2	B	900	BLA	8	0

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.

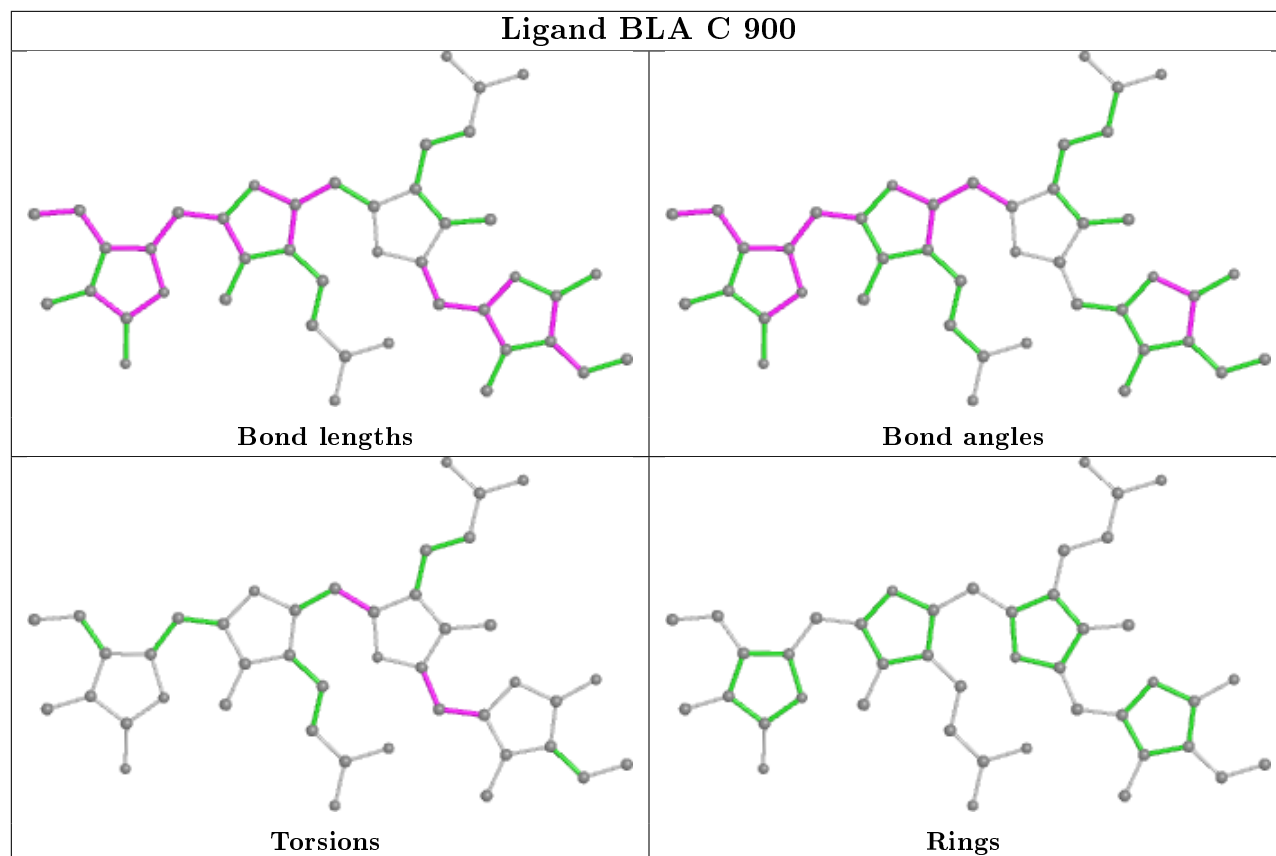
Ligand BLA G 900



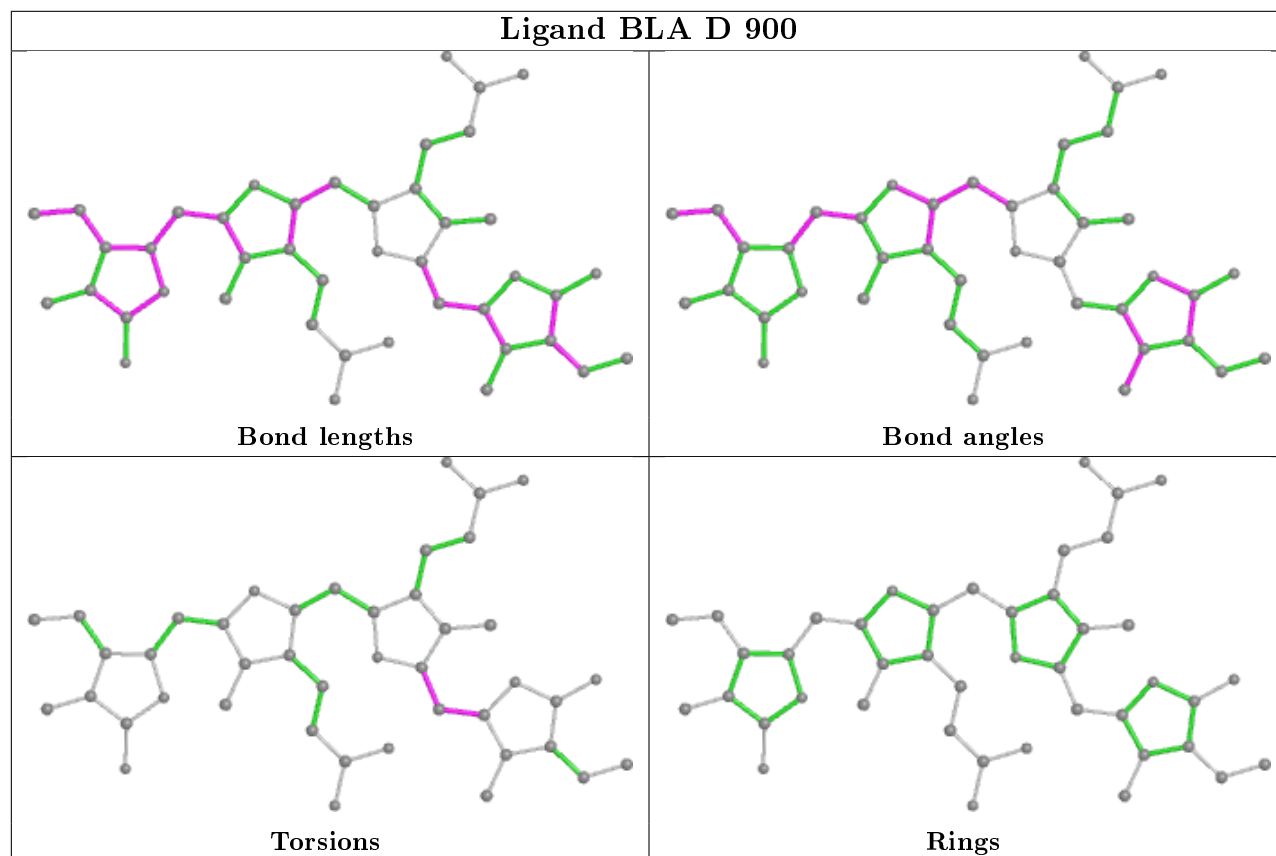
Ligand BLA H 900



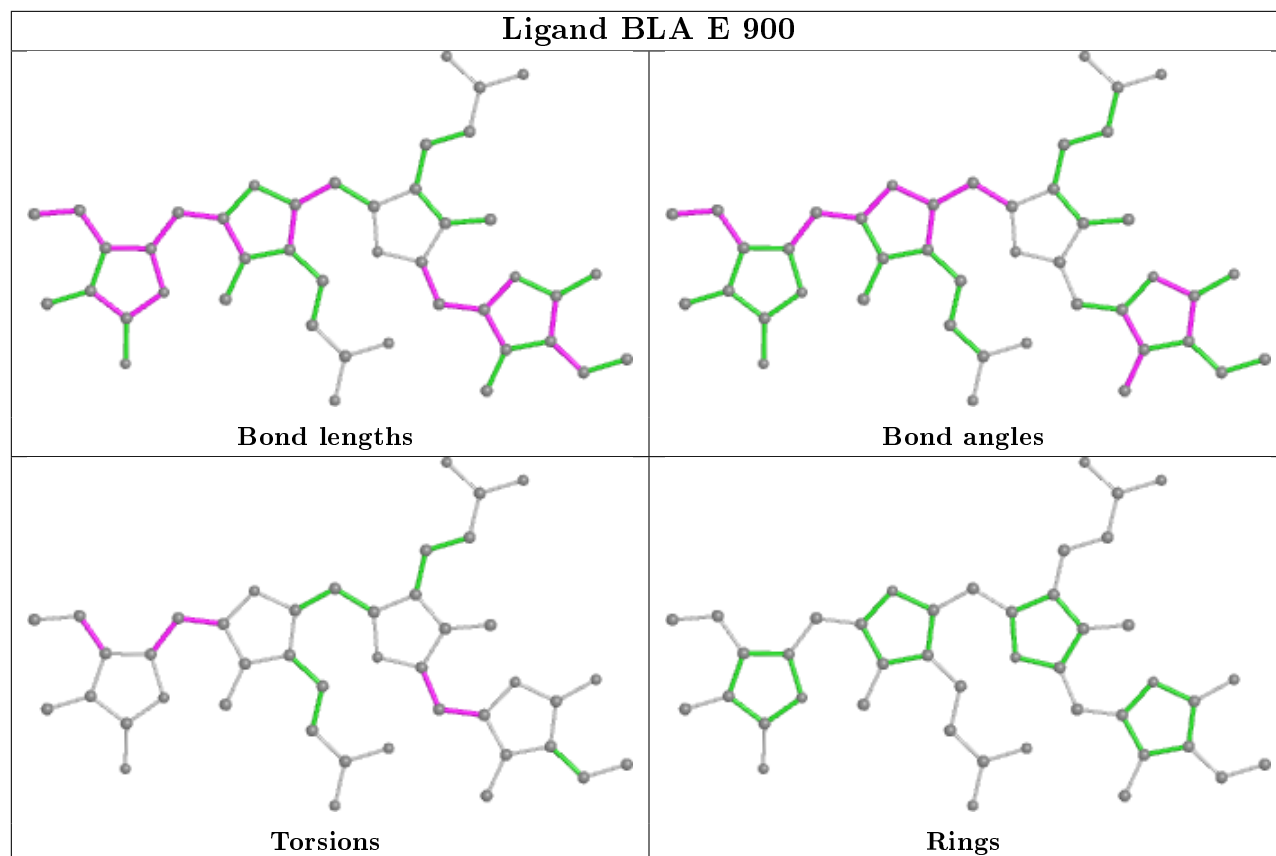
Ligand BLA C 900



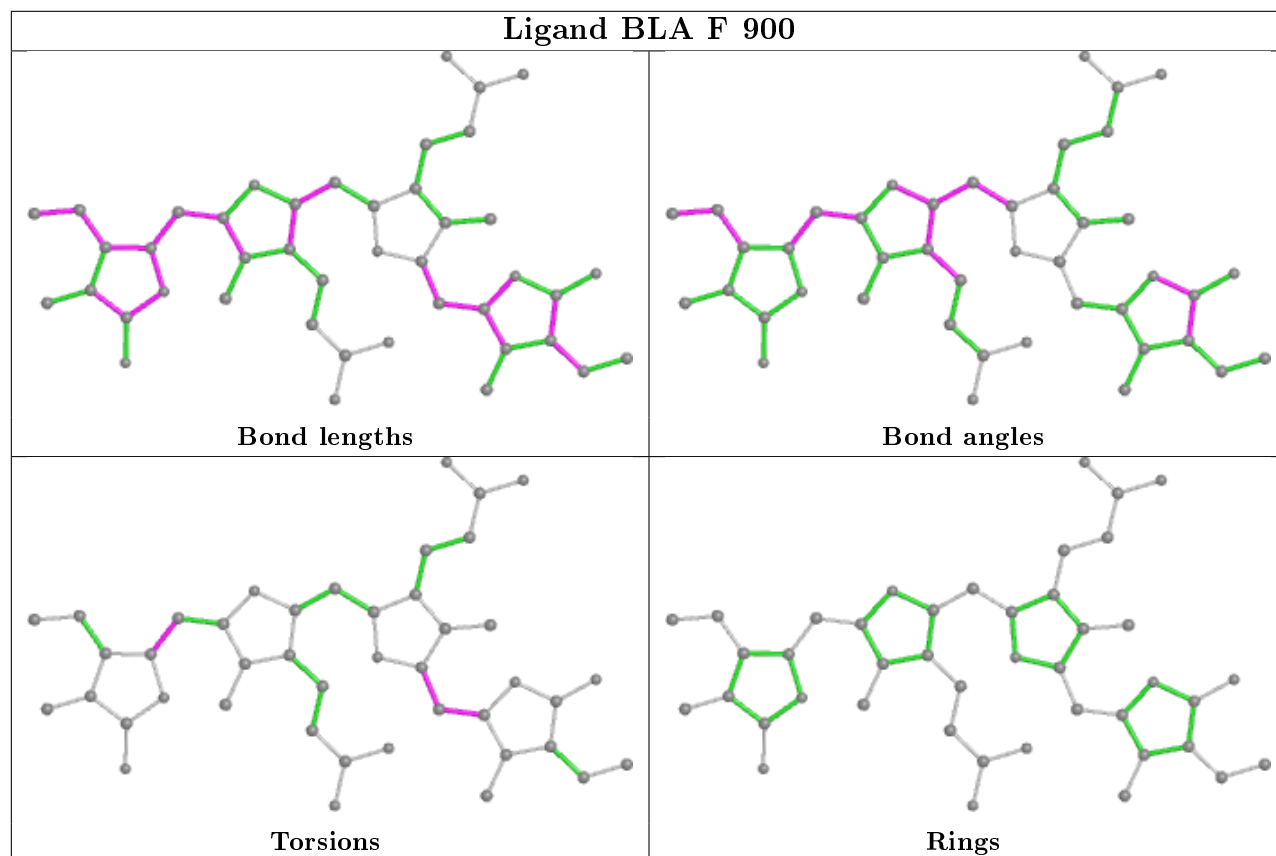
Ligand BLA D 900



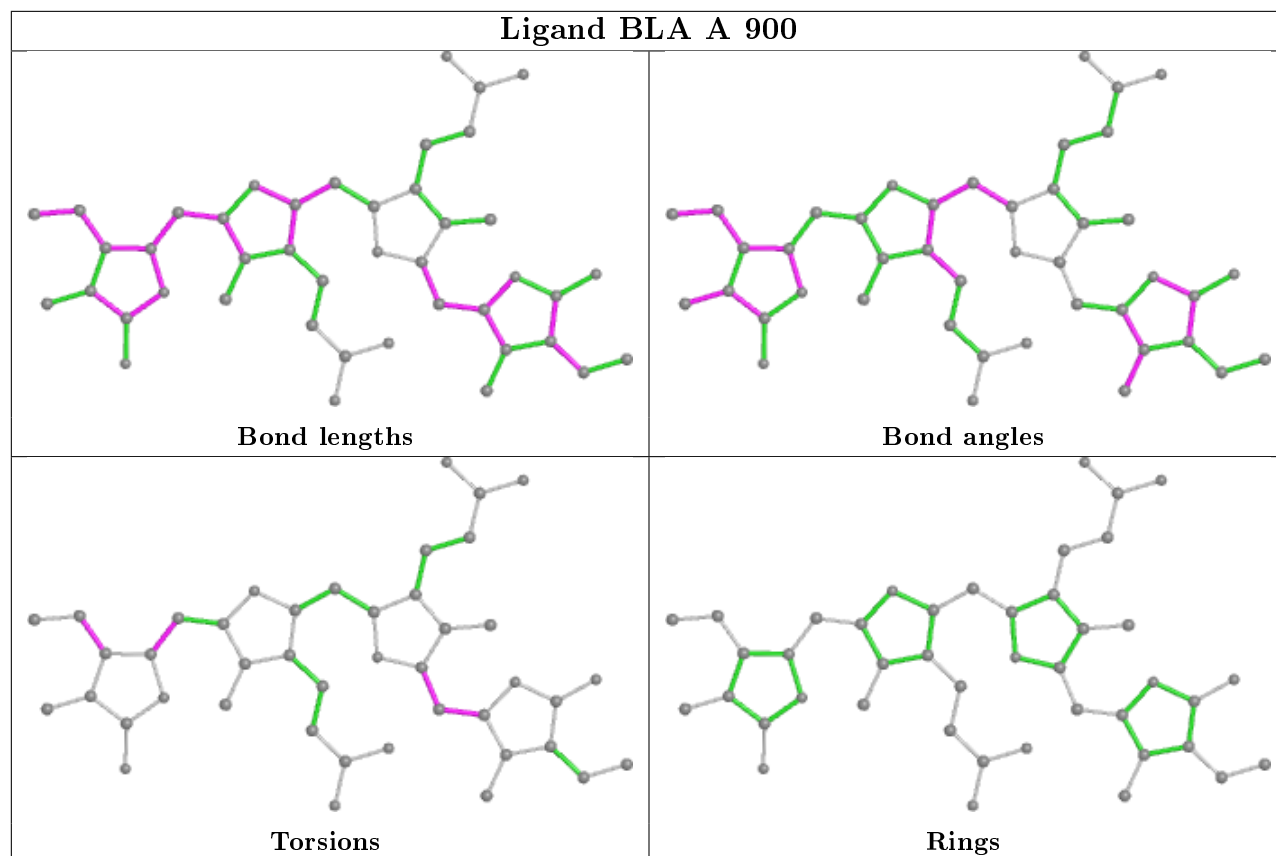
Ligand BLA E 900



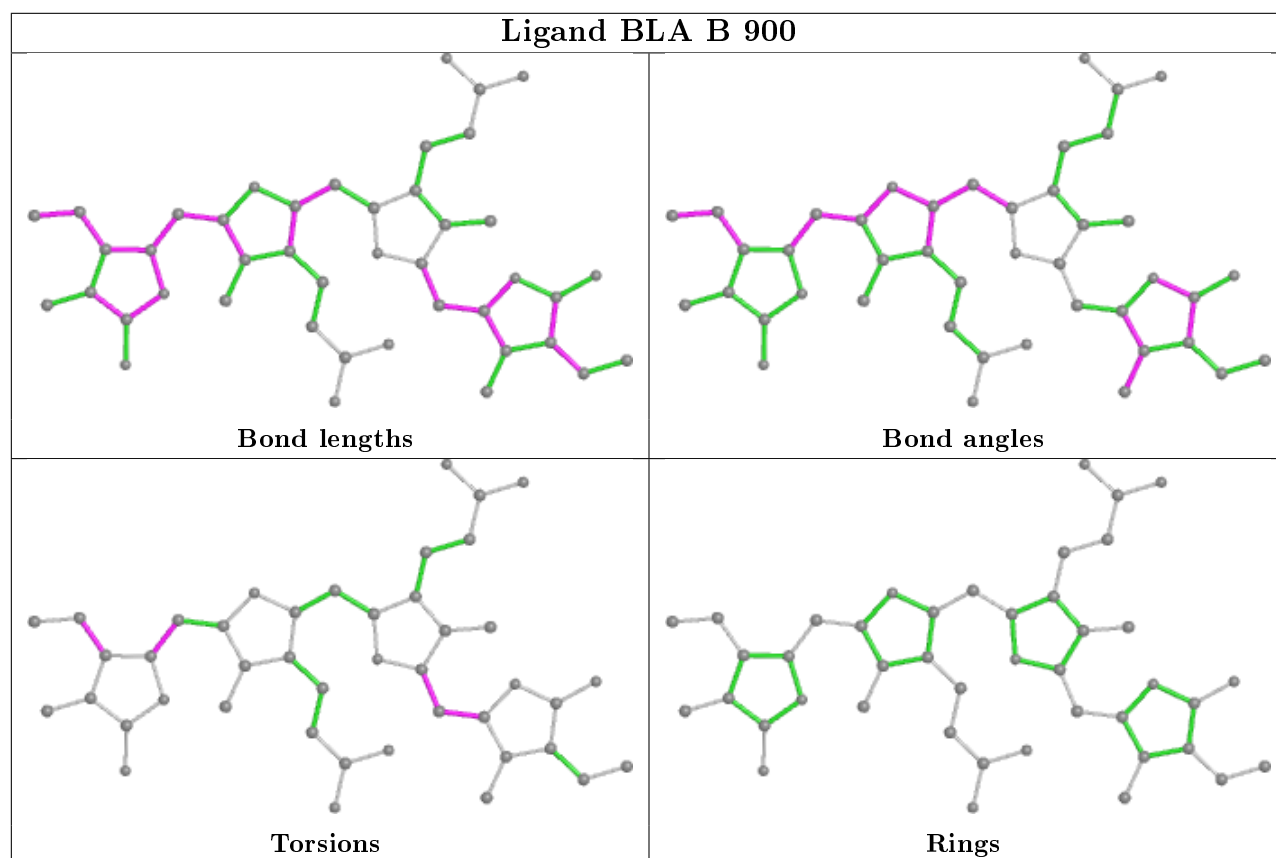
Ligand BLA F 900



Ligand BLA A 900



Ligand BLA B 900



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	479/505 (94%)	0.12	12 (2%) 57 63	37, 58, 109, 160	0
1	B	470/505 (93%)	0.68	42 (8%) 9 11	48, 88, 136, 183	0
1	C	482/505 (95%)	0.19	10 (2%) 63 70	39, 61, 102, 147	0
1	D	480/505 (95%)	0.62	46 (9%) 8 10	55, 92, 144, 191	0
1	E	479/505 (94%)	0.52	33 (6%) 16 20	49, 92, 134, 191	0
1	F	471/505 (93%)	0.58	54 (11%) 4 6	41, 81, 144, 171	0
1	G	482/505 (95%)	0.06	6 (1%) 79 84	37, 63, 105, 165	1 (0%)
1	H	481/505 (95%)	0.84	70 (14%) 2 3	55, 95, 158, 207	0
All	All	3824/4040 (94%)	0.45	273 (7%) 16 19	37, 79, 138, 207	1 (0%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	LEU	9.7
1	H	51	PHE	8.8
1	B	453	ARG	8.6
1	H	442	GLU	8.5
1	H	110	PHE	7.5
1	H	30	VAL	7.3
1	H	95	PHE	7.1
1	F	50	GLY	6.7
1	H	53	ALA	6.6
1	H	90	ILE	6.6
1	H	49	LEU	6.3
1	H	440	LYS	6.2
1	B	52	VAL	6.2
1	F	53	ALA	6.2
1	A	494	LEU	6.1
1	F	64	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	69	LEU	5.7
1	H	222	PHE	5.7
1	B	53	ALA	5.5
1	D	59	LEU	5.5
1	A	89	ARG	5.5
1	H	22	ALA	5.5
1	H	58	TYR	5.3
1	B	51	PHE	5.3
1	H	445	LEU	5.2
1	H	60	THR	5.1
1	H	230	ASN	5.1
1	B	332	ALA	5.0
1	H	231	GLU	4.8
1	H	223	PRO	4.8
1	F	51	PHE	4.8
1	E	214	VAL	4.8
1	H	91	GLY	4.7
1	B	331	ASP	4.7
1	C	494	LEU	4.7
1	H	227	PRO	4.7
1	A	445	LEU	4.7
1	H	32	LEU	4.6
1	B	59	LEU	4.6
1	D	90	ILE	4.6
1	A	330	ARG	4.6
1	D	51	PHE	4.6
1	B	468	ARG	4.5
1	F	89	ARG	4.5
1	A	93	HIS	4.5
1	F	30	VAL	4.5
1	F	222	PHE	4.5
1	B	58	TYR	4.4
1	B	224	ALA	4.3
1	D	64	VAL	4.3
1	D	53	ALA	4.3
1	B	69	LEU	4.3
1	F	32	LEU	4.2
1	D	66	PRO	4.2
1	E	494	LEU	4.2
1	H	28	ALA	4.2
1	F	90	ILE	4.2
1	H	29	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	63	GLN	4.1
1	E	330	ARG	4.1
1	A	90	ILE	4.1
1	H	45	ILE	4.1
1	F	49	LEU	4.0
1	F	225	LEU	4.0
1	H	52	VAL	4.0
1	H	89	ARG	4.0
1	B	496	HIS	4.0
1	D	49	LEU	3.9
1	H	233	PHE	3.9
1	F	45	ILE	3.8
1	E	454	LEU	3.8
1	D	30	VAL	3.8
1	H	94	LEU	3.8
1	H	47	ALA	3.7
1	B	9	LEU	3.7
1	E	230	ASN	3.6
1	F	33	ARG	3.6
1	B	62	GLU	3.6
1	D	48	LEU	3.6
1	B	222	PHE	3.6
1	B	93	HIS	3.6
1	H	64	VAL	3.6
1	H	39	LEU	3.6
1	D	444	LEU	3.6
1	F	58	TYR	3.5
1	C	441	PRO	3.5
1	D	116	ASP	3.5
1	D	432	VAL	3.5
1	E	384	ASP	3.5
1	H	220	ARG	3.4
1	B	36	GLY	3.4
1	C	442	GLU	3.4
1	F	29	LEU	3.4
1	F	233	PHE	3.4
1	A	329	ALA	3.3
1	H	93	HIS	3.3
1	B	55	PRO	3.3
1	E	221	VAL	3.3
1	H	115	ALA	3.3
1	H	419	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	221	VAL	3.3
1	D	95	PHE	3.3
1	F	115	ALA	3.3
1	C	53	ALA	3.3
1	B	29	LEU	3.2
1	F	34	ALA	3.2
1	F	395	TRP	3.2
1	H	439	GLY	3.2
1	D	467	VAL	3.2
1	D	32	LEU	3.2
1	G	444	LEU	3.2
1	D	62	GLU	3.1
1	H	42	SER	3.1
1	G	70	ARG	3.1
1	B	48	LEU	3.1
1	F	235	LEU	3.1
1	H	112	ILE	3.1
1	F	116	ASP	3.1
1	B	338	ALA	3.1
1	F	105	VAL	3.1
1	B	225	LEU	3.1
1	E	116	ASP	3.1
1	E	48	LEU	3.0
1	H	61	GLN	3.0
1	H	104	GLU	3.0
1	C	439	GLY	3.0
1	B	32	LEU	3.0
1	D	443	LYS	3.0
1	F	39	LEU	3.0
1	F	60	THR	3.0
1	A	442	GLU	3.0
1	D	52	VAL	3.0
1	E	445	LEU	3.0
1	D	440	LYS	3.0
1	D	9	LEU	3.0
1	D	114	THR	3.0
1	E	463	TRP	3.0
1	F	95	PHE	2.9
1	H	21	GLY	2.9
1	B	104	GLU	2.9
1	E	117	THR	2.9
1	D	61	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	37	MET	2.9
1	B	246	ILE	2.9
1	E	381	LEU	2.9
1	F	108	LEU	2.9
1	F	92	GLU	2.8
1	F	219	MET	2.8
1	H	219	MET	2.8
1	F	468	ARG	2.8
1	D	60	THR	2.8
1	F	59	LEU	2.8
1	H	92	GLU	2.8
1	B	49	LEU	2.8
1	C	406	GLY	2.8
1	H	46	GLN	2.8
1	B	460	PHE	2.8
1	B	235	LEU	2.7
1	H	116	ASP	2.7
1	E	383	ARG	2.7
1	H	98	ILE	2.7
1	F	334	ASP	2.7
1	B	446	THR	2.7
1	C	444	LEU	2.7
1	H	48	LEU	2.7
1	A	444	LEU	2.7
1	B	333	ASP	2.7
1	B	463	TRP	2.7
1	H	496	HIS	2.6
1	F	46	GLN	2.6
1	D	42	SER	2.6
1	F	229	THR	2.6
1	E	59	LEU	2.6
1	D	40	ALA	2.5
1	E	258	ALA	2.5
1	E	243	VAL	2.5
1	F	52	VAL	2.5
1	F	117	THR	2.5
1	H	235	LEU	2.5
1	B	450	SER	2.5
1	D	91	GLY	2.5
1	D	457	ARG	2.5
1	F	86	VAL	2.5
1	H	72	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	224	ALA	2.5
1	H	66	PRO	2.5
1	H	87	GLU	2.5
1	D	93	HIS	2.5
1	F	106	PHE	2.5
1	E	7	VAL	2.5
1	D	207	PRO	2.5
1	D	222	PHE	2.5
1	H	50	GLY	2.5
1	D	70	ARG	2.4
1	C	335	LEU	2.4
1	D	79	ASN	2.4
1	F	110	PHE	2.4
1	D	291	SER	2.4
1	B	469	GLY	2.4
1	H	74	GLU	2.4
1	G	332	ALA	2.4
1	F	227	PRO	2.3
1	C	128	GLN	2.3
1	D	63	GLN	2.3
1	E	5	THR	2.3
1	E	275	SER	2.3
1	B	39	LEU	2.3
1	H	69	LEU	2.3
1	F	40	ALA	2.3
1	H	443	LYS	2.3
1	D	112	ILE	2.3
1	F	41	ALA	2.3
1	E	233	PHE	2.3
1	H	108	LEU	2.3
1	B	447	ILE	2.2
1	A	180	GLU	2.2
1	H	179	ARG	2.2
1	G	299	CYS	2.2
1	E	279	MET	2.2
1	E	115	ALA	2.2
1	H	5	THR	2.2
1	A	493	CYS	2.2
1	E	256	VAL	2.2
1	E	466	VAL	2.2
1	F	38	VAL	2.2
1	H	97	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	40	ALA	2.2
1	F	94	LEU	2.2
1	F	57	SER	2.2
1	F	232	SER	2.2
1	H	418	ARG	2.2
1	D	294	ILE	2.2
1	F	224	ALA	2.2
1	D	72	LEU	2.2
1	B	296	SER	2.2
1	E	284	ILE	2.2
1	E	257	ARG	2.2
1	B	455	THR	2.1
1	D	211	ILE	2.1
1	H	31	THR	2.1
1	H	88	THR	2.1
1	B	207	PRO	2.1
1	E	274	PHE	2.1
1	F	62	GLU	2.1
1	H	107	TYR	2.1
1	H	229	THR	2.1
1	F	37	MET	2.1
1	E	222	PHE	2.1
1	H	43	GLU	2.1
1	F	7	VAL	2.1
1	B	31	THR	2.1
1	E	442	GLU	2.1
1	H	70	ARG	2.1
1	D	246	ILE	2.1
1	G	116	ASP	2.1
1	F	48	LEU	2.1
1	G	445	LEU	2.1
1	D	463	TRP	2.1
1	F	297	GLN	2.1
1	H	62	GLU	2.1
1	D	86	VAL	2.1
1	E	441	PRO	2.0
1	H	224	ALA	2.0
1	B	5	THR	2.0
1	A	492	LEU	2.0
1	D	361	GLY	2.0
1	C	207	PRO	2.0
1	F	230	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	58	TYR	2.0
1	D	97	VAL	2.0
1	D	89	ARG	2.0
1	B	182	LEU	2.0
1	E	281	PRO	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](#)

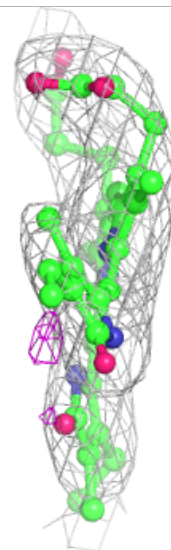
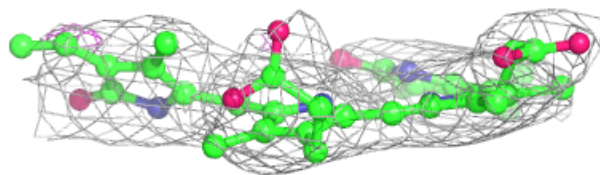
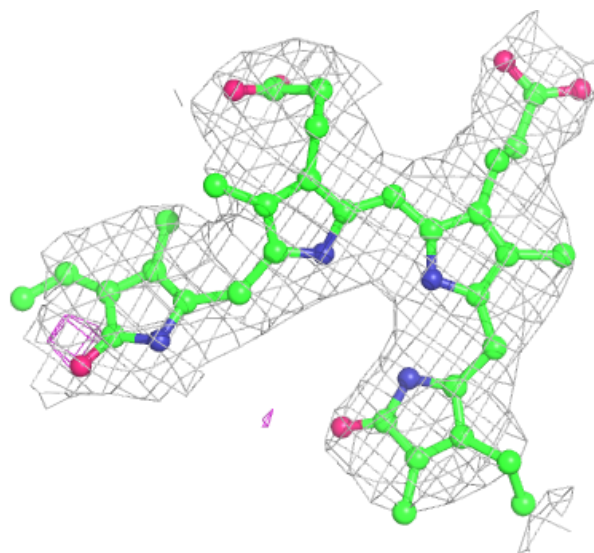
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BLA	H	900	43/43	0.92	0.21	64,83,93,105	0
2	BLA	E	900	43/43	0.93	0.31	72,92,104,113	0
2	BLA	B	900	43/43	0.93	0.21	60,76,95,107	0
2	BLA	D	900	43/43	0.94	0.17	62,81,95,101	0
2	BLA	G	900	43/43	0.95	0.18	37,58,68,89	0
2	BLA	F	900	43/43	0.96	0.17	39,60,70,84	0
2	BLA	A	900	43/43	0.96	0.17	34,49,64,77	0
2	BLA	C	900	43/43	0.96	0.18	34,54,68,85	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.

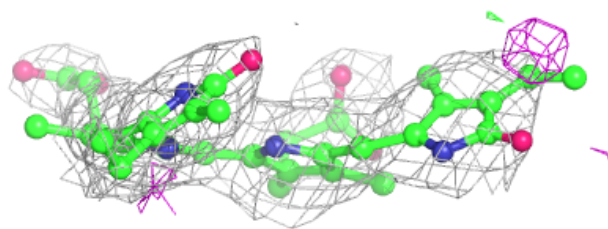
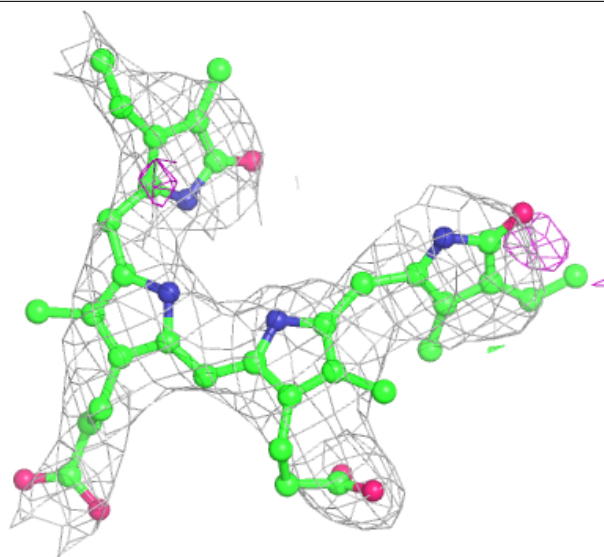
Electron density around BLA H 900:

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



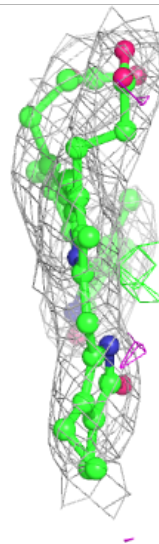
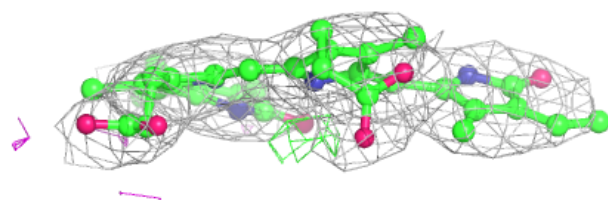
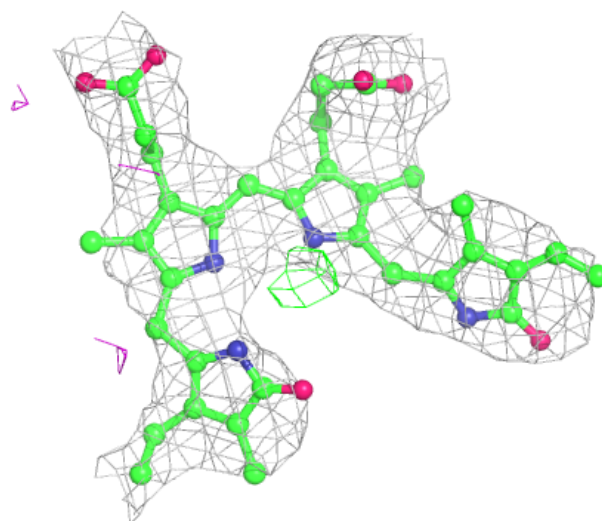
Electron density around BLA E 900:

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



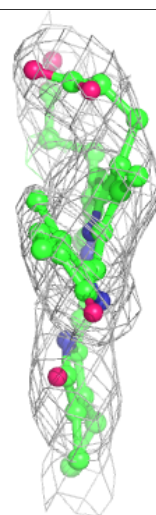
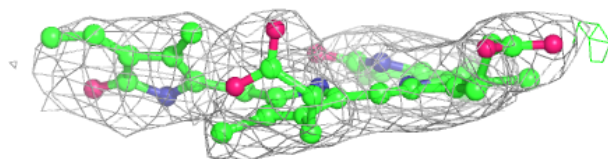
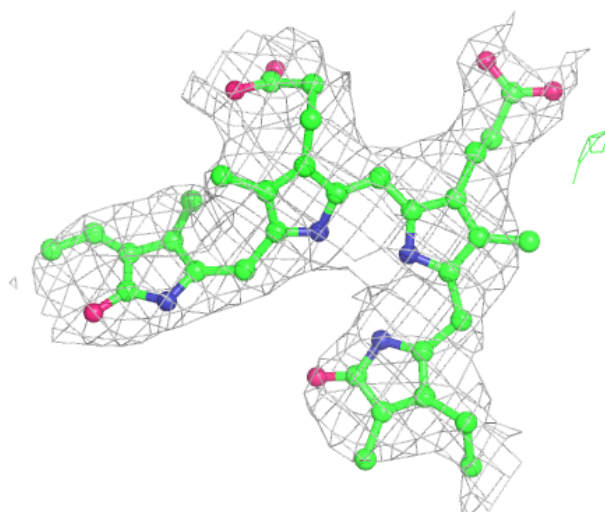
Electron density around BLA B 900:

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



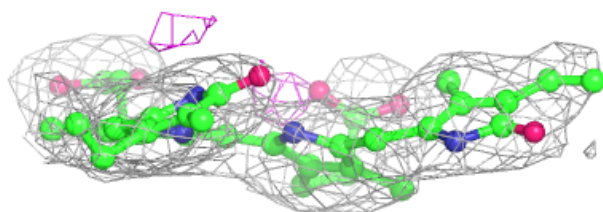
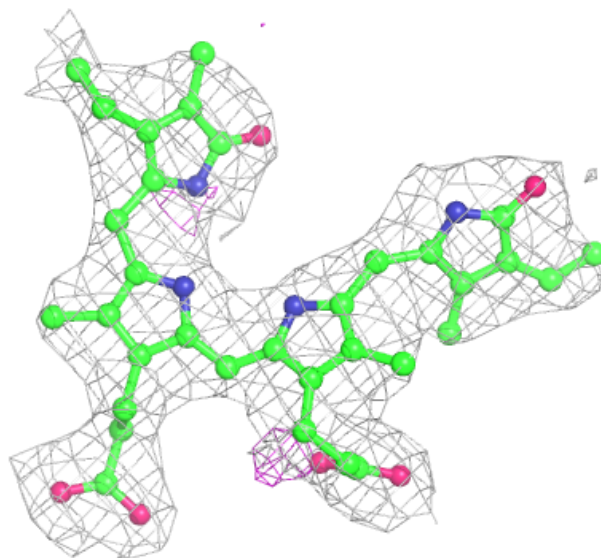
Electron density around BLA D 900:

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



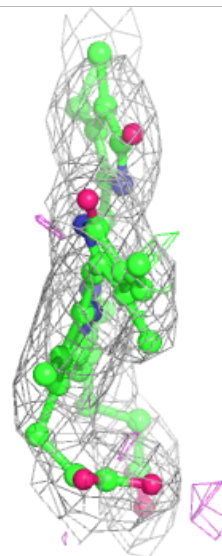
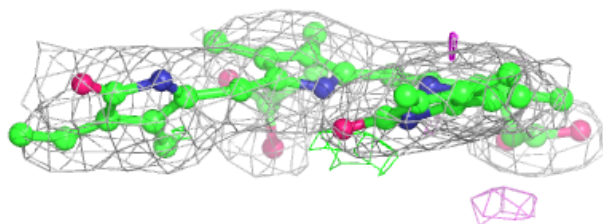
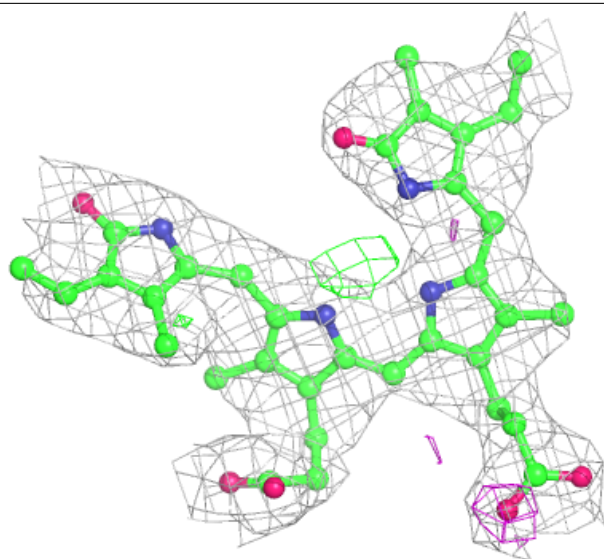
Electron density around BLA G 900:

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



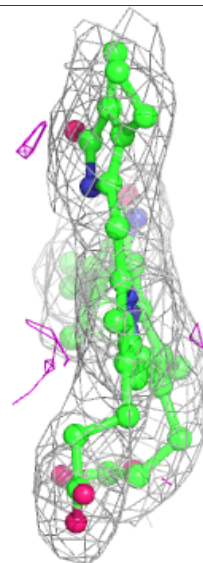
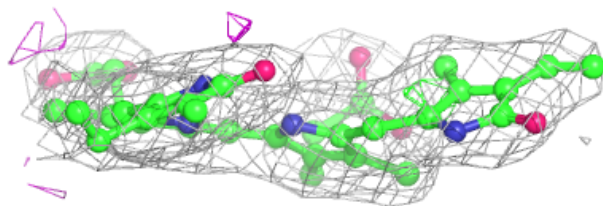
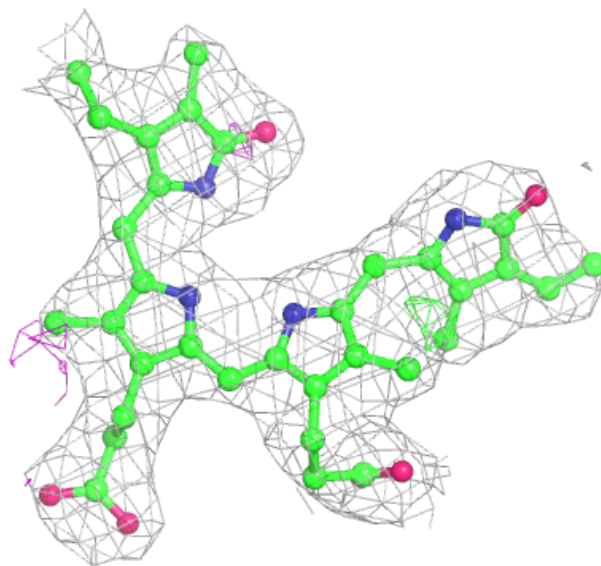
Electron density around BLA F 900:

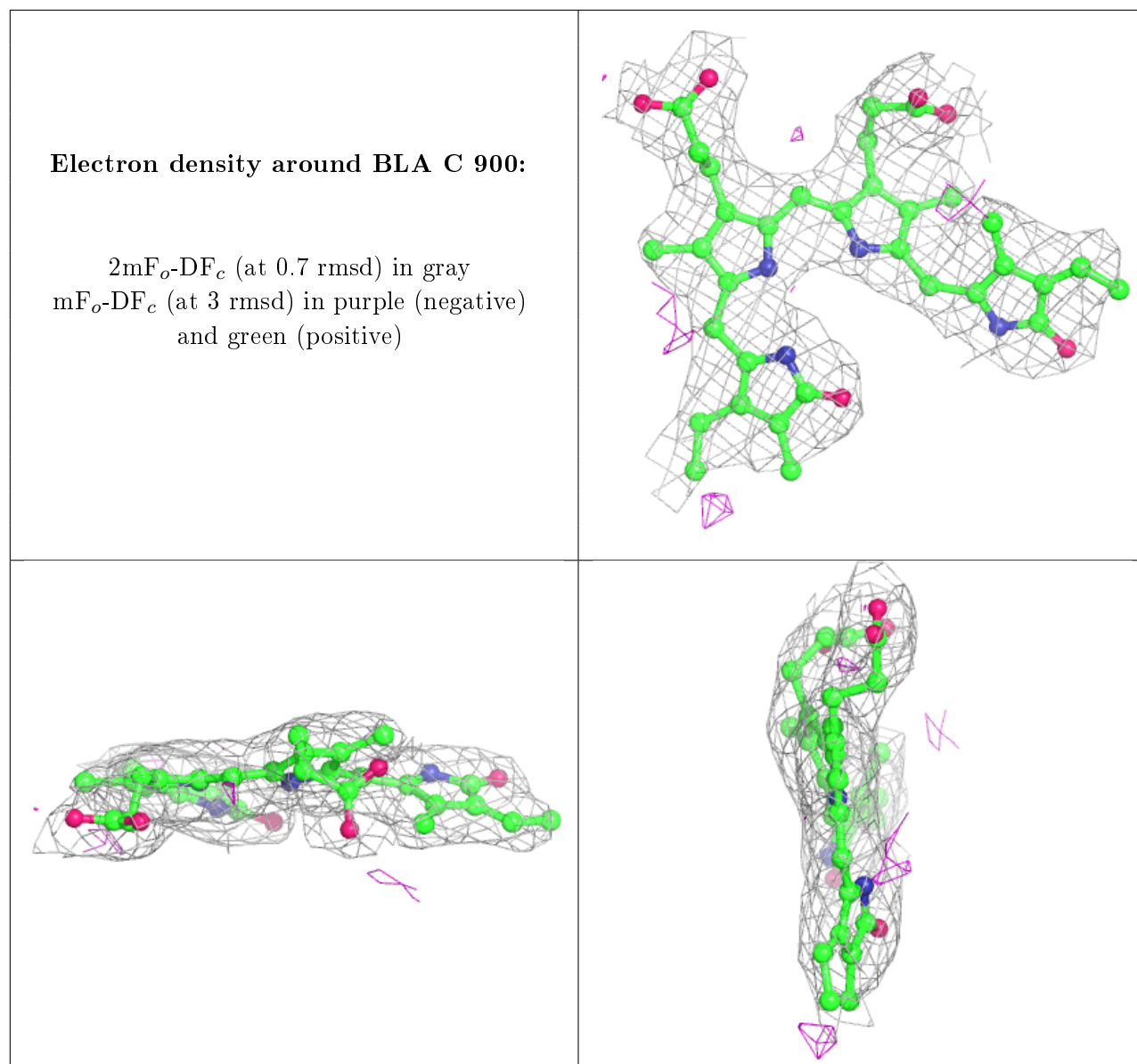
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLA A 900:

$2mF_o-DF_c$ (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.