Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 06:07 PM EDT

PDB ID	:	1SZZ
Title	:	Crystal structure of peptide deformylase from Leptospira Interrogans complexed with inhibitor actinonin
Authors	:	Zhou, Z.; Song, X.; Li, Y.; Gong, W.
Deposited on	:	2004-04-06
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

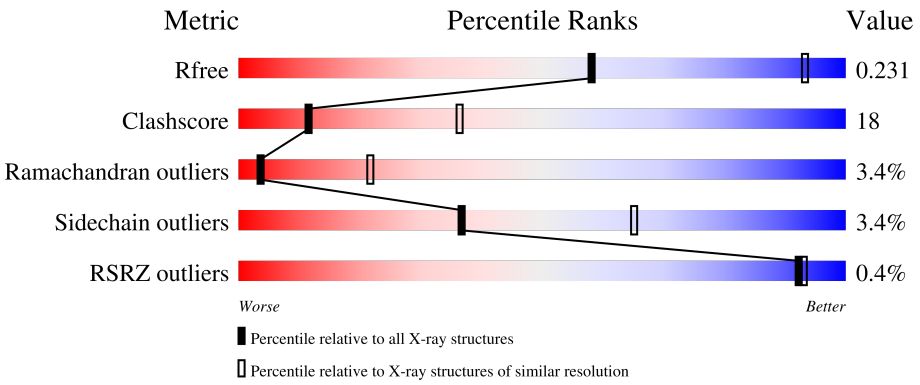
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	177	67% 26% • • •
1	B	177	61% 31% 5% • •
1	C	177	65% 29% • •
1	D	177	% 69% 23% • •
1	E	177	66% 28% • • •

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Mol	Chain	Length	Quality of chain
1	F	177	2% 66% 29%
1	G	177	62% 34%
1	H	177	69% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10753 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 Peptide deformylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1325	842	226	249	8	0	0	0
1	B	171	1321	841	225	247	8	0	0	0
1	C	171	1317	839	225	245	8	0	0	0
1	D	171	1319	838	228	245	8	0	0	0
1	E	171	1316	836	226	246	8	0	0	0
1	F	171	1310	834	225	243	8	0	0	0
1	G	171	1304	831	225	240	8	0	0	0
1	H	171	1304	831	225	240	8	0	0	0

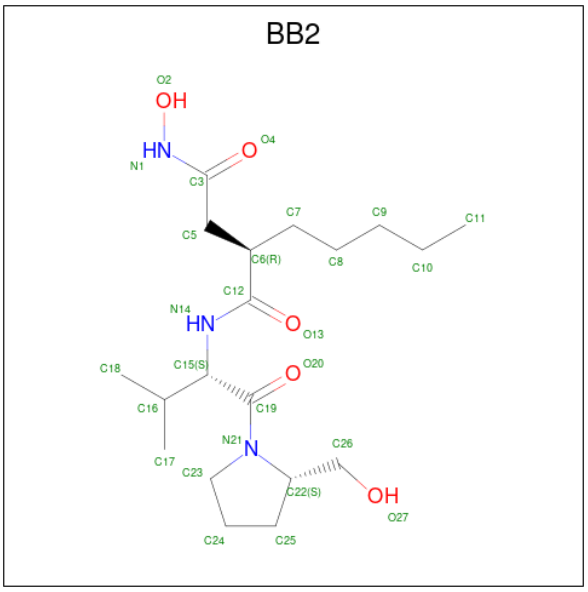
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	ASP	conflict	UNP Q93LE9
B	39	THR	ASP	conflict	UNP Q93LE9
C	39	THR	ASP	conflict	UNP Q93LE9
D	39	THR	ASP	conflict	UNP Q93LE9
E	39	THR	ASP	conflict	UNP Q93LE9
F	39	THR	ASP	conflict	UNP Q93LE9
G	39	THR	ASP	conflict	UNP Q93LE9
H	39	THR	ASP	conflict	UNP Q93LE9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0

- Molecule 3 is ACTINONIN (three-letter code: BB2) (formula: $C_{19}H_{35}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	19	3	5	0	0
3	B	1	27	19	3	5	0	0
3	C	1	27	19	3	5	0	0
3	D	1	27	19	3	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	E	1	27	19	3	5	0	0
3	F	1	27	19	3	5	0	0
3	G	1	27	19	3	5	0	0
3	H	1	27	19	3	5	0	0

- Molecule 4 is water.

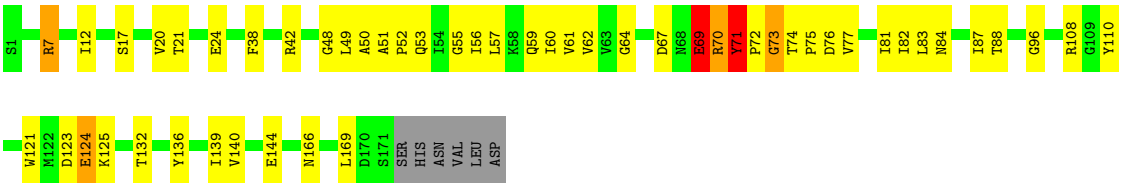
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	2	2	2	0	0
4	B	1	1	1	0	0
4	D	4	4	4	0	0
4	E	3	3	3	0	0
4	F	1	1	1	0	0
4	G	2	2	2	0	0

3 Residue-property plots (i)

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

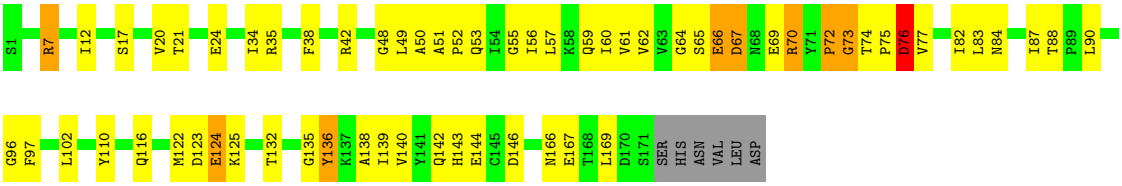
• Molecule 1: Peptide deformylase

Chain A:



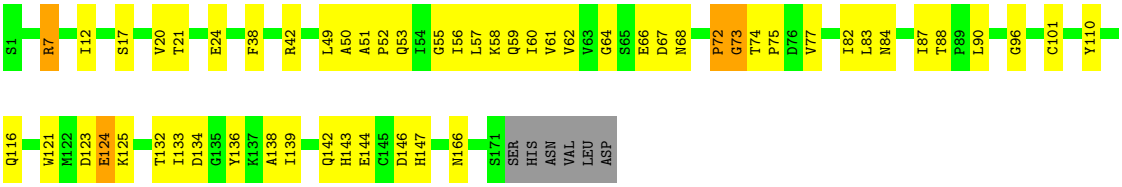
• Molecule 1: Peptide deformylase

Chain B:



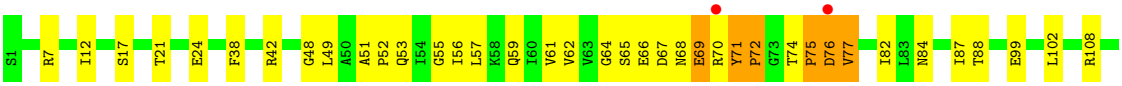
• Molecule 1: Peptide deformylase

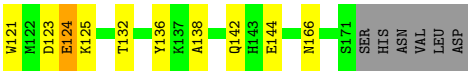
Chain C:



• Molecule 1: Peptide deformylase

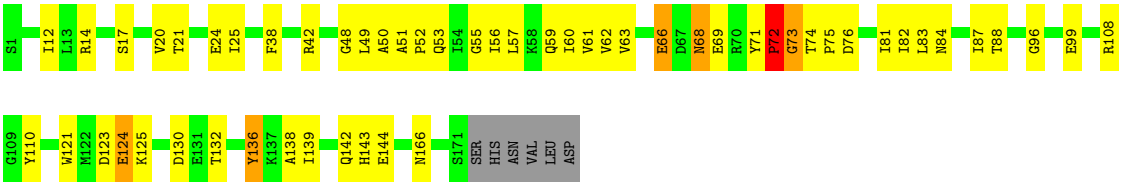
Chain D:





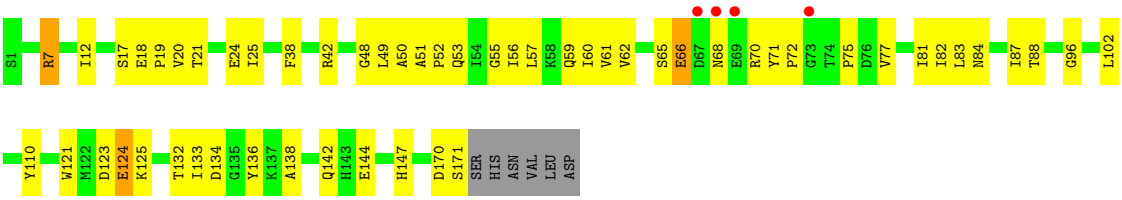
• Molecule 1: Peptide deformylase

Chain E:



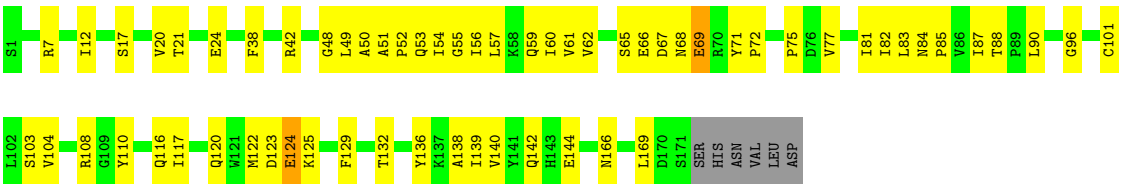
• Molecule 1: Peptide deformylase

Chain F:



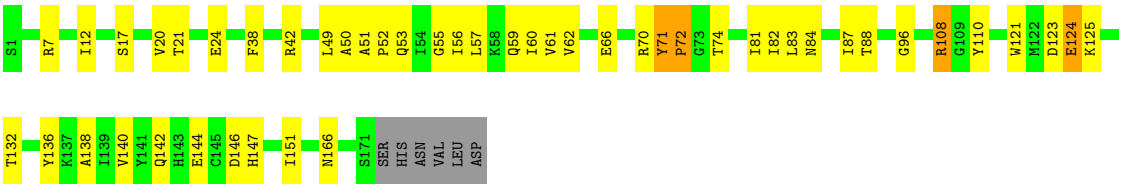
• Molecule 1: Peptide deformylase

Chain G:



• Molecule 1: Peptide deformylase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.49Å 118.93Å 95.76Å 90.00° 111.53° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 89.08 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.1 (20.00-3.30) 93.6 (89.08-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.33Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.241 0.235 , 0.231	Depositor DCC
R_{free} test set	1390 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	77.4	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BB2, ZN

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	0.50	0/1352	0.66	0/1834
1	B	0.51	0/1348	0.65	0/1829
1	C	0.53	1/1344 (0.1%)	0.66	0/1824
1	D	0.47	0/1345	0.66	0/1824
1	E	0.51	0/1342	0.67	0/1821
1	F	0.46	0/1336	0.65	0/1813
1	G	0.47	0/1330	0.67	0/1805
1	H	0.44	0/1330	0.64	0/1805
All	All	0.49	1/10727 (0.0%)	0.66	0/14555

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	CYS	CB-SG	-5.69	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1325	0	1289	47	0
1	B	1321	0	1288	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1317	0	1284	40	0
1	D	1319	0	1289	44	0
1	E	1316	0	1282	48	0
1	F	1310	0	1276	43	0
1	G	1304	0	1267	51	0
1	H	1304	0	1267	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	33	3	0
3	B	27	0	33	5	0
3	C	27	0	33	2	0
3	D	27	0	33	4	0
3	E	27	0	33	7	0
3	F	27	0	33	2	0
3	G	27	0	34	5	0
3	H	27	0	33	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	3	0
4	F	1	0	0	0	0
4	G	2	0	0	3	0
All	All	10753	0	10507	373	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 18.

All (373) 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:B:65:SER:HB3	1:B:77:VAL:H	1.08	1.16
1:B:65:SER:HB3	1:B:77:VAL:N	1.61	1.15
1:D:76:ASP:CG	1:D:77:VAL:H	1.70	0.91
1:A:108:ARG:HG3	1:A:166:ASN:HD21	1.39	0.86
1:G:108:ARG:HG3	1:G:166:ASN:ND2	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ASN:HA	4:G:724:HOH:O	1.77	0.83
1:G:108:ARG:HG3	1:G:166:ASN:HD21	1.44	0.82
1:H:61:VAL:HB	1:H:82:ILE:HB	1.64	0.80
1:E:99:GLU:HG2	3:E:517:BB2:C11	2.12	0.79
1:F:170:ASP:O	1:F:171:SER:HB2	1.81	0.79
1:D:21:THR:OG1	1:D:24:GLU:HG3	1.83	0.78
1:D:108:ARG:HG3	1:D:166:ASN:HD21	1.48	0.78
1:E:21:THR:OG1	1:E:24:GLU:HG3	1.84	0.78
1:B:21:THR:OG1	1:B:24:GLU:HG3	1.84	0.78
1:D:69:GLU:HG3	1:D:70:ARG:H	1.47	0.78
1:G:21:THR:OG1	1:G:24:GLU:HG3	1.84	0.77
1:F:61:VAL:HB	1:F:82:ILE:HB	1.66	0.77
1:C:21:THR:OG1	1:C:24:GLU:HG3	1.86	0.76
1:E:99:GLU:HG2	3:E:517:BB2:H111	1.68	0.76
1:G:139:ILE:HG22	3:G:519:BB2:H111	1.66	0.76
1:A:21:THR:OG1	1:A:24:GLU:HG3	1.87	0.75
1:H:59:GLN:HE21	1:H:84:ASN:HA	1.50	0.75
1:E:108:ARG:HG3	1:E:166:ASN:ND2	2.02	0.75
1:C:72:PRO:O	1:C:74:THR:N	2.20	0.75
1:G:61:VAL:HB	1:G:82:ILE:HB	1.68	0.74
1:H:21:THR:OG1	1:H:24:GLU:HG3	1.88	0.74
1:B:139:ILE:HG22	3:B:514:BB2:H111	1.70	0.74
1:E:20:VAL:HG23	1:E:84:ASN:HD21	1.52	0.73
1:H:20:VAL:HG23	1:H:84:ASN:HD21	1.54	0.73
1:E:63:VAL:N	4:E:721:HOH:O	2.23	0.72
1:B:65:SER:H	1:B:77:VAL:HB	1.55	0.72
1:F:21:THR:OG1	1:F:24:GLU:HG3	1.89	0.72
1:G:83:LEU:HB2	1:G:122:MET:O	1.90	0.72
1:B:72:PRO:C	1:B:74:THR:H	1.93	0.72
1:D:76:ASP:CG	1:D:77:VAL:N	2.43	0.71
1:C:59:GLN:HE21	1:C:84:ASN:HA	1.53	0.71
1:C:53:GLN:NE2	3:C:515:BB2:O2	2.23	0.70
1:E:61:VAL:HB	1:E:82:ILE:HB	1.73	0.70
1:B:61:VAL:HB	1:B:82:ILE:HB	1.74	0.70
1:A:61:VAL:HB	1:A:82:ILE:HB	1.74	0.69
1:D:74:THR:HB	1:D:75:PRO:HD2	1.76	0.68
1:H:108:ARG:HG2	1:H:166:ASN:ND2	2.07	0.68
1:B:56:ILE:N	1:B:56:ILE:HD12	2.08	0.68
1:B:72:PRO:O	1:B:74:THR:N	2.24	0.68
1:H:144:GLU:HA	1:H:144:GLU:OE2	1.94	0.67
1:B:75:PRO:O	1:B:76:ASP:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLU:HG2	3:D:516:BB2:H113	1.76	0.67
1:C:61:VAL:HB	1:C:82:ILE:HB	1.77	0.67
1:D:108:ARG:HG3	1:D:166:ASN:ND2	2.10	0.67
1:E:139:ILE:HG22	3:E:517:BB2:H112	1.76	0.67
1:F:49:LEU:HD12	1:F:53:GLN:OE1	1.94	0.66
1:G:59:GLN:HE21	1:G:84:ASN:HA	1.60	0.66
1:D:76:ASP:O	1:D:77:VAL:HG23	1.95	0.66
1:G:139:ILE:HG22	3:G:519:BB2:C11	2.26	0.65
1:F:56:ILE:HD12	1:F:56:ILE:N	2.12	0.65
1:A:56:ILE:HD12	1:A:56:ILE:N	2.12	0.65
1:A:12:ILE:HG23	1:A:57:LEU:HD11	1.79	0.65
1:C:56:ILE:HD12	1:C:56:ILE:N	2.10	0.65
1:B:144:GLU:OE2	1:B:144:GLU:HA	1.95	0.64
1:G:144:GLU:OE2	1:G:144:GLU:HA	1.98	0.64
1:G:56:ILE:N	1:G:56:ILE:HD12	2.12	0.63
1:E:56:ILE:N	1:E:56:ILE:HD12	2.13	0.63
1:B:65:SER:CB	1:B:77:VAL:H	1.99	0.63
1:F:20:VAL:HG23	1:F:84:ASN:HD21	1.63	0.63
1:H:56:ILE:HD12	1:H:56:ILE:N	2.15	0.62
1:F:57:LEU:N	1:F:57:LEU:HD12	2.13	0.62
1:F:144:GLU:HA	1:F:144:GLU:OE2	1.98	0.62
1:H:12:ILE:HG23	1:H:57:LEU:HD11	1.81	0.62
1:E:123:ASP:HB2	1:E:124:GLU:OE2	1.99	0.62
1:F:102:LEU:HG	3:F:518:BB2:H51	1.81	0.61
1:B:12:ILE:HG23	1:B:57:LEU:HD11	1.83	0.61
1:C:144:GLU:HA	1:C:144:GLU:OE2	1.98	0.61
1:A:71:TYR:C	1:A:73:GLY:H	2.04	0.61
1:B:139:ILE:HG22	3:B:514:BB2:C11	2.31	0.60
1:G:101:CYS:SG	1:G:103:SER:HB2	2.41	0.60
1:G:69:GLU:CB	1:G:72:PRO:HG3	2.31	0.60
1:F:71:TYR:N	1:F:72:PRO:HD3	2.16	0.59
1:A:108:ARG:HG3	1:A:166:ASN:ND2	2.13	0.59
1:D:144:GLU:OE2	1:D:144:GLU:HA	2.00	0.59
1:E:66:GLU:OE1	1:E:68:ASN:HB3	2.03	0.59
1:H:72:PRO:C	1:H:74:THR:H	2.05	0.59
1:A:139:ILE:HG22	3:A:513:BB2:C11	2.33	0.59
1:C:72:PRO:HG2	1:C:73:GLY:H	1.67	0.58
1:D:56:ILE:HD12	1:D:56:ILE:N	2.19	0.58
1:E:144:GLU:OE2	1:E:144:GLU:HA	2.02	0.58
1:B:65:SER:N	1:B:77:VAL:HB	2.19	0.58
1:F:65:SER:CB	1:F:77:VAL:H	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:SER:CB	1:G:77:VAL:H	2.17	0.58
1:D:49:LEU:HD12	1:D:53:GLN:OE1	2.04	0.58
1:D:57:LEU:N	1:D:57:LEU:HD12	2.18	0.57
1:D:66:GLU:O	1:D:68:ASN:N	2.32	0.57
1:D:12:ILE:HG23	1:D:57:LEU:HD11	1.85	0.57
1:A:71:TYR:N	1:A:72:PRO:CD	2.67	0.57
1:C:123:ASP:HB2	1:C:124:GLU:OE2	2.04	0.57
1:F:170:ASP:O	1:F:171:SER:CB	2.51	0.56
1:G:12:ILE:HG23	1:G:57:LEU:HD11	1.86	0.56
1:F:123:ASP:HB2	1:F:124:GLU:OE2	2.05	0.56
1:C:84:ASN:N	1:C:84:ASN:HD22	2.02	0.56
1:H:123:ASP:HB2	1:H:124:GLU:OE2	2.05	0.56
1:B:49:LEU:HD12	1:B:53:GLN:OE1	2.05	0.56
1:E:66:GLU:CD	1:E:68:ASN:HB3	2.25	0.56
1:G:51:ALA:N	1:G:52:PRO:HD2	2.20	0.56
1:C:90:LEU:HB2	1:C:116:GLN:HB3	1.88	0.56
1:E:73:GLY:O	1:E:75:PRO:HD3	2.05	0.56
1:A:59:GLN:HE21	1:A:84:ASN:HA	1.70	0.56
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.04	0.56
1:G:101:CYS:O	1:G:104:VAL:N	2.31	0.56
1:D:123:ASP:HB2	1:D:124:GLU:OE2	2.06	0.55
1:D:102:LEU:H	3:D:516:BB2:HN1	1.52	0.55
1:G:55:GLY:C	1:G:56:ILE:HD12	2.26	0.55
1:E:99:GLU:HG2	3:E:517:BB2:H113	1.88	0.55
1:A:123:ASP:HB2	1:A:124:GLU:OE2	2.06	0.55
1:C:12:ILE:HG23	1:C:57:LEU:HD11	1.88	0.55
1:G:123:ASP:HB2	1:G:124:GLU:OE2	2.05	0.55
1:E:62:VAL:HG13	4:E:721:HOH:O	2.07	0.55
1:B:60:ILE:HG12	1:B:83:LEU:CD2	2.38	0.54
1:G:129:PHE:HB2	4:G:723:HOH:O	2.07	0.54
1:E:12:ILE:HG23	1:E:57:LEU:HD11	1.88	0.54
1:A:140:VAL:HA	3:A:513:BB2:C11	2.36	0.54
1:E:57:LEU:HD12	1:E:57:LEU:N	2.23	0.54
1:A:20:VAL:HG23	1:A:84:ASN:HD21	1.73	0.54
1:G:57:LEU:HD12	1:G:57:LEU:N	2.22	0.54
1:B:84:ASN:N	1:B:84:ASN:HD22	2.05	0.54
1:B:97:PHE:HE2	3:B:514:BB2:H261	1.71	0.54
1:H:60:ILE:HG12	1:H:83:LEU:CD2	2.37	0.53
1:A:71:TYR:HB3	1:A:74:THR:CB	2.38	0.53
1:D:61:VAL:HB	1:D:82:ILE:HB	1.89	0.53
1:F:51:ALA:N	1:F:52:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:LEU:HD12	1:H:53:GLN:OE1	2.09	0.53
1:B:72:PRO:C	1:B:74:THR:N	2.61	0.53
1:F:84:ASN:HD22	1:F:84:ASN:N	2.04	0.53
1:G:60:ILE:HG12	1:G:83:LEU:CD2	2.38	0.53
1:G:84:ASN:N	1:G:84:ASN:HD22	2.05	0.53
1:G:20:VAL:HG23	1:G:84:ASN:HD21	1.74	0.53
1:B:59:GLN:HE21	1:B:84:ASN:HA	1.73	0.53
1:G:169:LEU:HB2	4:G:724:HOH:O	2.09	0.53
1:B:20:VAL:HG23	1:B:84:ASN:HD21	1.74	0.52
1:E:55:GLY:C	1:E:56:ILE:HD12	2.29	0.52
1:F:60:ILE:HG12	1:F:83:LEU:CD2	2.39	0.52
1:D:51:ALA:N	1:D:52:PRO:HD2	2.23	0.52
1:D:59:GLN:HE21	1:D:84:ASN:HA	1.75	0.52
1:F:59:GLN:HE21	1:F:84:ASN:HA	1.73	0.52
1:F:12:ILE:HG23	1:F:57:LEU:HD11	1.90	0.52
1:H:51:ALA:N	1:H:52:PRO:HD2	2.25	0.52
1:B:57:LEU:N	1:B:57:LEU:HD12	2.24	0.52
1:H:87:ILE:HG22	1:H:88:THR:N	2.24	0.52
1:H:42:ARG:HG3	1:H:42:ARG:HH11	1.75	0.52
1:B:72:PRO:HG2	1:B:73:GLY:H	1.75	0.52
1:A:84:ASN:HD22	1:A:84:ASN:N	2.07	0.51
1:C:96:GLY:HA3	1:C:110:TYR:OH	2.11	0.51
1:F:96:GLY:HA3	1:F:110:TYR:OH	2.10	0.51
1:G:140:VAL:HG22	3:G:519:BB2:H91	1.92	0.51
1:H:84:ASN:N	1:H:84:ASN:HD22	2.09	0.51
1:E:87:ILE:HG22	1:E:88:THR:N	2.26	0.51
1:G:144:GLU:OE1	3:G:519:BB2:N1	2.39	0.51
1:A:60:ILE:HG12	1:A:83:LEU:CD2	2.41	0.51
1:G:87:ILE:HG22	1:G:88:THR:N	2.25	0.51
1:H:55:GLY:C	1:H:56:ILE:HD12	2.32	0.51
1:A:69:GLU:O	1:A:70:ARG:O	2.28	0.51
1:D:68:ASN:O	1:D:69:GLU:CB	2.59	0.50
1:C:59:GLN:NE2	1:C:84:ASN:HA	2.25	0.50
1:G:84:ASN:N	1:G:84:ASN:ND2	2.59	0.50
1:C:87:ILE:HG22	1:C:88:THR:N	2.26	0.50
1:C:72:PRO:C	1:C:74:THR:H	2.14	0.50
1:D:138:ALA:O	1:D:142:GLN:HG3	2.11	0.50
1:F:70:ARG:C	1:F:72:PRO:HD3	2.32	0.50
1:G:87:ILE:CG2	1:G:88:THR:N	2.74	0.50
1:E:59:GLN:HE21	1:E:84:ASN:HA	1.76	0.50
1:C:57:LEU:HD12	1:C:57:LEU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:ALA:O	1:H:142:GLN:HG3	2.11	0.50
1:A:57:LEU:N	1:A:57:LEU:HD12	2.27	0.50
1:C:84:ASN:N	1:C:84:ASN:ND2	2.59	0.50
1:E:17:SER:HA	1:E:57:LEU:HB3	1.94	0.50
1:E:71:TYR:O	1:E:72:PRO:C	2.50	0.50
1:H:87:ILE:CG2	1:H:88:THR:N	2.75	0.50
1:B:123:ASP:HB2	1:B:124:GLU:OE2	2.12	0.49
1:E:87:ILE:CG2	1:E:88:THR:N	2.75	0.49
1:F:84:ASN:N	1:F:84:ASN:ND2	2.59	0.49
1:B:65:SER:N	1:B:77:VAL:O	2.44	0.49
1:B:84:ASN:N	1:B:84:ASN:ND2	2.60	0.49
1:D:102:LEU:N	3:D:516:BB2:O2	2.39	0.49
1:E:51:ALA:N	1:E:52:PRO:HD2	2.26	0.49
1:C:55:GLY:C	1:C:56:ILE:HD12	2.32	0.49
1:C:61:VAL:HG12	1:C:62:VAL:N	2.27	0.49
1:D:68:ASN:O	1:D:69:GLU:HB2	2.12	0.49
1:A:61:VAL:HG12	1:A:62:VAL:N	2.27	0.49
1:F:138:ALA:O	1:F:142:GLN:HG3	2.12	0.49
1:B:55:GLY:C	1:B:56:ILE:HD12	2.32	0.49
1:G:49:LEU:HD12	1:G:53:GLN:OE1	2.13	0.49
1:A:71:TYR:N	1:A:71:TYR:CD2	2.81	0.49
1:D:64:GLY:HA2	1:D:77:VAL:O	2.13	0.49
1:G:42:ARG:HG3	1:G:42:ARG:HH11	1.78	0.49
1:C:87:ILE:CG2	1:C:88:THR:N	2.76	0.49
1:A:55:GLY:C	1:A:56:ILE:HD12	2.34	0.48
1:B:7:ARG:HG3	1:B:7:ARG:HH11	1.78	0.48
1:E:108:ARG:HG3	1:E:166:ASN:HD21	1.76	0.48
1:D:65:SER:CB	1:D:76:ASP:O	2.61	0.48
1:D:70:ARG:O	1:D:71:TYR:CB	2.60	0.48
1:H:38:PHE:CZ	1:H:62:VAL:HG13	2.48	0.48
1:C:42:ARG:HG3	1:C:42:ARG:HH11	1.77	0.48
1:D:84:ASN:N	1:D:84:ASN:HD22	2.10	0.48
1:B:140:VAL:HA	3:B:514:BB2:H112	1.94	0.48
1:C:38:PHE:CZ	1:C:62:VAL:HG13	2.48	0.48
1:F:38:PHE:CZ	1:F:62:VAL:HG13	2.48	0.48
1:C:51:ALA:N	1:C:52:PRO:HD2	2.29	0.48
1:F:61:VAL:HG12	1:F:62:VAL:N	2.28	0.48
1:H:72:PRO:C	1:H:74:THR:N	2.66	0.48
1:B:138:ALA:O	1:B:142:GLN:HG3	2.14	0.47
1:E:42:ARG:HG3	1:E:42:ARG:HH11	1.79	0.47
1:E:143:HIS:CD2	3:E:517:BB2:N1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:N	1:A:52:PRO:HD2	2.29	0.47
1:A:71:TYR:C	1:A:73:GLY:N	2.67	0.47
1:B:90:LEU:HB2	1:B:116:GLN:HB3	1.95	0.47
1:B:51:ALA:N	1:B:52:PRO:HD2	2.29	0.47
1:C:138:ALA:O	1:C:142:GLN:HG3	2.14	0.47
1:E:84:ASN:N	1:E:84:ASN:HD22	2.10	0.47
1:D:71:TYR:O	1:D:72:PRO:C	2.53	0.47
1:G:96:GLY:HA3	1:G:110:TYR:OH	2.14	0.47
1:H:57:LEU:N	1:H:57:LEU:HD12	2.30	0.47
1:F:55:GLY:C	1:F:56:ILE:HD12	2.34	0.47
1:H:17:SER:HA	1:H:57:LEU:HB3	1.96	0.47
1:H:146:ASP:HB3	1:H:151:ILE:O	2.15	0.47
1:C:84:ASN:HD22	1:C:84:ASN:H	1.61	0.47
1:H:71:TYR:O	1:H:72:PRO:O	2.33	0.47
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.80	0.47
1:B:56:ILE:N	1:B:56:ILE:CD1	2.75	0.47
1:E:96:GLY:HA3	1:E:110:TYR:OH	2.15	0.47
1:D:48:GLY:HA2	1:D:62:VAL:O	2.15	0.46
1:C:49:LEU:HD12	1:C:53:GLN:OE1	2.15	0.46
1:F:48:GLY:HA2	1:F:62:VAL:O	2.15	0.46
1:H:96:GLY:HA3	1:H:110:TYR:OH	2.15	0.46
1:D:84:ASN:N	1:D:84:ASN:ND2	2.63	0.46
1:A:84:ASN:N	1:A:84:ASN:ND2	2.62	0.46
1:B:87:ILE:CG2	1:B:88:THR:N	2.79	0.46
1:C:60:ILE:HG12	1:C:83:LEU:CD2	2.45	0.46
1:A:87:ILE:HG22	1:A:88:THR:N	2.30	0.46
1:B:166:ASN:N	1:B:166:ASN:HD22	2.13	0.46
1:C:7:ARG:HG3	1:C:7:ARG:HH11	1.81	0.46
1:A:50:ALA:O	1:A:53:GLN:HB2	2.16	0.46
1:F:87:ILE:HG22	1:F:88:THR:N	2.30	0.46
1:G:84:ASN:HD22	1:G:84:ASN:H	1.64	0.46
1:A:70:ARG:C	1:A:71:TYR:CD2	2.89	0.46
1:B:87:ILE:HG22	1:B:88:THR:N	2.29	0.46
1:C:64:GLY:HA2	1:C:77:VAL:O	2.15	0.46
1:G:48:GLY:HA2	1:G:62:VAL:O	2.16	0.46
1:H:84:ASN:N	1:H:84:ASN:ND2	2.62	0.46
1:E:60:ILE:HG12	1:E:83:LEU:CD2	2.46	0.46
1:F:50:ALA:O	1:F:53:GLN:HB2	2.16	0.46
1:F:87:ILE:CG2	1:F:88:THR:N	2.78	0.46
1:H:70:ARG:O	1:H:71:TYR:CB	2.63	0.46
1:H:121:TRP:CE3	1:H:121:TRP:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD12	1:A:53:GLN:OE1	2.16	0.46
1:E:69:GLU:CB	1:E:74:THR:HG23	2.46	0.46
1:H:59:GLN:HB2	1:H:84:ASN:HD22	1.81	0.45
1:A:64:GLY:HA2	1:A:77:VAL:O	2.16	0.45
1:D:38:PHE:CZ	1:D:62:VAL:HG13	2.51	0.45
1:E:84:ASN:N	1:E:84:ASN:ND2	2.64	0.45
1:B:38:PHE:CZ	1:B:62:VAL:HG13	2.51	0.45
1:C:143:HIS:O	1:C:146:ASP:HB2	2.16	0.45
1:E:50:ALA:O	1:E:53:GLN:HB2	2.17	0.45
1:E:144:GLU:CD	3:E:517:BB2:HN1	2.18	0.45
1:G:38:PHE:CZ	1:G:62:VAL:HG13	2.50	0.45
1:H:61:VAL:HG12	1:H:62:VAL:N	2.32	0.45
1:E:138:ALA:O	1:E:142:GLN:HG3	2.16	0.45
1:A:87:ILE:CG2	1:A:88:THR:N	2.79	0.45
1:C:56:ILE:N	1:C:56:ILE:CD1	2.77	0.45
1:D:42:ARG:HG3	1:D:42:ARG:HH11	1.80	0.45
1:G:85:PRO:HA	1:G:120:GLN:O	2.16	0.45
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.82	0.45
1:E:48:GLY:HA2	1:E:62:VAL:O	2.17	0.45
1:F:56:ILE:N	1:F:56:ILE:CD1	2.78	0.45
1:G:138:ALA:O	1:G:142:GLN:HG3	2.17	0.45
1:H:147:HIS:NE2	3:H:520:BB2:O2	2.45	0.45
1:D:61:VAL:HG12	1:D:62:VAL:N	2.32	0.44
1:B:66:GLU:O	1:B:67:ASP:CB	2.64	0.44
1:B:96:GLY:HA3	1:B:110:TYR:OH	2.17	0.44
1:A:121:TRP:CE3	1:A:121:TRP:N	2.86	0.44
1:E:38:PHE:CZ	1:E:62:VAL:HG13	2.52	0.44
1:G:7:ARG:HH11	1:G:7:ARG:HG3	1.82	0.44
1:B:69:GLU:O	1:B:70:ARG:CB	2.65	0.44
1:B:83:LEU:HB2	1:B:122:MET:O	2.18	0.44
1:D:76:ASP:C	1:D:77:VAL:HG23	2.38	0.44
1:B:102:LEU:HG	3:B:514:BB2:H51	2.00	0.44
1:B:143:HIS:O	1:B:146:ASP:HB2	2.17	0.44
1:H:20:VAL:HG23	1:H:84:ASN:ND2	2.29	0.44
1:H:56:ILE:N	1:H:56:ILE:CD1	2.80	0.44
1:E:20:VAL:HG23	1:E:84:ASN:ND2	2.28	0.44
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.88	0.43
1:C:166:ASN:N	1:C:166:ASN:HD22	2.15	0.43
1:E:61:VAL:HG12	1:E:62:VAL:N	2.32	0.43
1:F:7:ARG:HG3	1:F:7:ARG:HH11	1.82	0.43
1:G:81:ILE:HB	1:G:124:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:SER:O	1:B:66:GLU:C	2.56	0.43
1:F:42:ARG:HH11	1:F:42:ARG:HG3	1.82	0.43
1:C:20:VAL:HG23	1:C:84:ASN:HD21	1.84	0.43
1:G:50:ALA:O	1:G:53:GLN:HB2	2.18	0.43
1:H:108:ARG:HG2	1:H:166:ASN:HD21	1.77	0.43
1:B:65:SER:CB	1:B:77:VAL:HB	2.48	0.43
1:A:56:ILE:N	1:A:56:ILE:CD1	2.80	0.43
1:A:81:ILE:HD12	1:A:81:ILE:N	2.34	0.43
1:D:87:ILE:HG22	1:D:88:THR:N	2.33	0.43
1:G:56:ILE:N	1:G:56:ILE:CD1	2.79	0.43
1:E:25:ILE:C	1:E:25:ILE:HD12	2.39	0.43
1:F:17:SER:HA	1:F:57:LEU:HB3	1.99	0.43
1:F:84:ASN:HD22	1:F:84:ASN:H	1.64	0.43
1:B:17:SER:HA	1:B:57:LEU:HB3	2.00	0.43
1:B:34:ILE:O	1:B:35:ARG:C	2.56	0.43
1:B:61:VAL:HG12	1:B:62:VAL:N	2.34	0.43
1:D:7:ARG:HG3	1:D:7:ARG:HH11	1.84	0.43
1:E:81:ILE:N	1:E:81:ILE:HD12	2.34	0.43
1:G:87:ILE:HG23	1:G:117:ILE:HB	1.99	0.43
1:B:84:ASN:HD22	1:B:84:ASN:H	1.66	0.43
1:F:147:HIS:CD2	3:F:518:BB2:O2	2.72	0.43
1:D:87:ILE:CG2	1:D:88:THR:N	2.82	0.42
1:A:17:SER:HA	1:A:57:LEU:HB3	2.01	0.42
1:A:71:TYR:O	1:A:73:GLY:N	2.40	0.42
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.87	0.42
1:D:55:GLY:C	1:D:56:ILE:HD12	2.38	0.42
1:E:14:ARG:NE	4:E:723:HOH:O	2.41	0.42
1:E:56:ILE:N	1:E:56:ILE:CD1	2.79	0.42
1:F:81:ILE:HD12	1:F:81:ILE:N	2.35	0.42
1:G:90:LEU:HB2	1:G:116:GLN:HB3	2.00	0.42
1:A:48:GLY:HA2	1:A:62:VAL:O	2.19	0.42
1:A:96:GLY:HA3	1:A:110:TYR:OH	2.18	0.42
1:A:7:ARG:HG3	1:A:7:ARG:HH11	1.83	0.42
1:C:133:ILE:HG22	1:C:134:ASP:N	2.35	0.42
1:D:17:SER:HA	1:D:57:LEU:HB3	2.02	0.42
1:G:65:SER:CB	1:G:77:VAL:N	2.82	0.42
1:H:140:VAL:HG22	3:H:520:BB2:H113	2.02	0.42
1:G:38:PHE:HE1	1:G:81:ILE:HD11	1.85	0.42
1:B:7:ARG:HG3	1:B:7:ARG:NH1	2.34	0.42
1:A:38:PHE:CZ	1:A:62:VAL:HG13	2.55	0.42
1:A:140:VAL:HA	3:A:513:BB2:H111	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLY:O	1:B:136:TYR:C	2.59	0.41
1:D:76:ASP:O	1:D:77:VAL:CG2	2.65	0.41
1:H:7:ARG:HG3	1:H:7:ARG:HH11	1.84	0.41
1:A:74:THR:HA	1:A:75:PRO:HD2	1.94	0.41
1:C:58:LYS:O	1:C:60:ILE:N	2.53	0.41
1:F:57:LEU:N	1:F:57:LEU:CD1	2.81	0.41
1:G:61:VAL:HG12	1:G:62:VAL:N	2.36	0.41
1:C:139:ILE:HG22	3:C:515:BB2:C11	2.51	0.41
1:D:121:TRP:N	1:D:121:TRP:CE3	2.89	0.41
1:H:51:ALA:HB2	1:H:60:ILE:HB	2.03	0.41
1:A:70:ARG:O	1:A:71:TYR:CB	2.68	0.41
1:F:121:TRP:N	1:F:121:TRP:CE3	2.89	0.41
1:F:60:ILE:HG12	1:F:83:LEU:HD22	2.02	0.41
3:E:517:BB2:N14	3:E:517:BB2:H82	2.36	0.41
1:F:66:GLU:H	1:F:66:GLU:HG2	1.60	0.41
1:G:17:SER:HA	1:G:57:LEU:HB3	2.03	0.41
1:B:48:GLY:HA2	1:B:62:VAL:O	2.21	0.41
1:C:17:SER:HA	1:C:57:LEU:HB3	2.01	0.41
1:E:121:TRP:N	1:E:121:TRP:CE3	2.89	0.41
1:E:136:TYR:O	1:E:139:ILE:HB	2.21	0.41
1:G:51:ALA:O	1:G:54:ILE:CG1	2.69	0.41
1:H:81:ILE:HD12	1:H:81:ILE:N	2.35	0.41
1:B:166:ASN:O	1:B:167:GLU:C	2.59	0.41
1:D:56:ILE:N	1:D:56:ILE:CD1	2.84	0.41
1:D:99:GLU:HG2	3:D:516:BB2:C11	2.47	0.40
1:E:49:LEU:HD12	1:E:53:GLN:OE1	2.20	0.40
3:H:520:BB2:H231	3:H:520:BB2:H173	2.02	0.40
1:A:84:ASN:HD22	1:A:84:ASN:H	1.69	0.40
1:F:25:ILE:HD12	1:F:25:ILE:C	2.42	0.40
1:A:69:GLU:C	1:A:70:ARG:O	2.59	0.40
1:B:50:ALA:O	1:B:53:GLN:HB2	2.20	0.40
1:B:166:ASN:N	1:B:166:ASN:ND2	2.69	0.40
1:G:139:ILE:CG2	3:G:519:BB2:H111	2.43	0.40
1:C:50:ALA:O	1:C:53:GLN:HB2	2.21	0.40
1:E:84:ASN:HD22	1:E:84:ASN:H	1.69	0.40
1:F:133:ILE:HG22	1:F:134:ASP:N	2.37	0.40
1:C:121:TRP:CE3	1:C:121:TRP:N	2.89	0.40
1:F:18:GLU:HB2	1:F:19:PRO:HD2	2.04	0.40
1:G:66:GLU:O	1:G:68:ASN:N	2.54	0.40
1:H:50:ALA:O	1:H:53:GLN:HB2	2.21	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	169/177 (96%)	145 (86%)	19 (11%)	5 (3%)	4	24
1	B	169/177 (96%)	145 (86%)	16 (10%)	8 (5%)	2	14
1	C	169/177 (96%)	143 (85%)	19 (11%)	7 (4%)	3	17
1	D	169/177 (96%)	145 (86%)	16 (10%)	8 (5%)	2	14
1	E	169/177 (96%)	143 (85%)	21 (12%)	5 (3%)	4	24
1	F	169/177 (96%)	145 (86%)	20 (12%)	4 (2%)	6	28
1	G	169/177 (96%)	145 (86%)	19 (11%)	5 (3%)	4	24
1	H	169/177 (96%)	146 (86%)	19 (11%)	4 (2%)	6	28
All	All	1352/1416 (96%)	1157 (86%)	149 (11%)	46 (3%)	3	22

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	B	66	GLU
1	B	67	ASP
1	B	72	PRO
1	B	76	ASP
1	C	73	GLY
1	D	69	GLU
1	D	71	TYR
1	D	77	VAL
1	E	66	GLU
1	E	72	PRO
1	F	66	GLU
1	G	67	ASP
1	G	75	PRO
1	H	71	TYR
1	H	72	PRO
1	A	69	GLU

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Mol	Chain	Res	Type
1	A	70	ARG
1	A	136	TYR
1	B	73	GLY
1	C	68	ASN
1	C	72	PRO
1	D	67	ASP
1	D	75	PRO
1	D	76	ASP
1	F	75	PRO
1	B	136	TYR
1	C	75	PRO
1	C	136	TYR
1	D	72	PRO
1	D	136	TYR
1	F	136	TYR
1	B	70	ARG
1	C	67	ASP
1	E	136	TYR
1	G	69	GLU
1	G	71	TYR
1	G	136	TYR
1	H	66	GLU
1	H	136	TYR
1	C	66	GLU
1	F	68	ASN
1	E	130	ASP
1	A	73	GLY
1	E	73	GLY
1	B	64	GLY

5.3.2 Protein sidechains (i)

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	141/159 (89%)	133 (94%)	8 (6%)	20	51
1	B	140/159 (88%)	135 (96%)	5 (4%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	139/159 (87%)	134 (96%)	5 (4%)	35	63
1	D	139/159 (87%)	136 (98%)	3 (2%)	52	74
1	E	139/159 (87%)	133 (96%)	6 (4%)	29	59
1	F	137/159 (86%)	133 (97%)	4 (3%)	42	69
1	G	135/159 (85%)	132 (98%)	3 (2%)	52	74
1	H	135/159 (85%)	131 (97%)	4 (3%)	41	68
All	All	1105/1272 (87%)	1067 (97%)	38 (3%)	37	65

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	67	ASP
1	A	69	GLU
1	A	71	TYR
1	A	76	ASP
1	A	124	GLU
1	A	125	LYS
1	A	132	THR
1	B	7	ARG
1	B	76	ASP
1	B	124	GLU
1	B	125	LYS
1	B	132	THR
1	C	7	ARG
1	C	124	GLU
1	C	125	LYS
1	C	132	THR
1	C	147	HIS
1	D	124	GLU
1	D	125	LYS
1	D	132	THR
1	E	68	ASN
1	E	72	PRO
1	E	76	ASP
1	E	124	GLU
1	E	125	LYS
1	E	132	THR
1	F	7	ARG
1	F	124	GLU

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Mol	Chain	Res	Type
1	F	125	LYS
1	F	132	THR
1	G	124	GLU
1	G	125	LYS
1	G	132	THR
1	H	108	ARG
1	H	124	GLU
1	H	125	LYS
1	H	132	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	68	ASN
1	A	84	ASN
1	A	166	ASN
1	B	59	GLN
1	B	84	ASN
1	B	166	ASN
1	C	59	GLN
1	C	84	ASN
1	C	166	ASN
1	D	59	GLN
1	D	84	ASN
1	D	166	ASN
1	E	59	GLN
1	E	68	ASN
1	E	84	ASN
1	E	147	HIS
1	E	166	ASN
1	F	59	GLN
1	F	84	ASN
1	F	166	ASN
1	G	59	GLN
1	G	84	ASN
1	G	166	ASN
1	H	59	GLN
1	H	84	ASN
1	H	166	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BB2	B	514	2	27,27,27	1.86	3 (11%)	34,35,35	1.41	3 (8%)
3	BB2	C	515	2	27,27,27	1.91	3 (11%)	34,35,35	1.60	7 (20%)
3	BB2	H	520	2	27,27,27	1.75	3 (11%)	34,35,35	1.34	4 (11%)
3	BB2	D	516	2	27,27,27	1.95	4 (14%)	34,35,35	1.45	5 (14%)
3	BB2	A	513	2	27,27,27	1.70	3 (11%)	34,35,35	1.61	5 (14%)
3	BB2	F	518	2	27,27,27	1.85	3 (11%)	34,35,35	1.33	4 (11%)
3	BB2	G	519	2	27,27,27	2.11	6 (22%)	34,35,35	1.47	4 (11%)
3	BB2	E	517	2	27,27,27	1.91	3 (11%)	34,35,35	1.60	7 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BB2	B	514	2	-	7/33/43/43	0/1/1/1
3	BB2	C	515	2	-	11/33/43/43	0/1/1/1
3	BB2	H	520	2	-	6/33/43/43	0/1/1/1
3	BB2	D	516	2	-	7/33/43/43	0/1/1/1
3	BB2	A	513	2	-	6/33/43/43	0/1/1/1
3	BB2	F	518	2	-	5/33/43/43	0/1/1/1
3	BB2	G	519	2	-	3/33/43/43	0/1/1/1
3	BB2	E	517	2	-	11/33/43/43	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	515	BB2	O2-N1	-7.49	1.21	1.40
3	E	517	BB2	O2-N1	-7.49	1.21	1.40
3	F	518	BB2	O2-N1	-7.48	1.21	1.40
3	H	520	BB2	O2-N1	-7.11	1.22	1.40
3	D	516	BB2	O2-N1	-7.08	1.22	1.40
3	B	514	BB2	O2-N1	-7.06	1.22	1.40
3	A	513	BB2	O2-N1	-6.81	1.22	1.40
3	G	519	BB2	O2-N1	-6.76	1.22	1.40
3	G	519	BB2	C5-C6	4.95	1.63	1.53
3	B	514	BB2	O27-C26	-3.90	1.25	1.42
3	F	518	BB2	O27-C26	-3.77	1.26	1.42
3	D	516	BB2	O27-C26	-3.68	1.26	1.42
3	D	516	BB2	C6-C12	3.67	1.58	1.51
3	A	513	BB2	O27-C26	-3.59	1.27	1.42
3	D	516	BB2	C5-C6	3.53	1.60	1.53
3	H	520	BB2	O27-C26	-3.41	1.28	1.42
3	F	518	BB2	C5-C6	3.34	1.60	1.53
3	E	517	BB2	O27-C26	-3.29	1.28	1.42
3	C	515	BB2	O27-C26	-3.28	1.28	1.42
3	G	519	BB2	O27-C26	-3.24	1.28	1.42
3	B	514	BB2	C5-C6	3.20	1.60	1.53
3	G	519	BB2	C5-C3	3.12	1.58	1.51
3	C	515	BB2	C5-C6	2.98	1.59	1.53
3	E	517	BB2	C5-C6	2.97	1.59	1.53
3	G	519	BB2	C3-N1	2.91	1.35	1.32
3	H	520	BB2	C5-C6	2.75	1.59	1.53
3	A	513	BB2	C5-C6	2.60	1.58	1.53
3	G	519	BB2	C6-C12	2.53	1.56	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	517	BB2	C5-C6-C12	5.77	118.12	109.77
3	C	515	BB2	C5-C6-C12	5.77	118.12	109.77
3	D	516	BB2	C5-C6-C12	4.85	116.80	109.77
3	B	514	BB2	C5-C6-C12	4.78	116.69	109.77
3	A	513	BB2	C5-C6-C12	4.75	116.65	109.77
3	A	513	BB2	C5-C3-N1	4.07	121.30	115.14
3	G	519	BB2	C5-C6-C12	4.01	115.57	109.77
3	G	519	BB2	O2-N1-C3	3.80	125.41	119.79
3	F	518	BB2	O4-C3-C5	-3.75	116.01	121.50
3	B	514	BB2	C5-C3-N1	3.72	120.78	115.14
3	A	513	BB2	O4-C3-C5	-3.45	116.45	121.50
3	G	519	BB2	C5-C3-N1	3.38	120.27	115.14
3	E	517	BB2	C5-C3-N1	3.37	120.25	115.14
3	H	520	BB2	O4-C3-C5	-3.37	116.56	121.50
3	C	515	BB2	C5-C3-N1	3.37	120.24	115.14
3	G	519	BB2	O4-C3-C5	-3.36	116.57	121.50
3	D	516	BB2	C5-C3-N1	3.35	120.22	115.14
3	H	520	BB2	C5-C6-C12	3.34	114.61	109.77
3	H	520	BB2	O2-N1-C3	3.32	124.70	119.79
3	H	520	BB2	C5-C3-N1	3.15	119.91	115.14
3	F	518	BB2	C5-C3-N1	3.12	119.86	115.14
3	F	518	BB2	O2-N1-C3	3.10	124.37	119.79
3	F	518	BB2	C5-C6-C12	3.08	114.23	109.77
3	D	516	BB2	O2-N1-C3	3.06	124.31	119.79
3	A	513	BB2	C15-N14-C12	2.89	129.26	121.89
3	D	516	BB2	O4-C3-C5	-2.86	117.30	121.50
3	A	513	BB2	O2-N1-C3	2.81	123.95	119.79
3	B	514	BB2	O4-C3-C5	-2.79	117.41	121.50
3	E	517	BB2	O4-C3-C5	-2.47	117.88	121.50
3	C	515	BB2	O4-C3-C5	-2.42	117.95	121.50
3	C	515	BB2	O2-N1-C3	2.32	123.21	119.79
3	E	517	BB2	O2-N1-C3	2.30	123.20	119.79
3	E	517	BB2	O27-C26-C22	2.21	120.28	111.50
3	C	515	BB2	O27-C26-C22	2.20	120.26	111.50
3	E	517	BB2	C16-C15-C19	2.13	115.04	110.73
3	C	515	BB2	C16-C15-C19	2.13	115.02	110.73
3	C	515	BB2	C15-N14-C12	2.05	127.13	121.89
3	E	517	BB2	C15-N14-C12	2.05	127.12	121.89
3	D	516	BB2	C7-C6-C5	-2.03	102.83	109.85

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	513	BB2	C3-C5-C6-C12
3	A	513	BB2	C3-C5-C6-C7
3	B	514	BB2	C19-C15-C16-C17
3	C	515	BB2	C3-C5-C6-C12
3	C	515	BB2	C3-C5-C6-C7
3	C	515	BB2	N21-C22-C26-O27
3	C	515	BB2	C25-C22-C26-O27
3	D	516	BB2	C3-C5-C6-C12
3	D	516	BB2	C3-C5-C6-C7
3	D	516	BB2	N21-C22-C26-O27
3	D	516	BB2	C25-C22-C26-O27
3	E	517	BB2	C3-C5-C6-C12
3	E	517	BB2	C3-C5-C6-C7
3	E	517	BB2	N21-C22-C26-O27
3	E	517	BB2	C25-C22-C26-O27
3	F	518	BB2	N21-C22-C26-O27
3	F	518	BB2	C25-C22-C26-O27
3	G	519	BB2	C3-C5-C6-C7
3	B	514	BB2	N14-C15-C16-C18
3	B	514	BB2	N14-C15-C16-C17
3	B	514	BB2	C19-C15-C16-C18
3	H	520	BB2	N14-C15-C16-C18
3	H	520	BB2	C19-C15-C16-C18
3	H	520	BB2	C19-C15-C16-C17
3	C	515	BB2	N14-C15-C16-C18
3	E	517	BB2	N14-C15-C16-C18
3	B	514	BB2	O13-C12-N14-C15
3	D	516	BB2	O13-C12-N14-C15
3	A	513	BB2	C7-C8-C9-C10
3	H	520	BB2	N14-C15-C16-C17
3	C	515	BB2	N14-C15-C16-C17
3	E	517	BB2	N14-C15-C16-C17
3	B	514	BB2	C6-C12-N14-C15
3	D	516	BB2	C6-C12-N14-C15
3	C	515	BB2	C11-C10-C9-C8
3	E	517	BB2	C11-C10-C9-C8
3	C	515	BB2	C19-C15-C16-C18
3	E	517	BB2	C19-C15-C16-C18
3	G	519	BB2	C11-C10-C9-C8
3	C	515	BB2	C19-C15-C16-C17
3	E	517	BB2	C19-C15-C16-C17
3	H	520	BB2	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	H	520	BB2	C7-C8-C9-C10
3	D	516	BB2	C11-C10-C9-C8
3	B	514	BB2	C11-C10-C9-C8
3	F	518	BB2	C7-C8-C9-C10
3	F	518	BB2	O4-C3-C5-C6
3	F	518	BB2	N1-C3-C5-C6
3	G	519	BB2	O4-C3-C5-C6
3	A	513	BB2	C11-C10-C9-C8
3	A	513	BB2	O13-C12-C6-C5
3	C	515	BB2	O13-C12-C6-C5
3	E	517	BB2	O13-C12-C6-C5
3	A	513	BB2	N14-C12-C6-C7
3	C	515	BB2	N14-C12-C6-C7
3	E	517	BB2	N14-C12-C6-C7

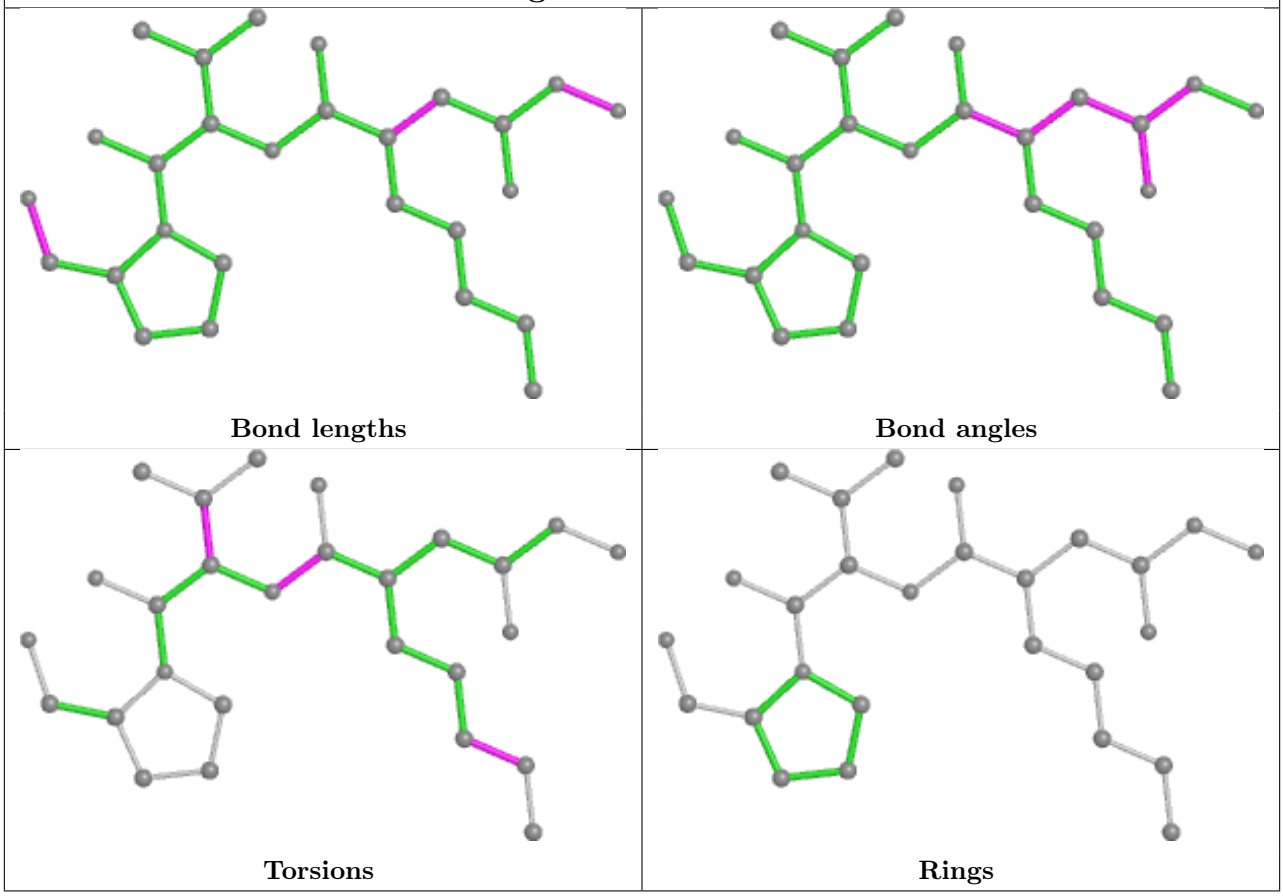
There are no ring outliers.

8 monomers are involved in 31 short contacts:

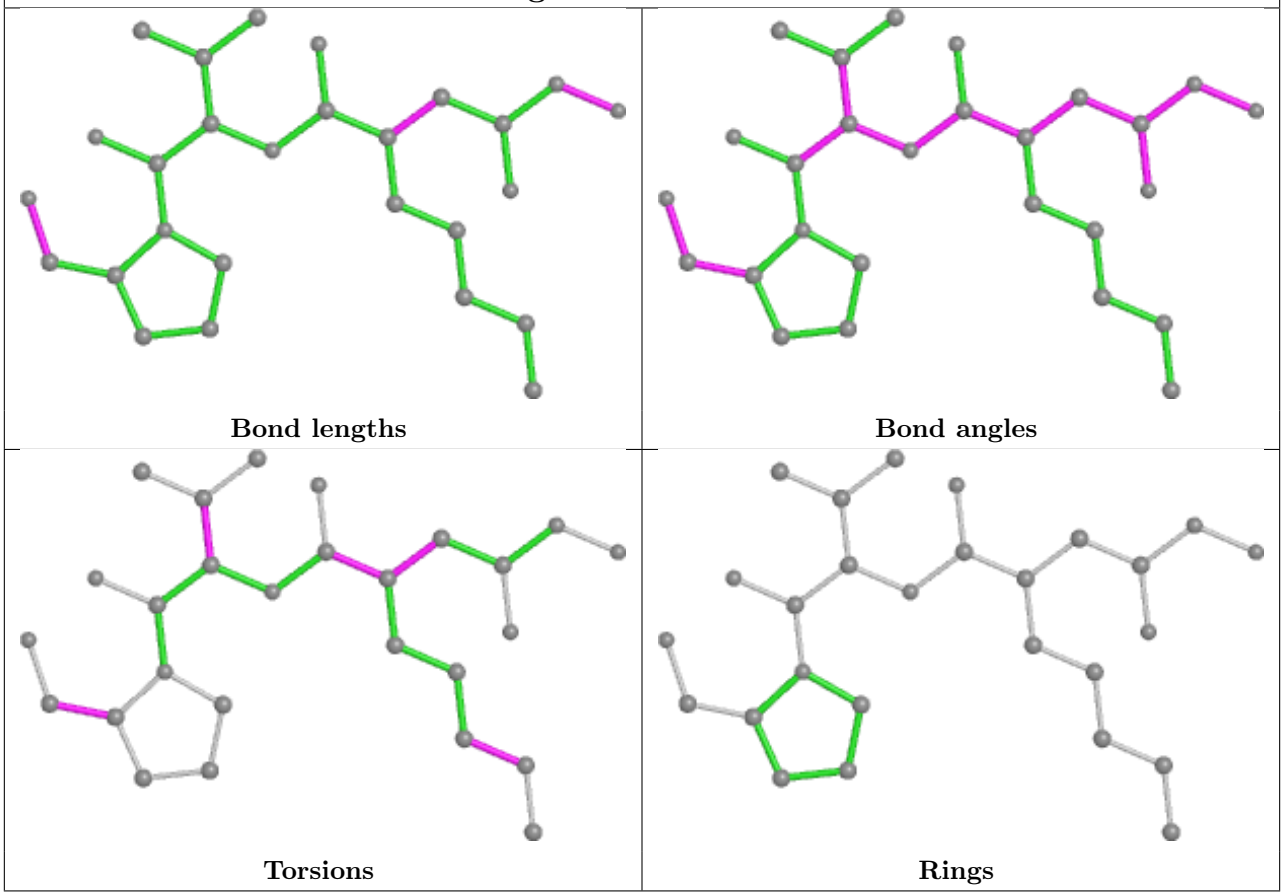
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	514	BB2	5	0
3	C	515	BB2	2	0
3	H	520	BB2	3	0
3	D	516	BB2	4	0
3	A	513	BB2	3	0
3	F	518	BB2	2	0
3	G	519	BB2	5	0
3	E	517	BB2	7	0

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 then 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.

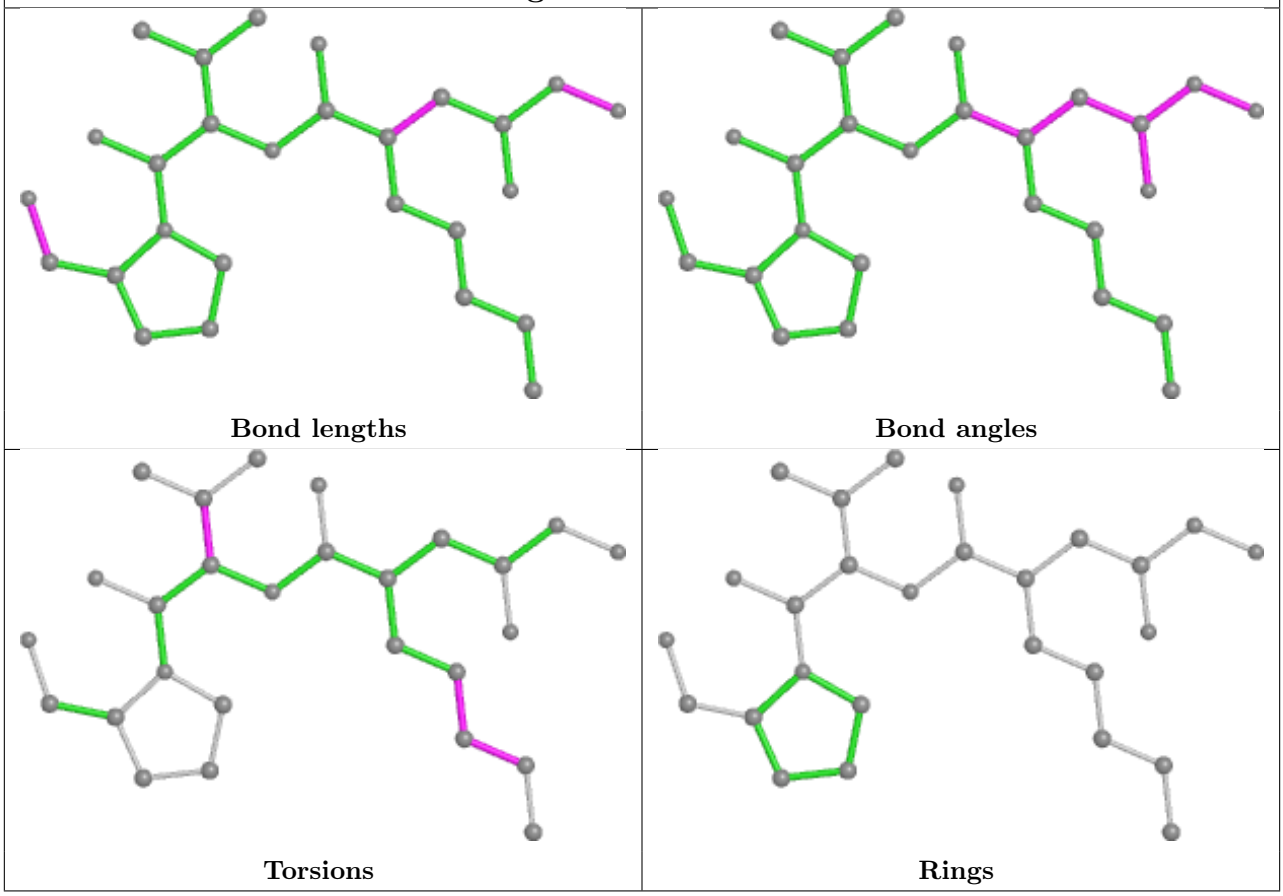
Ligand BB2 B 514



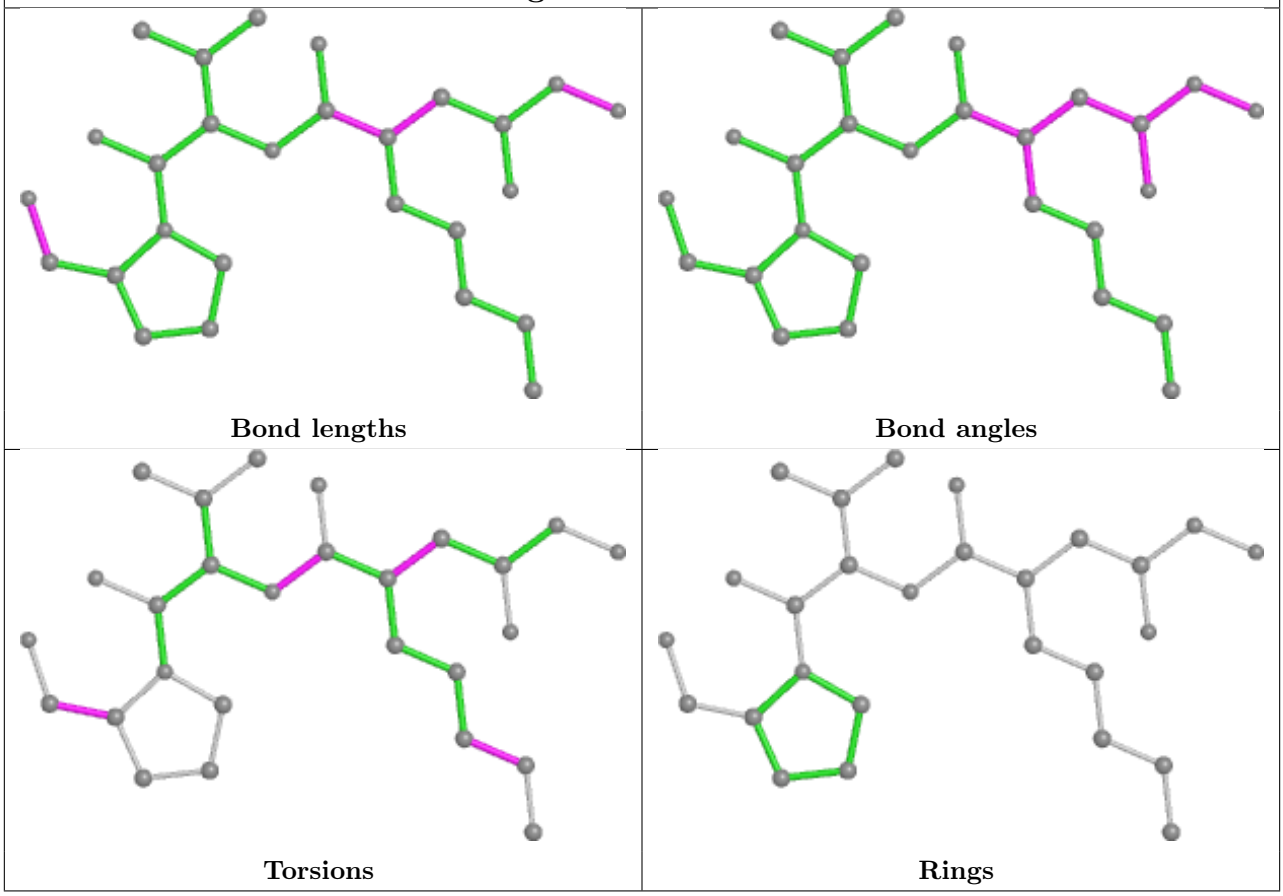
Ligand BB2 C 515



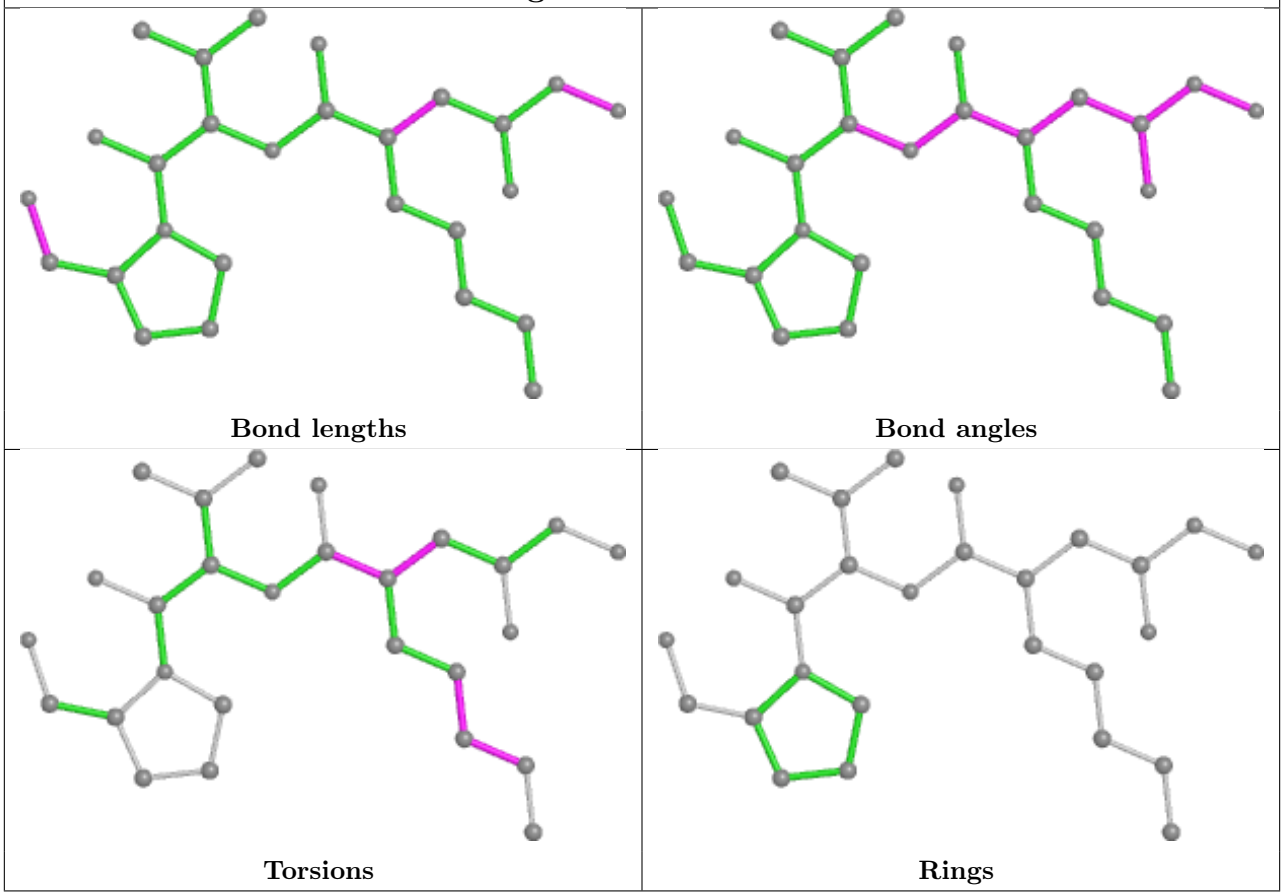
Ligand BB2 H 520



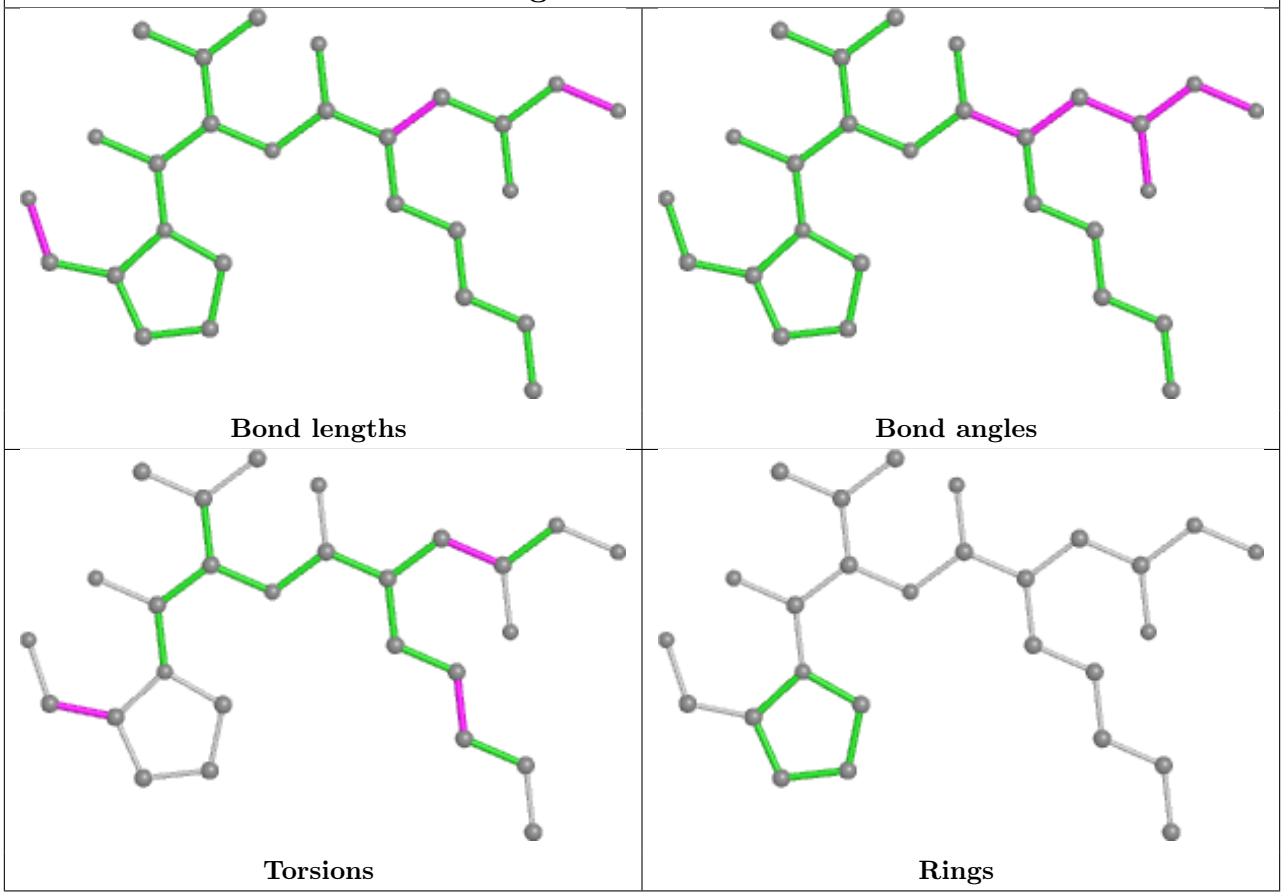
Ligand BB2 D 516



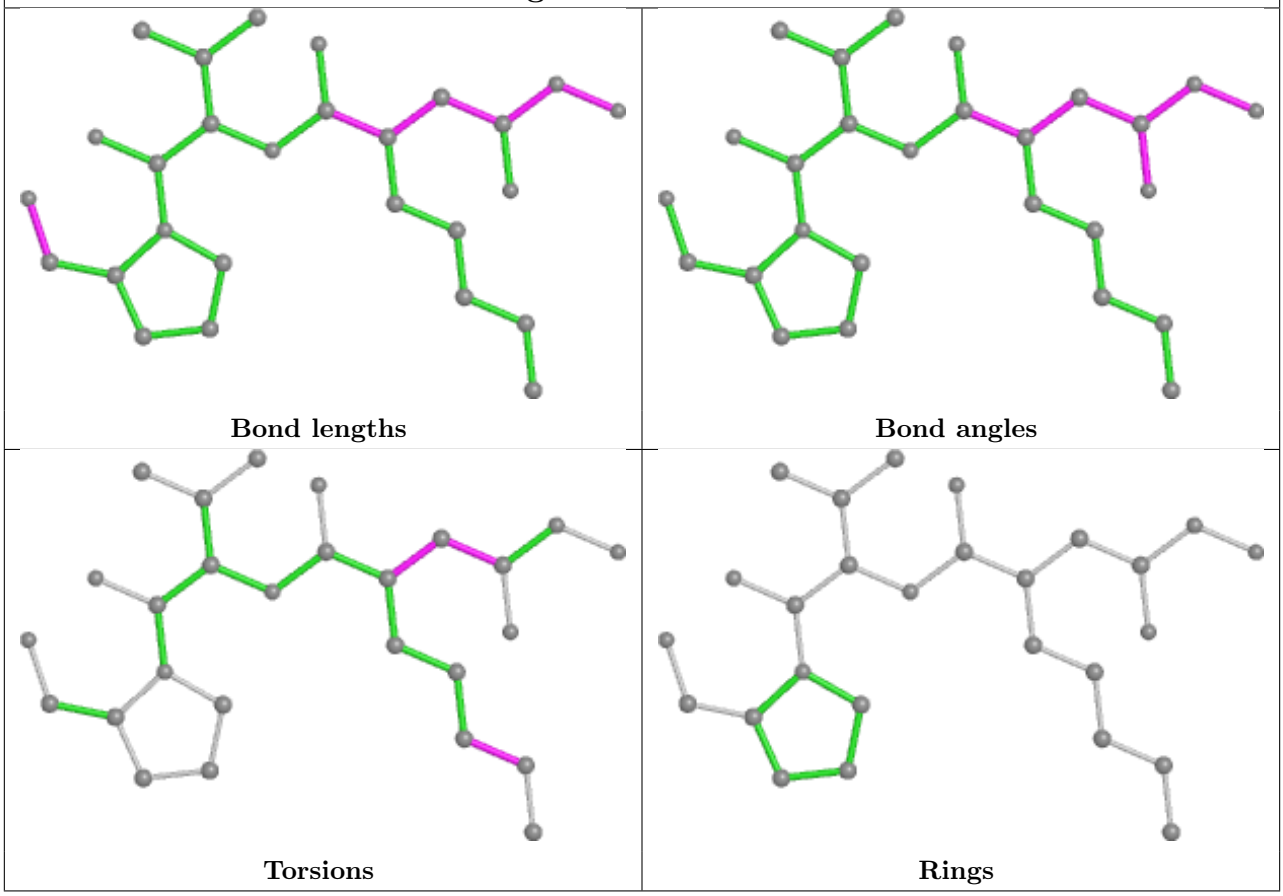
Ligand BB2 A 513

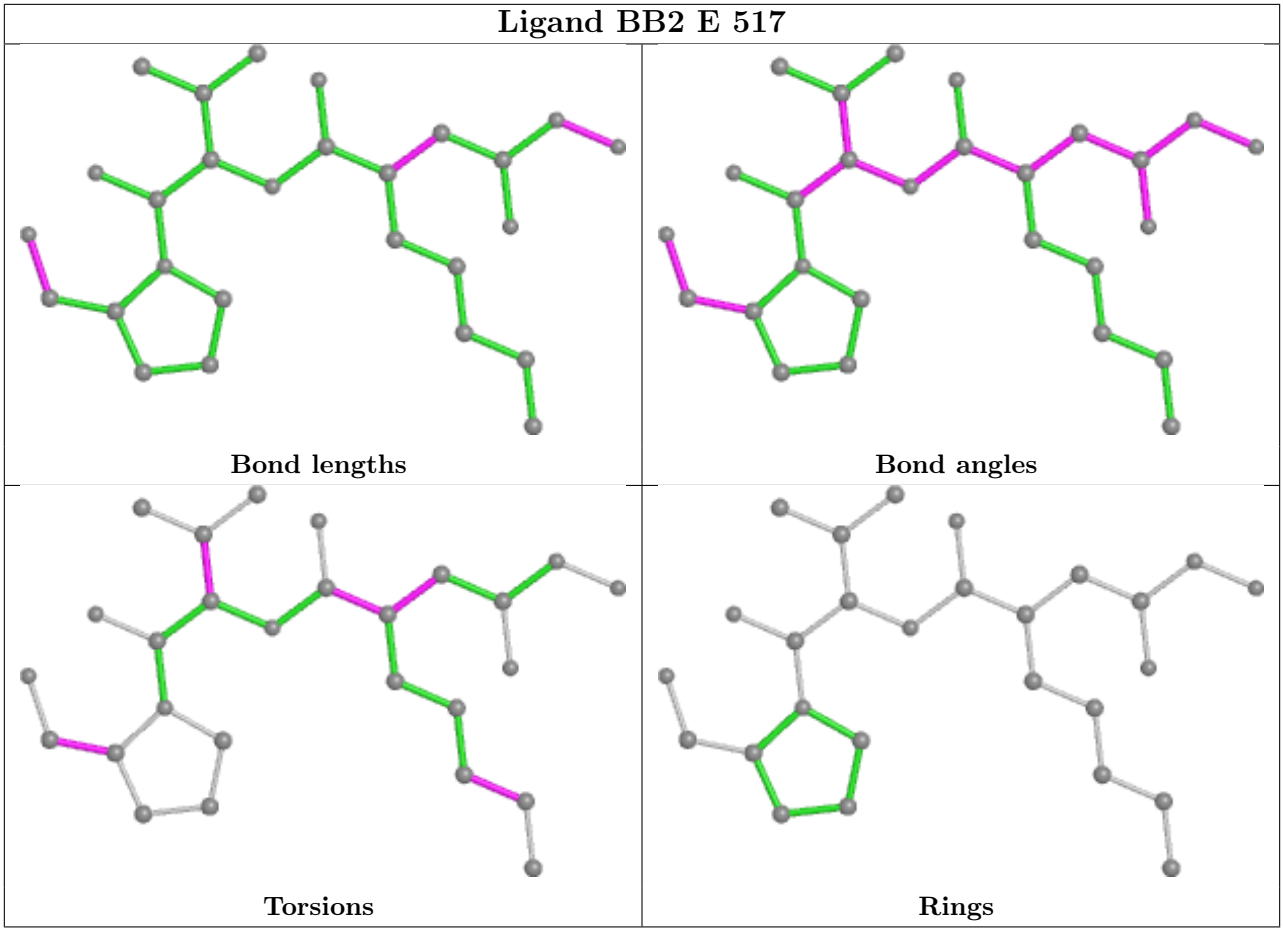


Ligand BB2 F 518



Ligand BB2 G 519





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	171/177 (96%)	-0.34	0	100	100	1, 22, 48, 67	0
1	B	171/177 (96%)	-0.33	0	100	100	2, 21, 47, 61	0
1	C	171/177 (96%)	-0.34	0	100	100	2, 21, 46, 53	0
1	D	171/177 (96%)	-0.22	2 (1%)	79	78	2, 24, 57, 69	0
1	E	171/177 (96%)	-0.33	0	100	100	3, 23, 50, 67	0
1	F	171/177 (96%)	-0.21	4 (2%)	60	59	3, 24, 64, 76	0
1	G	171/177 (96%)	-0.22	0	100	100	3, 24, 53, 67	0
1	H	171/177 (96%)	-0.34	0	100	100	4, 24, 55, 71	0
All	All	1368/1416 (96%)	-0.29	6 (0%)	92	93	1, 23, 52, 76	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	68	ASN	4.3
1	F	69	GLU	3.4
1	D	70	ARG	3.1
1	F	73	GLY	2.5
1	F	67	ASP	2.3
1	D	76	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

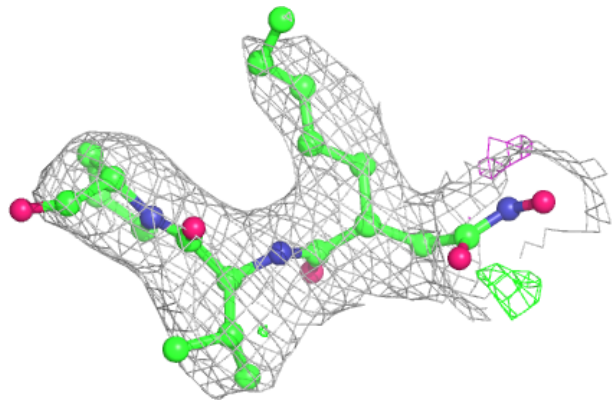
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

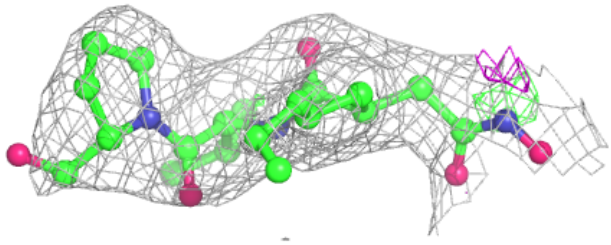
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BB2	E	517	27/27	0.94	0.27	1,2,15,18	0
3	BB2	G	519	27/27	0.94	0.30	25,41,57,59	0
3	BB2	F	518	27/27	0.95	0.23	1,27,41,46	0
3	BB2	A	513	27/27	0.96	0.27	1,1,7,8	0
2	ZN	E	720	1/1	0.96	0.12	12,12,12,12	0
3	BB2	H	520	27/27	0.96	0.22	17,23,33,34	0
2	ZN	G	722	1/1	0.97	0.06	19,19,19,19	0
3	BB2	B	514	27/27	0.97	0.27	1,1,13,16	0
3	BB2	C	515	27/27	0.97	0.23	1,1,12,13	0
3	BB2	D	516	27/27	0.97	0.24	1,18,34,37	0
2	ZN	F	721	1/1	0.98	0.09	13,13,13,13	0
2	ZN	D	719	1/1	0.98	0.10	6,6,6,6	0
2	ZN	B	717	1/1	0.99	0.13	7,7,7,7	0
2	ZN	C	718	1/1	0.99	0.13	13,13,13,13	0
2	ZN	A	716	1/1	0.99	0.13	7,7,7,7	0
2	ZN	H	723	1/1	0.99	0.08	18,18,18,18	0

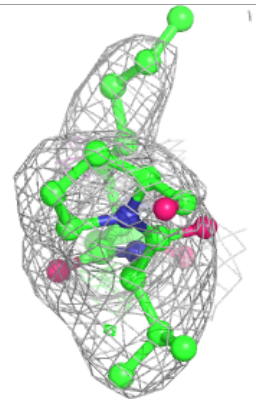
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BB2 E 517:

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

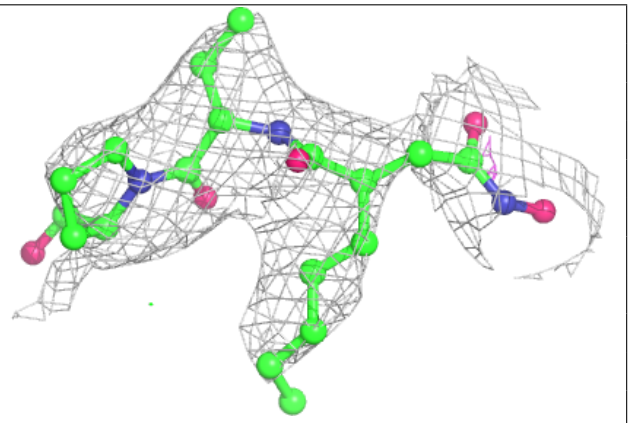


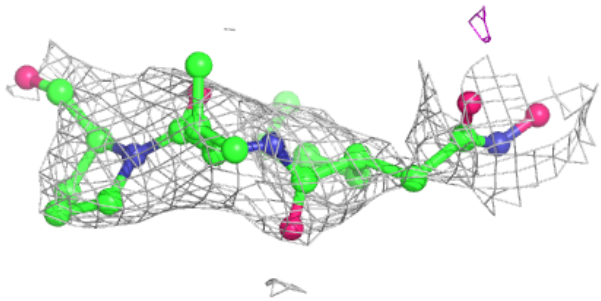


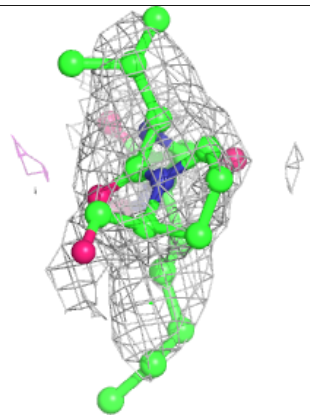


Electron density around BB2 G 519:

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

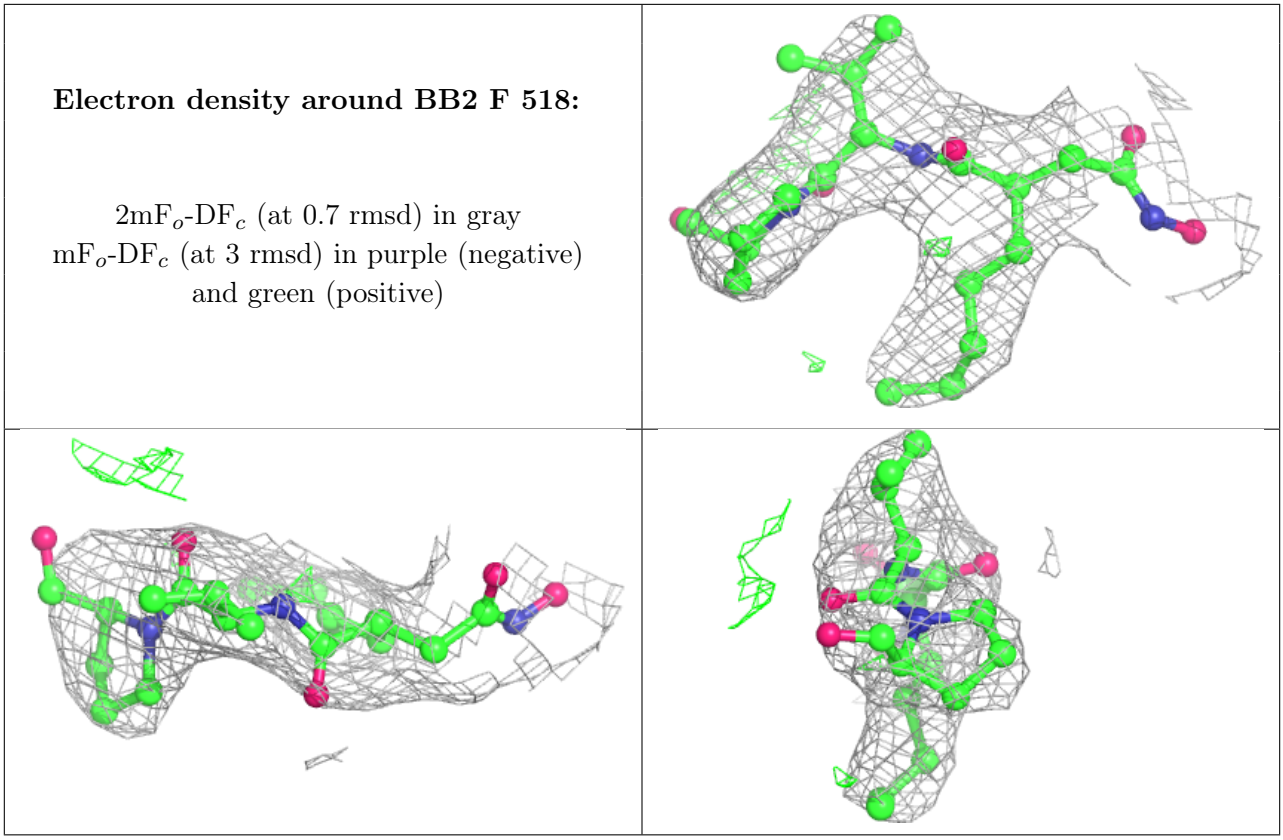






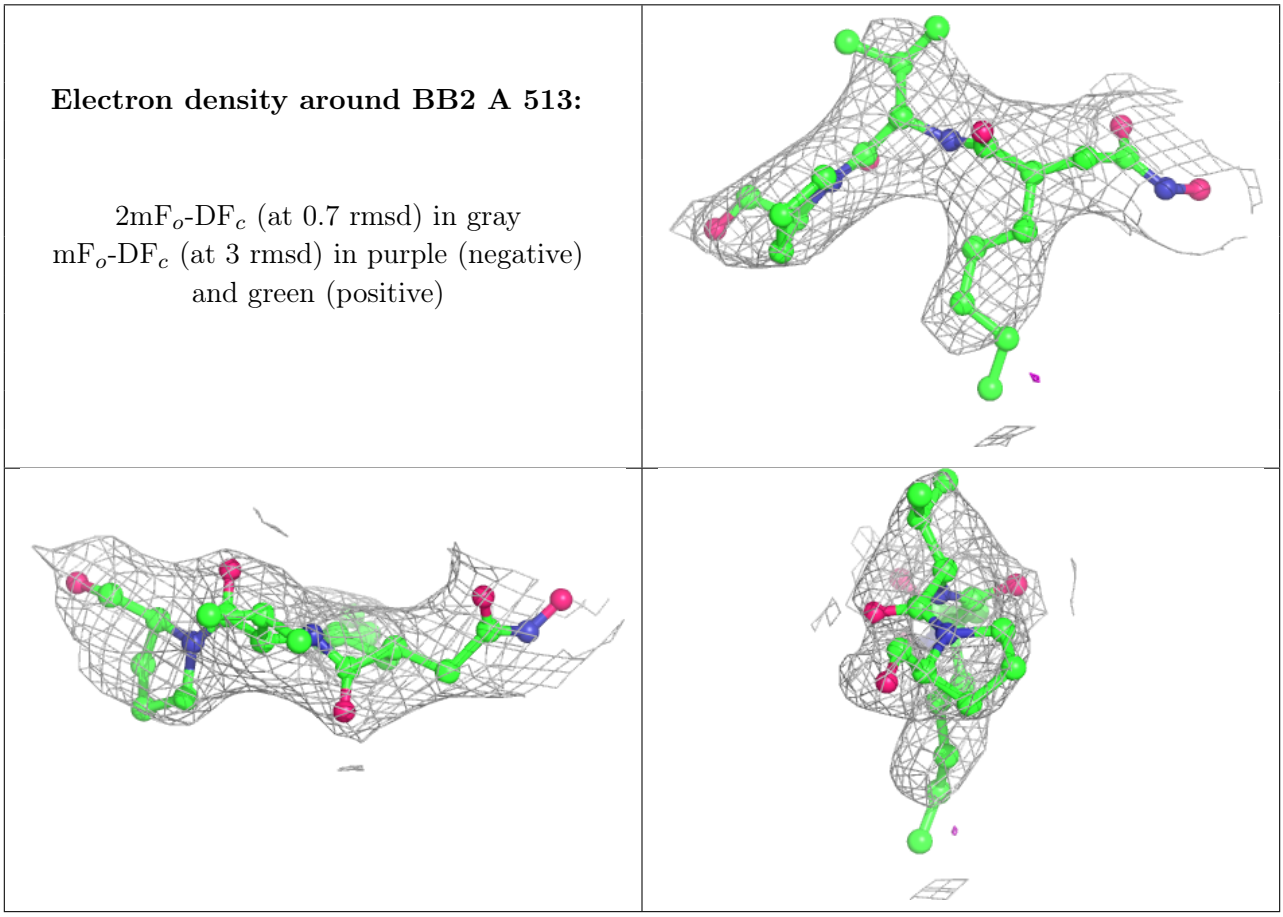
Electron density around BB2 F 518:

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



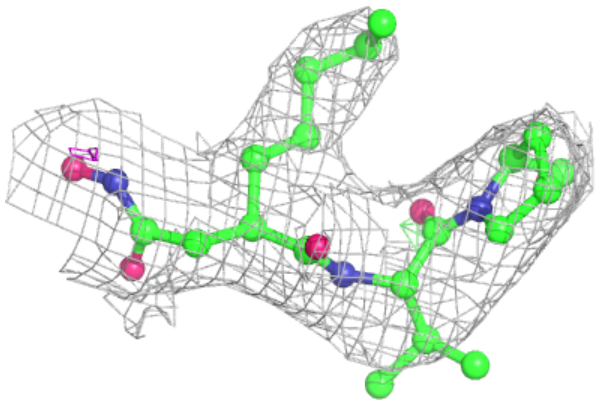
Electron density around BB2 A 513:

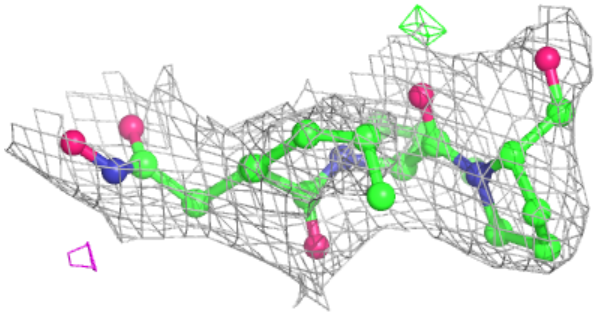
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

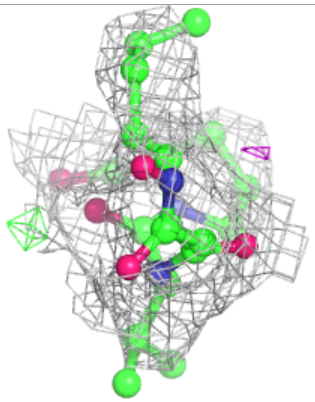


Electron density around BB2 H 520:

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

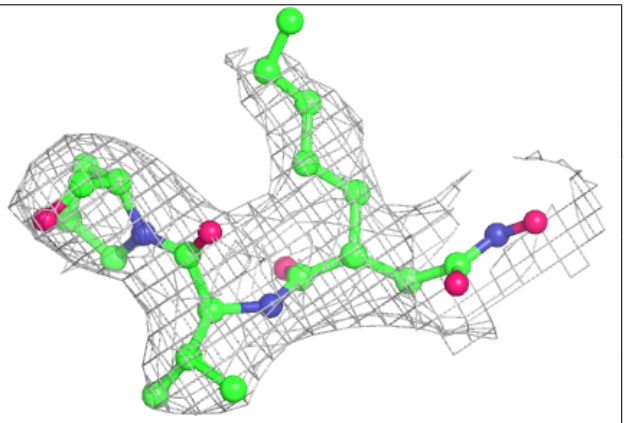


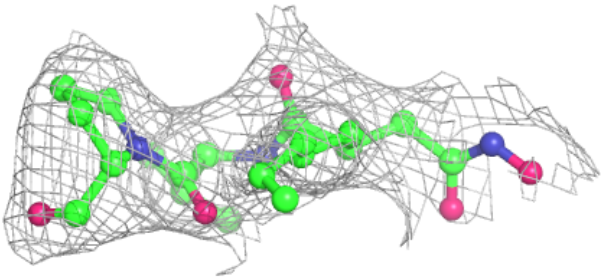


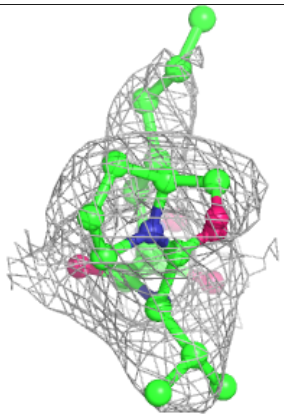


Electron density around BB2 B 514:

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

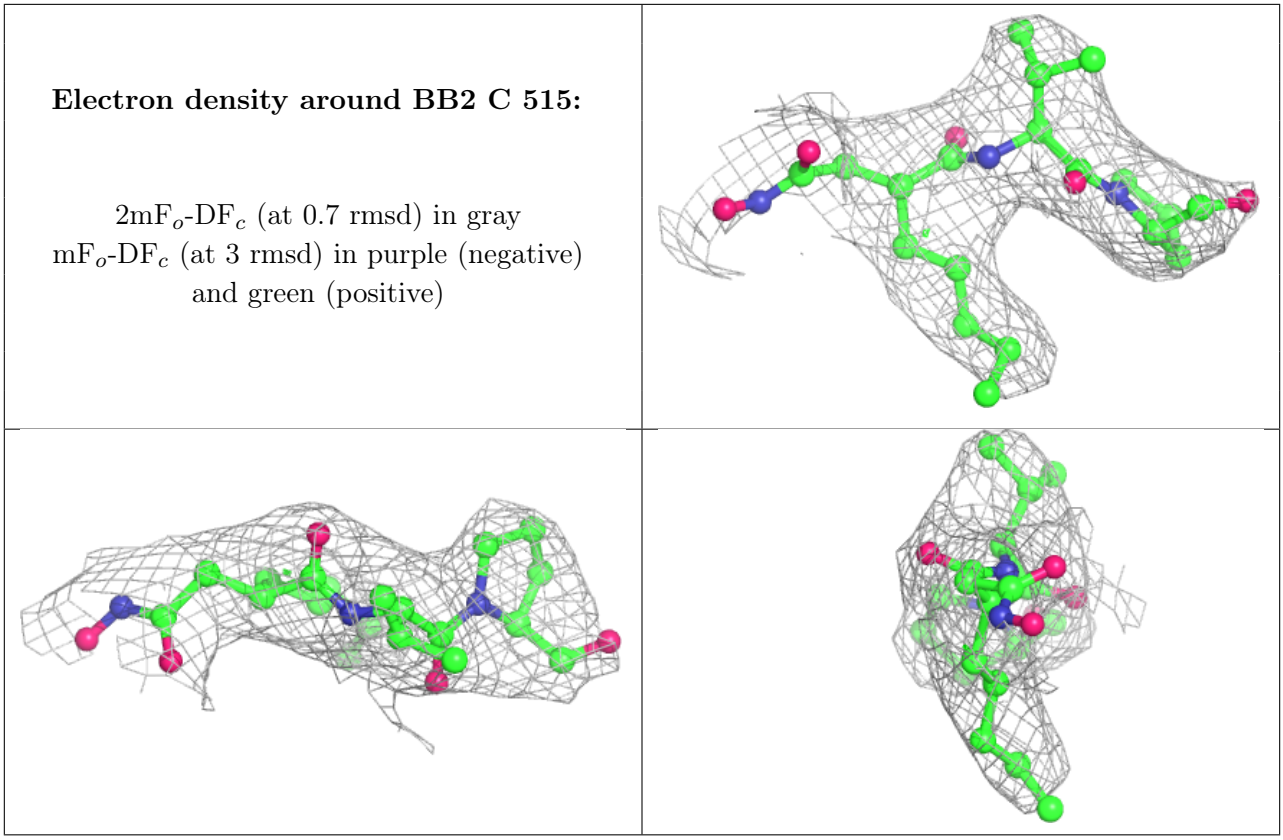






Electron density around BB2 C 515:

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



Electron density around BB2 D 516:

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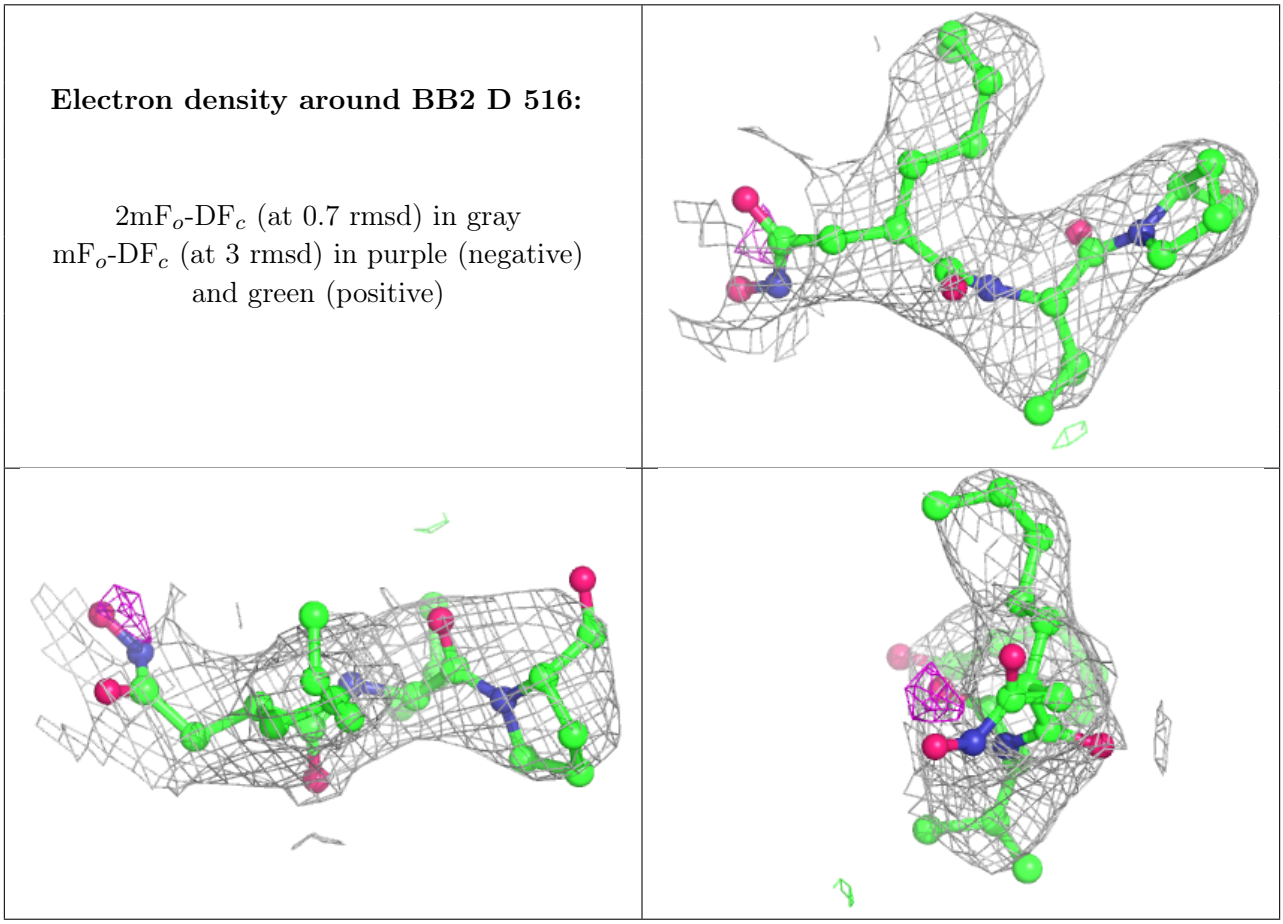
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.