



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2022 – 12:20 PM JST

PDB ID : 7E1H  
Title : crystal structure of RD-BEF  
Authors : Hong, S.; Zhang, X.; Zhang, P.  
Deposited on : 2021-02-01  
Resolution : 2.81 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](mailto: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.

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

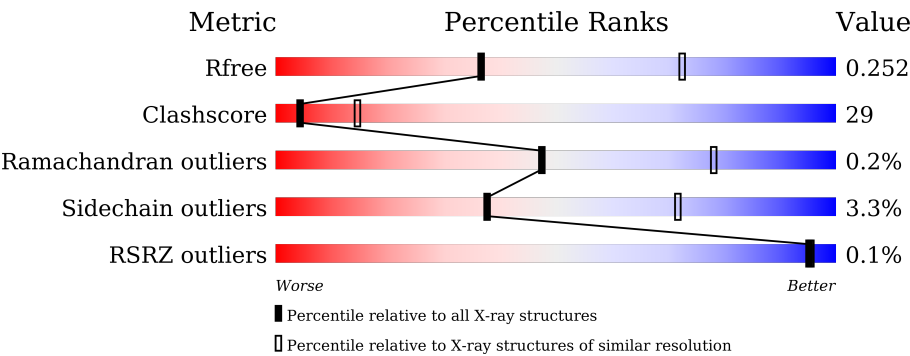
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.81 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.








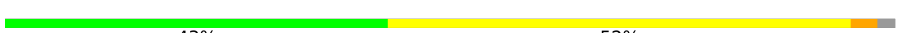
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	117	<div><div></div><div></div><div></div><div></div><div></div></div> <div>59%38%..</div>
1	B	117	<div><div></div><div></div><div></div><div></div><div></div></div> <div>56%43%. </div>
1	C	117	<div><div></div><div></div><div></div><div></div><div></div></div> <div>50%45%.. </div>
1	D	117	<div><div></div><div></div><div></div><div></div><div></div></div> <div>56%43%. </div>
1	E	117	<div><div></div><div></div><div></div><div></div><div></div></div> <div>56%41%.. </div>
1	F	117	<div><div></div><div></div><div></div><div></div><div></div></div> <div>56%41%.. </div>

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Mol	Chain	Length	Quality of chain
1	G	117	
1	H	117	
1	I	117	
1	J	117	
1	K	117	
1	L	117	
1	M	117	
1	N	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BEF	B	201	-	-	X	-

## 2 Entry composition

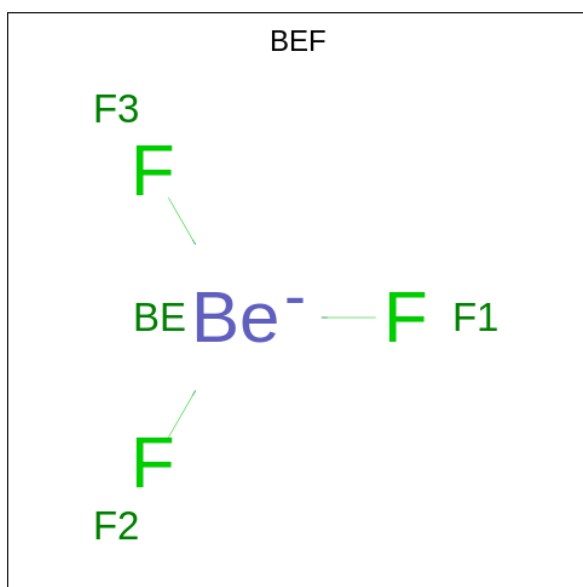
There are 4 unique types of molecules in this entry. The entry contains 15650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA-binding response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			913	584	155	173	1			
1	B	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	C	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	D	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	E	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	F	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	G	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	H	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	I	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	J	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	K	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	L	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	M	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			
1	N	115	Total	C	N	O	S	0	0	0
			904	578	153	172	1			

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total	O	0	0
			169	169		
4	B	156	Total	O	0	0
			156	156		
4	C	252	Total	O	0	0
			252	252		

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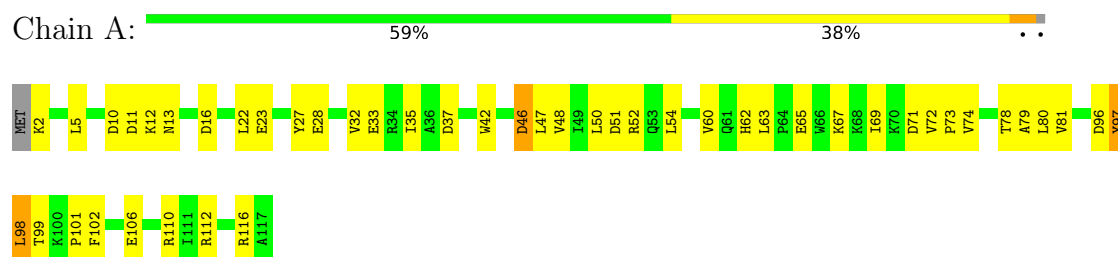
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	279	Total 279	O 279	0	0
4	E	165	Total 165	O 165	0	0
4	F	264	Total 264	O 264	0	0
4	G	219	Total 219	O 219	0	0
4	H	143	Total 143	O 143	0	0
4	I	199	Total 199	O 199	0	0
4	J	213	Total 213	O 213	0	0
4	K	219	Total 219	O 219	0	0
4	L	243	Total 243	O 243	0	0
4	M	252	Total 252	O 252	0	0
4	N	197	Total 197	O 197	0	0

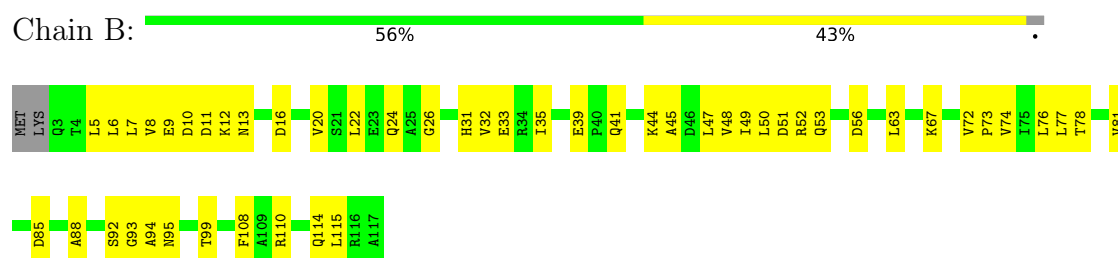
### 3 Residue-property plots [i](#)

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.

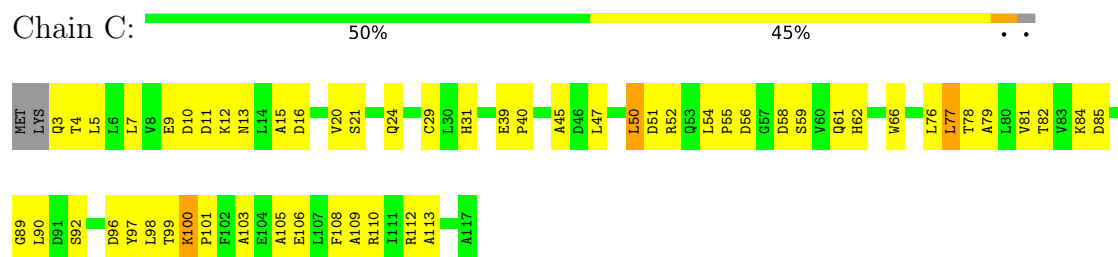
- Molecule 1: DNA-binding response regulator



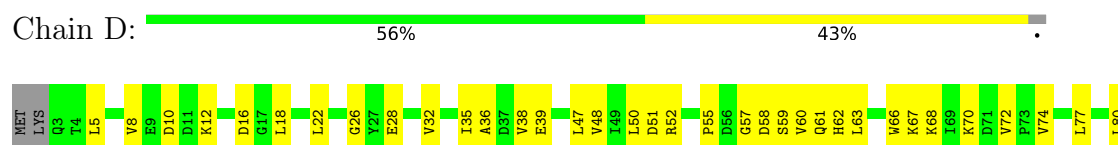
- Molecule 1: DNA-binding response regulator



- Molecule 1: DNA-binding response regulator



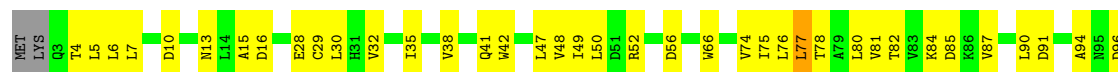
- Molecule 1: DNA-binding response regulator





- Molecule 1: DNA-binding response regulator

Chain E: 56% 41% ..



- Molecule 1: DNA-binding response regulator

Chain F: 56% 41% ..



- Molecule 1: DNA-binding response regulator

Chain G: 44% 54% ..



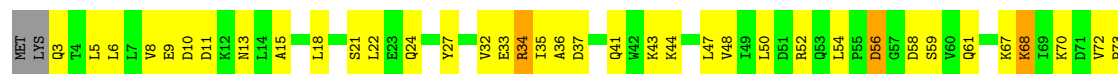
- Molecule 1: DNA-binding response regulator

Chain H: 49% 48% ..



- Molecule 1: DNA-binding response regulator

Chain I: 51% 44% ..

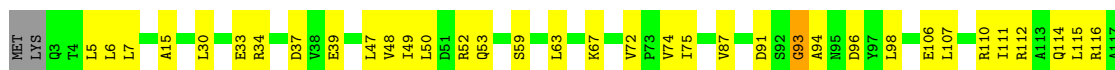






- Molecule 1: DNA-binding response regulator

Chain J: 68% 29% ..



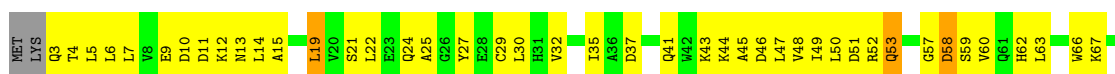
- Molecule 1: DNA-binding response regulator

Chain K: 56% 39% ..



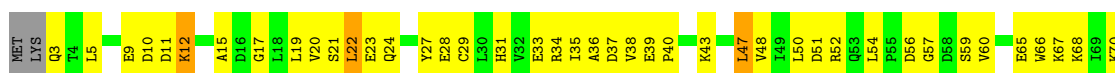
- Molecule 1: DNA-binding response regulator

Chain L: 44% 51% ..



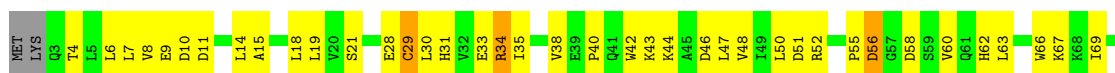
- Molecule 1: DNA-binding response regulator

Chain M: 43% 52% ..



- Molecule 1: DNA-binding response regulator

Chain N: 50% 46% ..



P73	V74	L75	L76	L77	T78	A79	L80	V81	T82	D85	L88	T99	K100	P101	F102	F108	A109	R110	I111	R112	A117
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.86Å 130.86Å 271.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.47 – 2.81 29.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	78.2 (29.47-2.81) 88.7 (29.69-2.81)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.226 , 0.253 0.221 , 0.252	Depositor DCC
$R_{free}$ test set	2011 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.447 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-h-k,-l	Depositor
Outliers	0 of 59252 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5854e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.25	0/927	0.47	0/1258
1	B	0.27	0/918	0.49	0/1247
1	C	0.29	0/918	0.51	0/1247
1	D	0.26	0/918	0.48	0/1247
1	E	0.25	0/918	0.46	0/1247
1	F	0.26	0/918	0.47	0/1247
1	G	0.29	0/918	0.50	0/1247
1	H	0.29	0/918	0.51	0/1247
1	I	0.24	0/918	0.47	0/1247
1	J	0.25	0/918	0.47	0/1247
1	K	0.28	0/918	0.49	0/1247
1	L	0.32	0/918	0.55	0/1247
1	M	0.37	0/918	0.59	0/1247
1	N	0.27	0/918	0.48	0/1247
All	All	0.28	0/12861	0.50	0/17469

There are no bond length outliers.

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	913	0	941	41	0
1	B	904	0	928	50	0
1	C	904	0	928	65	0
1	D	904	0	928	46	1
1	E	904	0	928	45	0
1	F	904	0	928	52	0
1	G	904	0	928	72	0
1	H	904	0	928	54	0
1	I	904	0	928	53	0
1	J	904	0	928	31	0
1	K	904	0	928	58	0
1	L	904	0	928	63	0
1	M	904	0	928	92	0
1	N	904	0	928	54	0
2	A	4	0	0	0	0
2	B	4	0	0	2	0
2	E	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
4	A	169	0	0	17	1
4	B	156	0	0	21	0
4	C	252	0	0	30	0
4	D	279	0	0	15	1
4	E	165	0	0	14	3
4	F	264	0	0	23	0
4	G	219	0	0	31	2
4	H	143	0	0	21	1
4	I	199	0	0	23	1
4	J	213	0	0	14	1
4	K	219	0	0	21	2
4	L	243	0	0	25	0
4	M	252	0	0	31	0
4	N	197	0	0	10	1
All	All	15650	0	13005	746	7

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 29.

All (746) 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:K:95:ASN:HB3	1:K:114:GLN:NE2	1.62	1.13
1:A:28:GLU:OE2	4:A:301:HOH:O	1.65	1.11
1:A:12:LYS:NZ	4:A:302:HOH:O	1.81	1.10
1:G:96:ASP:N	4:G:203:HOH:O	1.89	1.04
1:K:95:ASN:HB3	1:K:114:GLN:HE22	0.84	1.01
1:J:33:GLU:O	1:J:34:ARG:NH1	1.94	1.00
1:H:82:THR:HG22	4:H:204:HOH:O	1.64	0.97
1:F:3:GLN:OE1	4:F:201:HOH:O	1.84	0.95
1:E:29:CYS:O	4:E:301:HOH:O	1.82	0.95
1:G:52:ARG:HB2	1:G:78:THR:HG21	1.48	0.94
1:G:91:ASP:OD1	4:G:201:HOH:O	1.84	0.93
1:G:100:LYS:O	4:G:202:HOH:O	1.84	0.93
1:K:95:ASN:CB	1:K:114:GLN:HE22	1.80	0.93
1:L:103:ALA:O	4:L:201:HOH:O	1.87	0.91
1:K:107:LEU:O	4:K:201:HOH:O	1.89	0.91
1:I:24:GLN:O	4:I:201:HOH:O	1.88	0.91
1:G:10:ASP:O	4:G:204:HOH:O	1.89	0.91
1:G:95:ASN:OD1	4:G:205:HOH:O	1.89	0.91
1:L:63:LEU:HD12	4:L:210:HOH:O	1.72	0.90
1:A:50:LEU:HG	4:A:308:HOH:O	1.72	0.89
1:F:92:SER:O	4:F:202:HOH:O	1.93	0.87
1:G:23:GLU:OE1	4:G:206:HOH:O	1.92	0.87
1:G:78:THR:HG23	1:G:80:LEU:H	1.38	0.86
1:J:111:ILE:O	4:J:201:HOH:O	1.93	0.86
1:L:43:LYS:NZ	4:L:202:HOH:O	2.07	0.86
1:A:116:ARG:O	4:A:303:HOH:O	1.94	0.86
1:K:17:GLY:O	4:K:202:HOH:O	1.92	0.85
1:J:112:ARG:NH1	4:J:202:HOH:O	2.09	0.84
1:M:116:ARG:NH2	4:M:209:HOH:O	2.09	0.84
1:M:116:ARG:O	4:M:202:HOH:O	1.94	0.84
1:C:58:ASP:OD1	4:C:202:HOH:O	1.95	0.83
1:K:72:VAL:O	4:K:204:HOH:O	1.95	0.83
1:D:52:ARG:O	4:D:201:HOH:O	1.96	0.83
1:H:71:ASP:O	4:H:201:HOH:O	1.96	0.83
1:C:7:LEU:HD22	1:C:31:HIS:CE1	2.13	0.83
1:K:85:ASP:OD1	4:K:203:HOH:O	1.95	0.83
1:A:101:PRO:O	4:A:304:HOH:O	1.95	0.83
1:G:106:GLU:OE1	4:G:207:HOH:O	1.95	0.82
1:L:67:LYS:NZ	1:L:72:VAL:O	2.12	0.82
1:I:37:ASP:OD1	4:I:203:HOH:O	1.98	0.81
1:M:60:VAL:HG23	1:M:92:SER:HB2	1.61	0.81
1:M:33:GLU:O	4:M:204:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:LEU:HD22	1:M:111:ILE:HG23	1.60	0.80
1:C:112:ARG:NH2	4:C:207:HOH:O	2.15	0.80
1:N:21:SER:HB3	1:N:108:PHE:HZ	1.45	0.80
1:E:116:ARG:NE	4:E:305:HOH:O	2.14	0.79
1:H:116:ARG:NH1	4:H:203:HOH:O	2.15	0.79
1:M:68:LYS:O	4:M:205:HOH:O	2.01	0.79
1:M:34:ARG:HH11	1:M:36:ALA:HB2	1.48	0.79
1:M:83:VAL:HA	1:M:86:LYS:HB2	1.64	0.79
1:I:6:LEU:O	4:I:204:HOH:O	2.01	0.79
1:M:106:GLU:HG2	4:M:216:HOH:O	1.82	0.78
1:C:10:ASP:OD2	4:C:203:HOH:O	2.02	0.78
1:B:26:GLY:O	4:B:302:HOH:O	2.01	0.78
1:H:84:LYS:N	4:H:204:HOH:O	2.17	0.78
1:C:96:ASP:OD1	1:C:110:ARG:NH1	2.17	0.78
1:F:48:VAL:O	4:F:203:HOH:O	2.02	0.77
1:B:81:VAL:O	4:B:303:HOH:O	2.03	0.77
1:I:43:LYS:NZ	4:I:202:HOH:O	1.92	0.76
1:D:116:ARG:O	4:D:202:HOH:O	2.04	0.76
1:C:59:SER:N	4:C:202:HOH:O	2.19	0.76
1:J:53:GLN:NE2	4:J:205:HOH:O	2.19	0.76
1:A:112:ARG:NH1	4:A:311:HOH:O	2.15	0.76
1:E:5:LEU:HD22	1:E:47:LEU:HB3	1.66	0.76
1:A:65:GLU:O	4:A:306:HOH:O	2.03	0.75
1:A:42:TRP:O	4:A:305:HOH:O	2.03	0.75
1:M:84:LYS:NZ	4:M:211:HOH:O	2.12	0.75
1:E:90:LEU:O	4:E:302:HOH:O	2.05	0.75
1:D:114:GLN:O	4:D:203:HOH:O	2.04	0.75
1:G:44:LYS:NZ	4:G:214:HOH:O	2.21	0.74
1:B:20:VAL:HG13	1:K:34:ARG:HH12	1.53	0.74
1:G:99:THR:OG1	4:G:210:HOH:O	2.02	0.74
1:C:13:ASN:ND2	4:C:213:HOH:O	2.21	0.74
1:F:112:ARG:O	4:F:204:HOH:O	2.05	0.74
1:I:67:LYS:NZ	1:I:72:VAL:O	2.16	0.73
1:B:39:GLU:OE2	4:B:304:HOH:O	2.06	0.73
1:G:30:LEU:O	4:G:211:HOH:O	2.05	0.73
1:M:21:SER:OG	4:M:206:HOH:O	2.06	0.73
1:I:10:ASP:HA	1:I:33:GLU:HG2	1.69	0.72
1:G:35:ILE:HB	1:G:56:ASP:HB3	1.72	0.72
1:M:112:ARG:NH2	4:M:218:HOH:O	2.23	0.72
1:M:3:GLN:O	4:M:208:HOH:O	2.07	0.72
1:G:43:LYS:HD2	1:G:70:LYS:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:22:LEU:HD13	1:M:29:CYS:HB2	1.70	0.72
1:A:11:ASP:OD1	1:I:114:GLN:NE2	2.22	0.72
1:L:13:ASN:ND2	4:L:213:HOH:O	2.22	0.72
1:D:90:LEU:HD11	1:D:97:TYR:HB2	1.70	0.71
1:C:39:GLU:OE1	4:C:205:HOH:O	2.07	0.71
1:L:62:HIS:CD2	4:L:265:HOH:O	2.42	0.71
1:L:52:ARG:O	4:L:203:HOH:O	2.09	0.71
1:H:9:GLU:HG3	1:H:11:ASP:H	1.55	0.71
1:B:67:LYS:NZ	1:B:93:GLY:O	2.24	0.71
1:K:58:ASP:O	4:K:205:HOH:O	2.07	0.71
1:C:61:GLN:NE2	4:C:217:HOH:O	2.24	0.71
1:H:48:VAL:HB	1:H:74:VAL:HG12	1.72	0.71
1:K:52:ARG:O	4:K:207:HOH:O	2.09	0.71
1:G:96:ASP:O	4:G:203:HOH:O	2.09	0.70
1:L:62:HIS:HD2	4:L:265:HOH:O	1.73	0.70
1:F:112:ARG:NH2	4:F:208:HOH:O	2.20	0.70
1:A:69:ILE:N	4:A:306:HOH:O	2.09	0.70
1:G:3:GLN:NE2	4:G:218:HOH:O	2.25	0.70
1:E:96:ASP:O	4:E:304:HOH:O	2.09	0.70
1:C:3:GLN:N	4:C:219:HOH:O	2.25	0.69
1:M:48:VAL:O	4:M:210:HOH:O	2.10	0.69
1:I:9:GLU:OE2	4:I:206:HOH:O	2.09	0.69
1:C:100:LYS:HB3	1:L:116:ARG:HH22	1.54	0.69
1:I:90:LEU:O	4:I:205:HOH:O	2.10	0.69
1:A:37:ASP:OD2	4:A:309:HOH:O	2.08	0.69
1:I:15:ALA:HA	1:I:18:LEU:HB3	1.73	0.69
1:B:12:LYS:HD3	1:B:33:GLU:OE1	1.92	0.69
1:D:62:HIS:NE2	4:D:208:HOH:O	2.26	0.69
1:N:110:ARG:NH2	4:N:203:HOH:O	2.16	0.69
1:G:13:ASN:ND2	4:G:217:HOH:O	2.25	0.69
1:I:34:ARG:HB2	1:I:56:ASP:HB2	1.75	0.69
1:H:100:LYS:NZ	4:N:203:HOH:O	2.24	0.69
1:C:84:LYS:O	4:C:206:HOH:O	2.10	0.69
1:H:8:VAL:HG12	1:H:32:VAL:HG23	1.73	0.69
1:L:41:GLN:OE1	4:L:205:HOH:O	2.10	0.68
1:K:58:ASP:OD1	1:K:60:VAL:N	2.25	0.68
1:I:35:ILE:HB	1:I:56:ASP:HB3	1.76	0.68
1:K:51:ASP:OD1	4:K:208:HOH:O	2.11	0.68
1:H:62:HIS:ND1	4:H:209:HOH:O	2.27	0.68
1:H:84:LYS:HG2	4:H:204:HOH:O	1.93	0.68
1:I:86:LYS:HE2	1:I:97:TYR:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TYR:O	1:B:110:ARG:NH2	2.26	0.67
1:E:96:ASP:OD1	1:F:110:ARG:NH2	2.27	0.67
1:F:31:HIS:H	1:M:36:ALA:HB1	1.59	0.67
1:K:52:ARG:HE	1:K:78:THR:HG23	1.59	0.67
1:M:5:LEU:HD22	4:M:208:HOH:O	1.94	0.67
1:H:34:ARG:NH2	4:H:211:HOH:O	2.28	0.67
1:G:95:ASN:N	4:G:203:HOH:O	2.27	0.67
1:I:50:LEU:O	1:I:77:LEU:N	2.28	0.67
1:A:54:LEU:O	1:I:97:TYR:OH	2.11	0.67
1:K:111:ILE:HG13	4:K:201:HOH:O	1.94	0.67
1:L:11:ASP:OD2	4:L:206:HOH:O	2.13	0.67
1:N:66:TRP:HA	1:N:69:ILE:HD12	1.77	0.67
1:D:10:ASP:HB3	1:D:55:PRO:HD3	1.76	0.66
1:A:33:GLU:O	4:A:310:HOH:O	2.12	0.66
1:G:12:LYS:O	1:G:16:ASP:N	2.28	0.66
1:L:7:LEU:HA	1:L:49:ILE:HG23	1.77	0.66
1:K:35:ILE:HD12	1:K:56:ASP:HB2	1.77	0.66
1:M:10:ASP:OD1	4:M:212:HOH:O	2.14	0.66
1:F:48:VAL:HG23	4:F:269:HOH:O	1.95	0.66
1:C:52:ARG:NH1	4:C:211:HOH:O	2.28	0.66
1:B:74:VAL:HG12	4:B:328:HOH:O	1.96	0.65
1:D:52:ARG:HE	1:D:80:LEU:HD12	1.62	0.65
1:D:116:ARG:NH1	4:D:211:HOH:O	2.27	0.65
1:J:74:VAL:HB	1:J:94:ALA:HA	1.78	0.65
1:M:100:LYS:HG2	1:M:102:PHE:HE2	1.61	0.65
1:M:116:ARG:N	4:M:214:HOH:O	2.29	0.65
1:L:13:ASN:O	4:L:207:HOH:O	2.14	0.65
1:M:51:ASP:OD2	4:M:213:HOH:O	2.15	0.65
1:A:5:LEU:HD22	1:A:47:LEU:HB3	1.79	0.65
1:F:82:THR:N	4:F:215:HOH:O	2.30	0.64
1:G:67:LYS:NZ	1:G:71:ASP:OD1	2.28	0.64
1:G:53:GLN:O	4:G:212:HOH:O	2.14	0.64
1:M:34:ARG:NH1	1:M:36:ALA:HB2	2.11	0.64
1:G:35:ILE:HG23	1:G:66:TRP:HH2	1.61	0.64
1:G:74:VAL:N	4:G:205:HOH:O	2.25	0.64
1:N:47:LEU:HD12	1:N:73:PRO:HB2	1.79	0.64
1:N:52:ARG:HH11	1:N:60:VAL:HG21	1.63	0.64
1:K:110:ARG:O	4:K:209:HOH:O	2.15	0.64
1:C:5:LEU:HB2	1:C:29:CYS:SG	2.38	0.64
1:F:9:GLU:OE1	4:F:206:HOH:O	2.15	0.64
1:F:80:LEU:O	4:F:205:HOH:O	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:BEF:F1	4:B:319:HOH:O	2.05	0.64
1:D:8:VAL:HG22	1:D:32:VAL:HB	1.79	0.64
1:M:112:ARG:HG2	4:M:214:HOH:O	1.98	0.64
1:B:73:PRO:HB3	1:B:114:GLN:HB3	1.80	0.64
1:A:27:TYR:OH	4:A:307:HOH:O	2.04	0.63
1:D:62:HIS:ND1	4:D:213:HOH:O	2.31	0.63
1:J:5:LEU:HD22	1:J:47:LEU:HB3	1.80	0.63
1:J:39:GLU:HB3	4:J:209:HOH:O	1.98	0.63
1:A:116:ARG:NH1	1:B:94:ALA:O	2.32	0.63
1:N:8:VAL:HG22	4:N:204:HOH:O	1.98	0.63
1:K:102:PHE:HE1	1:K:107:LEU:HD22	1.64	0.63
1:M:75:ILE:N	4:M:210:HOH:O	2.31	0.63
1:A:2:LYS:NZ	4:A:315:HOH:O	2.32	0.62
1:L:60:VAL:HA	1:L:63:LEU:HB2	1.81	0.62
1:J:63:LEU:HD21	1:J:94:ALA:H	1.64	0.62
1:A:51:ASP:O	4:A:308:HOH:O	2.15	0.62
1:B:53:GLN:NE2	4:B:316:HOH:O	2.32	0.62
1:B:92:SER:O	4:B:308:HOH:O	2.16	0.62
4:C:203:HOH:O	1:L:97:TYR:HE1	1.82	0.62
1:K:81:VAL:HG13	1:K:86:LYS:HE3	1.82	0.62
1:N:100:LYS:HG2	1:N:101:PRO:HA	1.81	0.62
1:D:61:GLN:OE1	1:D:62:HIS:NE2	2.33	0.62
1:C:112:ARG:NH2	1:D:91:ASP:OD1	2.23	0.62
1:L:22:LEU:O	1:L:27:TYR:HB2	1.99	0.62
1:B:94:ALA:HB3	4:B:343:HOH:O	1.97	0.62
1:L:48:VAL:HG22	1:L:74:VAL:HG22	1.81	0.62
1:B:53:GLN:OE1	1:J:110:ARG:NH2	2.32	0.61
1:C:85:ASP:HB2	4:C:229:HOH:O	2.00	0.61
1:M:48:VAL:HB	1:M:74:VAL:HG22	1.80	0.61
1:F:6:LEU:N	4:F:216:HOH:O	2.32	0.61
1:F:45:ALA:O	1:F:70:LYS:NZ	2.33	0.61
1:N:21:SER:HB3	1:N:108:PHE:CZ	2.31	0.61
1:F:4:THR:HB	1:F:45:ALA:HA	1.81	0.61
1:C:96:ASP:OD2	4:C:208:HOH:O	2.16	0.61
1:G:4:THR:OG1	1:G:46:ASP:N	2.33	0.61
1:K:74:VAL:N	1:K:95:ASN:OD1	2.31	0.61
1:K:102:PHE:CE1	1:K:107:LEU:HB2	2.35	0.61
1:D:52:ARG:HH11	1:D:60:VAL:HG21	1.65	0.60
1:M:112:ARG:O	4:M:214:HOH:O	2.16	0.60
1:F:32:VAL:HG13	1:F:37:ASP:HB2	1.83	0.60
1:M:15:ALA:O	1:M:19:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:OE2	1:A:110:ARG:NH1	2.35	0.60
1:M:22:LEU:O	1:M:27:TYR:N	2.34	0.60
1:L:49:ILE:HG13	4:L:260:HOH:O	2.01	0.60
1:D:48:VAL:HB	1:D:74:VAL:HG22	1.84	0.60
1:M:67:LYS:NZ	4:M:203:HOH:O	1.96	0.60
1:F:19:LEU:HD21	1:F:31:HIS:HB2	1.83	0.60
1:B:95:ASN:ND2	4:B:317:HOH:O	2.34	0.60
1:D:57:GLY:O	4:D:201:HOH:O	2.16	0.60
1:M:51:ASP:OD1	1:M:78:THR:OG1	2.16	0.59
1:B:48:VAL:HG23	1:B:72:VAL:HG11	1.83	0.59
1:E:82:THR:OG1	1:E:85:ASP:OD2	2.19	0.59
1:G:3:GLN:N	4:G:222:HOH:O	2.35	0.59
1:C:52:ARG:HG2	4:C:202:HOH:O	2.02	0.59
1:D:62:HIS:HB2	1:D:66:TRP:CZ2	2.38	0.59
1:L:21:SER:OG	4:L:208:HOH:O	2.16	0.59
1:M:34:ARG:HE	1:M:56:ASP:CB	2.16	0.59
1:M:89:GLY:HA2	1:M:92:SER:HB3	1.83	0.59
1:L:35:ILE:HG12	1:L:59:SER:HB2	1.85	0.59
1:N:48:VAL:HB	1:N:74:VAL:HG12	1.85	0.59
1:H:52:ARG:HD3	1:H:78:THR:HG21	1.84	0.59
1:I:68:LYS:NZ	4:I:214:HOH:O	2.36	0.59
1:L:15:ALA:O	1:L:19:LEU:HB2	2.03	0.59
4:C:235:HOH:O	1:D:90:LEU:HD13	2.02	0.58
1:E:50:LEU:HD22	1:E:74:VAL:HG21	1.85	0.58
1:J:112:ARG:O	4:J:203:HOH:O	2.17	0.58
1:K:73:PRO:HB3	1:K:114:GLN:OE1	2.04	0.58
1:M:22:LEU:HD23	1:M:22:LEU:H	1.67	0.58
1:M:9:GLU:HG2	1:M:15:ALA:HB2	1.85	0.58
1:K:60:VAL:HA	1:K:63:LEU:HB2	1.86	0.58
1:I:74:VAL:HG13	1:I:94:ALA:HA	1.85	0.58
4:C:213:HOH:O	1:L:95:ASN:ND2	2.26	0.58
1:E:16:ASP:OD1	4:E:306:HOH:O	2.17	0.58
1:G:75:ILE:N	4:G:215:HOH:O	2.23	0.58
1:I:36:ALA:N	4:I:203:HOH:O	2.35	0.58
1:N:62:HIS:HB2	1:N:66:TRP:CZ2	2.39	0.58
1:F:27:TYR:N	4:F:209:HOH:O	2.20	0.58
1:B:51:ASP:OD2	1:B:52:ARG:N	2.32	0.58
1:H:63:LEU:HD13	4:H:226:HOH:O	2.03	0.58
1:K:74:VAL:HG12	4:K:204:HOH:O	2.04	0.58
1:L:41:GLN:NE2	4:L:227:HOH:O	2.37	0.58
1:L:93:GLY:N	4:L:204:HOH:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ASN:HA	1:A:16:ASP:HB2	1.86	0.58
1:C:106:GLU:N	4:C:225:HOH:O	2.35	0.58
1:H:63:LEU:HD11	4:H:284:HOH:O	2.03	0.57
1:K:102:PHE:HE1	1:K:107:LEU:HB2	1.69	0.57
1:G:39:GLU:HB2	1:G:66:TRP:HE1	1.69	0.57
1:K:44:LYS:HG2	4:K:234:HOH:O	2.02	0.57
1:K:102:PHE:CE1	1:K:107:LEU:HD22	2.39	0.57
1:J:87:VAL:O	1:J:91:ASP:N	2.37	0.57
1:L:6:LEU:HB3	1:L:48:VAL:HG12	1.86	0.57
1:E:116:ARG:NH1	1:F:90:LEU:O	2.23	0.57
1:G:107:LEU:O	1:G:111:ILE:N	2.35	0.57
1:M:82:THR:OG1	1:M:85:ASP:OD1	2.22	0.57
1:N:14:LEU:HD11	1:N:102:PHE:HE1	1.69	0.57
1:H:60:VAL:HA	1:H:63:LEU:HD12	1.86	0.57
1:M:34:ARG:HD3	1:M:36:ALA:H	1.69	0.57
1:N:38:VAL:HG21	1:N:66:TRP:CZ2	2.39	0.57
1:J:106:GLU:OE1	4:J:204:HOH:O	2.18	0.56
1:C:90:LEU:N	4:C:226:HOH:O	2.38	0.56
1:D:112:ARG:NH2	4:D:216:HOH:O	2.35	0.56
1:I:34:ARG:NH2	4:I:215:HOH:O	2.37	0.56
1:E:94:ALA:HB1	4:E:304:HOH:O	2.04	0.56
1:J:37:ASP:OD1	1:J:37:ASP:N	2.35	0.56
1:K:95:ASN:CB	1:K:114:GLN:NE2	2.52	0.56
1:C:9:GLU:HG3	1:C:11:ASP:H	1.70	0.56
1:I:22:LEU:HB3	1:I:27:TYR:HD2	1.71	0.56
1:F:8:VAL:HA	1:F:32:VAL:O	2.06	0.56
1:G:18:LEU:HA	1:G:21:SER:HB3	1.86	0.56
1:M:22:LEU:HD12	1:M:27:TYR:O	2.04	0.56
1:M:77:LEU:HD21	1:M:102:PHE:CZ	2.41	0.56
1:N:18:LEU:HA	1:N:21:SER:HB2	1.88	0.56
1:H:20:VAL:O	1:H:24:GLN:N	2.39	0.56
1:F:85:ASP:HB2	4:F:215:HOH:O	2.06	0.56
1:M:51:ASP:OD1	1:M:52:ARG:N	2.38	0.56
1:I:37:ASP:N	4:I:203:HOH:O	2.30	0.55
1:B:12:LYS:NZ	4:B:307:HOH:O	2.14	0.55
1:I:56:ASP:O	4:I:208:HOH:O	2.18	0.55
1:M:37:ASP:OD1	1:M:37:ASP:N	2.32	0.55
1:N:8:VAL:CG2	1:N:50:LEU:HA	2.36	0.55
1:F:47:LEU:HG	4:F:203:HOH:O	2.06	0.55
1:F:52:ARG:NH1	1:F:85:ASP:HB3	2.22	0.55
1:L:51:ASP:HA	1:L:77:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:9:GLU:HG3	1:N:11:ASP:H	1.71	0.55
1:L:53:GLN:HE22	1:L:79:ALA:HB3	1.69	0.55
1:D:58:ASP:HA	4:D:201:HOH:O	2.07	0.55
1:M:50:LEU:O	1:M:77:LEU:N	2.40	0.55
1:C:79:ALA:HA	4:C:204:HOH:O	2.06	0.55
1:E:38:VAL:O	1:E:42:TRP:N	2.39	0.55
1:H:35:ILE:HB	1:H:56:ASP:HB3	1.88	0.55
1:I:56:ASP:OD2	4:I:208:HOH:O	2.18	0.55
1:M:35:ILE:HG23	1:M:66:TRP:CZ2	2.42	0.55
1:M:9:GLU:OE2	1:M:11:ASP:N	2.29	0.54
1:G:52:ARG:H	1:G:78:THR:HB	1.71	0.54
1:A:23:GLU:N	1:A:23:GLU:OE2	2.40	0.54
1:E:15:ALA:HB3	4:E:321:HOH:O	2.07	0.54
1:H:7:LEU:HD12	4:H:224:HOH:O	2.06	0.54
1:N:8:VAL:HG23	1:N:50:LEU:HA	1.90	0.54
1:K:88:ALA:O	1:K:92:SER:N	2.35	0.54
1:B:81:VAL:HG12	1:B:99:THR:HB	1.88	0.54
1:C:52:ARG:HD3	1:C:78:THR:HG21	1.88	0.54
1:J:63:LEU:HD21	1:J:94:ALA:N	2.23	0.54
1:B:44:LYS:NZ	4:B:315:HOH:O	2.31	0.54
1:B:73:PRO:HG2	4:B:356:HOH:O	2.08	0.54
1:H:33:GLU:O	1:H:34:ARG:NH1	2.39	0.54
1:L:47:LEU:N	4:L:226:HOH:O	2.40	0.54
1:E:109:ALA:HB2	1:F:87:VAL:HG13	1.89	0.54
1:J:115:LEU:N	4:J:201:HOH:O	2.11	0.54
1:B:52:ARG:HD3	1:B:78:THR:HG21	1.90	0.54
1:M:65:GLU:OE2	4:M:215:HOH:O	2.17	0.54
1:M:98:LEU:HD13	1:M:107:LEU:HD12	1.90	0.53
1:B:63:LEU:HD21	1:B:94:ALA:HB2	1.90	0.53
1:B:85:ASP:OD1	4:B:309:HOH:O	2.19	0.53
1:D:91:ASP:HA	4:D:210:HOH:O	2.08	0.53
1:H:15:ALA:HA	1:H:18:LEU:HB3	1.89	0.53
1:G:52:ARG:HG3	1:G:76:LEU:HD22	1.90	0.53
1:L:9:GLU:OE1	1:L:10:ASP:N	2.41	0.53
1:A:47:LEU:HD12	1:A:73:PRO:HB2	1.89	0.53
1:J:52:ARG:HB3	4:J:205:HOH:O	2.08	0.53
1:B:5:LEU:HD22	1:B:47:LEU:HB3	1.89	0.53
1:G:51:ASP:OD2	1:G:52:ARG:N	2.42	0.53
1:L:3:GLN:N	4:L:231:HOH:O	2.41	0.53
1:N:19:LEU:HD23	1:N:29:CYS:SG	2.48	0.53
1:F:74:VAL:HA	4:F:203:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:ASN:HB2	4:H:205:HOH:O	2.09	0.53
1:L:50:LEU:O	1:L:77:LEU:N	2.40	0.53
1:C:110:ARG:HG2	4:C:235:HOH:O	2.08	0.53
1:N:52:ARG:HG2	1:N:76:LEU:HD22	1.91	0.53
1:B:93:GLY:HA3	4:B:308:HOH:O	2.08	0.53
1:C:89:GLY:O	1:C:92:SER:OG	2.20	0.53
1:E:78:THR:HG22	1:E:80:LEU:H	1.73	0.53
1:F:52:ARG:HD3	1:F:80:LEU:HD22	1.91	0.53
1:I:86:LYS:O	1:I:90:LEU:N	2.42	0.53
1:K:5:LEU:HD12	1:K:27:TYR:HB3	1.91	0.53
1:N:47:LEU:HD13	1:N:111:ILE:HG23	1.91	0.53
1:L:116:ARG:HB3	4:L:266:HOH:O	2.09	0.53
1:C:110:ARG:NE	4:C:224:HOH:O	2.30	0.52
1:D:106:GLU:OE2	1:D:110:ARG:NH1	2.43	0.52
1:K:87:VAL:O	1:K:91:ASP:HB2	2.08	0.52
1:C:56:ASP:O	4:C:209:HOH:O	2.19	0.52
1:G:50:LEU:HB2	1:G:76:LEU:HD23	1.90	0.52
1:I:94:ALA:N	4:I:205:HOH:O	2.05	0.52
1:M:77:LEU:CD2	1:M:102:PHE:HZ	2.22	0.52
1:E:10:ASP:OD1	1:E:10:ASP:N	2.42	0.52
1:E:28:GLU:O	4:E:307:HOH:O	2.19	0.52
1:L:113:ALA:HA	1:L:116:ARG:NH2	2.25	0.52
1:C:105:ALA:HA	1:C:108:PHE:HB2	1.92	0.52
1:D:77:LEU:HD12	4:D:218:HOH:O	2.08	0.52
1:D:5:LEU:N	1:D:28:GLU:O	2.41	0.52
1:K:75:ILE:HD13	1:K:110:ARG:HB3	1.92	0.52
1:L:47:LEU:HD22	1:L:111:ILE:HG23	1.91	0.52
1:C:109:ALA:O	1:C:113:ALA:N	2.42	0.52
1:M:54:LEU:HB2	4:M:219:HOH:O	2.10	0.52
1:J:47:LEU:HB2	1:J:115:LEU:HD11	1.91	0.52
1:M:21:SER:HB3	1:M:108:PHE:HZ	1.75	0.52
1:N:34:ARG:HB3	1:N:56:ASP:HB2	1.91	0.51
1:B:99:THR:HA	4:B:323:HOH:O	2.08	0.51
1:K:53:GLN:HB2	4:K:278:HOH:O	2.11	0.51
1:B:8:VAL:HG12	1:B:32:VAL:HG22	1.92	0.51
1:E:90:LEU:HA	1:E:94:ALA:HB3	1.91	0.51
1:I:6:LEU:HB3	1:I:48:VAL:HG22	1.93	0.51
1:A:96:ASP:OD1	1:A:97:TYR:N	2.42	0.51
1:C:9:GLU:OE2	1:C:51:ASP:OD2	2.29	0.51
1:G:20:VAL:O	1:G:24:GLN:HB2	2.10	0.51
1:G:110:ARG:HG3	1:H:90:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:ARG:CG	1:M:35:ILE:H	2.24	0.51
1:F:78:THR:HG23	4:F:205:HOH:O	2.11	0.51
1:J:7:LEU:HD12	4:J:206:HOH:O	2.10	0.51
1:N:52:ARG:NH2	1:N:85:ASP:OD2	2.43	0.51
1:N:82:THR:HG1	1:N:85:ASP:H	1.58	0.51
1:C:5:LEU:HD23	1:C:47:LEU:HB3	1.92	0.51
1:K:74:VAL:HG13	1:K:94:ALA:HA	1.93	0.51
1:K:110:ARG:HB2	4:K:201:HOH:O	2.10	0.51
1:M:43:LYS:HD2	4:M:273:HOH:O	2.10	0.51
1:A:69:ILE:HG13	4:A:306:HOH:O	2.11	0.51
1:C:81:VAL:HG22	1:C:99:THR:HB	1.93	0.51
1:C:100:LYS:HB3	1:L:116:ARG:NH2	2.25	0.51
1:E:110:ARG:HH12	1:F:97:TYR:HB3	1.76	0.51
1:F:72:VAL:HG21	4:F:269:HOH:O	2.10	0.51
1:F:67:LYS:NZ	1:F:95:ASN:OD1	2.41	0.50
1:G:52:ARG:HB3	1:G:80:LEU:HD12	1.93	0.50
1:N:80:LEU:HB3	1:N:85:ASP:OD1	2.11	0.50
1:B:20:VAL:O	1:B:24:GLN:HB2	2.12	0.50
1:I:34:ARG:HG3	4:I:203:HOH:O	2.11	0.50
1:H:83:VAL:N	4:H:204:HOH:O	2.44	0.50
1:E:35:ILE:HD12	1:E:56:ASP:HB3	1.94	0.50
1:M:22:LEU:HD13	1:M:29:CYS:CB	2.40	0.50
1:M:22:LEU:HG	1:M:23:GLU:HG3	1.92	0.50
1:D:48:VAL:HG23	1:D:72:VAL:HG11	1.93	0.50
1:H:85:ASP:OD2	4:H:206:HOH:O	2.19	0.50
1:J:50:LEU:HD21	1:J:59:SER:HB2	1.93	0.50
1:C:82:THR:N	4:C:229:HOH:O	2.45	0.50
1:C:101:PRO:HA	1:L:116:ARG:CZ	2.42	0.50
1:I:86:LYS:N	4:I:207:HOH:O	2.14	0.50
1:M:70:LYS:HE2	1:M:72:VAL:HG22	1.94	0.50
1:C:101:PRO:HB3	1:L:116:ARG:HD2	1.93	0.50
1:A:32:VAL:HG13	1:A:37:ASP:HB3	1.94	0.50
1:L:45:ALA:HB3	4:L:220:HOH:O	2.11	0.50
1:A:48:VAL:HG23	1:A:72:VAL:HG11	1.93	0.50
1:D:90:LEU:HD11	1:D:97:TYR:CB	2.41	0.50
1:F:39:GLU:OE2	4:F:207:HOH:O	2.20	0.50
1:K:13:ASN:N	4:K:212:HOH:O	2.22	0.50
1:A:28:GLU:CD	4:A:301:HOH:O	2.30	0.49
1:K:19:LEU:O	1:K:23:GLU:HG3	2.12	0.49
1:K:111:ILE:HA	4:K:209:HOH:O	2.11	0.49
1:M:34:ARG:NE	1:M:56:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:ARG:HE	1:M:56:ASP:HB2	1.76	0.49
1:N:4:THR:OG1	1:N:46:ASP:N	2.45	0.49
1:G:81:VAL:HG11	1:G:99:THR:HB	1.93	0.49
1:M:9:GLU:HB3	1:M:31:HIS:NE2	2.27	0.49
1:M:37:ASP:HA	1:M:40:PRO:HD2	1.93	0.49
1:N:50:LEU:HB3	1:N:76:LEU:HD23	1.94	0.49
1:A:67:LYS:NZ	1:A:71:ASP:OD1	2.31	0.49
1:C:9:GLU:OE2	1:C:51:ASP:CB	2.60	0.49
1:C:85:ASP:O	4:C:211:HOH:O	2.19	0.49
1:J:67:LYS:HE2	1:J:72:VAL:O	2.12	0.49
1:A:98:LEU:HD21	1:A:102:PHE:HB2	1.94	0.49
1:G:50:LEU:HD11	1:G:63:LEU:HD13	1.94	0.49
1:H:52:ARG:NH1	1:H:97:TYR:OH	2.45	0.49
1:A:35:ILE:HG21	1:A:62:HIS:CE1	2.47	0.49
1:A:81:VAL:HG12	1:A:99:THR:HB	1.95	0.49
1:E:117:ALA:HB2	4:E:309:HOH:O	2.12	0.49
1:L:83:VAL:O	1:L:87:VAL:HG23	2.12	0.49
1:C:21:SER:HA	1:C:24:GLN:HB2	1.95	0.49
1:K:98:LEU:HD13	1:K:102:PHE:CD1	2.48	0.49
1:N:7:LEU:HD21	1:N:15:ALA:HB1	1.95	0.49
1:B:78:THR:OG1	2:B:201:BEF:F3	2.11	0.49
1:D:58:ASP:OD2	1:D:59:SER:N	2.45	0.49
1:C:50:LEU:O	1:C:76:LEU:HD23	2.12	0.49
1:K:95:ASN:ND2	1:K:114:GLN:OE1	2.46	0.49
1:G:6:LEU:HA	4:G:211:HOH:O	2.13	0.48
1:G:75:ILE:HG21	1:G:107:LEU:HD11	1.95	0.48
1:H:74:VAL:HG23	1:H:94:ALA:HA	1.94	0.48
1:M:100:LYS:O	4:M:217:HOH:O	2.19	0.48
1:B:88:ALA:O	4:B:310:HOH:O	2.20	0.48
1:G:52:ARG:HB2	1:G:78:THR:CG2	2.32	0.48
1:K:33:GLU:O	4:K:210:HOH:O	2.20	0.48
1:M:20:VAL:O	1:M:24:GLN:NE2	2.46	0.48
1:A:78:THR:HG23	1:A:80:LEU:H	1.79	0.48
1:D:8:VAL:HB	1:D:50:LEU:HD12	1.95	0.48
1:M:34:ARG:HB3	4:M:227:HOH:O	2.13	0.48
1:G:82:THR:HG21	4:G:275:HOH:O	2.14	0.48
1:E:111:ILE:HG13	1:E:112:ARG:N	2.28	0.48
1:B:115:LEU:HD23	4:B:356:HOH:O	2.14	0.48
1:C:78:THR:O	4:C:204:HOH:O	2.20	0.48
1:K:47:LEU:HD11	4:K:209:HOH:O	2.12	0.48
1:M:17:GLY:O	4:M:206:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLN:NE2	4:B:313:HOH:O	2.31	0.48
1:C:96:ASP:O	4:C:212:HOH:O	2.20	0.48
1:D:112:ARG:NH2	4:D:221:HOH:O	2.45	0.48
1:K:17:GLY:O	4:K:211:HOH:O	2.20	0.48
1:L:30:LEU:HD23	1:L:30:LEU:HA	1.72	0.48
1:N:7:LEU:HA	4:N:204:HOH:O	2.13	0.48
1:C:4:THR:HB	1:C:45:ALA:HA	1.95	0.48
1:C:96:ASP:CG	1:C:110:ARG:HH11	2.16	0.48
1:N:7:LEU:N	1:N:30:LEU:O	2.28	0.48
1:D:70:LYS:NZ	4:D:206:HOH:O	2.32	0.48
1:F:44:LYS:NZ	1:M:39:GLU:OE2	2.47	0.48
1:B:6:LEU:HB2	1:B:45:ALA:HB2	1.95	0.47
1:B:35:ILE:HB	1:B:56:ASP:HB3	1.94	0.47
1:G:4:THR:OG1	1:G:46:ASP:OD2	2.19	0.47
1:J:67:LYS:NZ	1:J:93:GLY:O	2.39	0.47
1:L:13:ASN:O	4:L:209:HOH:O	2.20	0.47
1:N:14:LEU:O	1:N:18:LEU:HD12	2.14	0.47
1:N:35:ILE:O	1:N:38:VAL:HG22	2.14	0.47
1:E:30:LEU:HD22	1:E:41:GLN:HE22	1.78	0.47
1:E:81:VAL:HG12	1:E:99:THR:HB	1.95	0.47
1:E:111:ILE:O	1:E:115:LEU:HG	2.14	0.47
1:F:47:LEU:HB2	1:F:115:LEU:HD21	1.97	0.47
1:M:77:LEU:CD2	1:M:102:PHE:CZ	2.97	0.47
1:D:67:LYS:NZ	1:D:72:VAL:O	2.41	0.47
1:L:52:ARG:NH2	1:L:58:ASP:OD2	2.48	0.47
1:D:99:THR:N	4:D:218:HOH:O	2.47	0.47
1:G:67:LYS:NZ	4:G:205:HOH:O	2.26	0.47
1:G:90:LEU:HA	1:G:94:ALA:HB3	1.96	0.47
1:I:3:GLN:N	4:I:221:HOH:O	2.47	0.47
1:B:72:VAL:O	1:B:74:VAL:HG23	2.14	0.47
1:F:5:LEU:O	1:F:29:CYS:HA	2.14	0.47
1:I:58:ASP:OD1	1:I:59:SER:N	2.47	0.47
1:J:75:ILE:HG13	4:J:212:HOH:O	2.14	0.47
1:M:82:THR:O	1:M:86:LYS:N	2.42	0.47
1:M:106:GLU:O	1:M:109:ALA:HB3	2.14	0.47
1:C:50:LEU:HD11	1:C:66:TRP:HZ3	1.80	0.47
1:D:47:LEU:HD13	1:D:115:LEU:HG	1.96	0.47
1:G:25:ALA:O	4:G:213:HOH:O	2.20	0.47
1:B:7:LEU:HA	1:B:49:ILE:HB	1.96	0.47
1:H:18:LEU:O	1:H:22:LEU:HD12	2.15	0.47
1:I:82:THR:OG1	1:I:85:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:ARG:HD3	4:J:205:HOH:O	2.15	0.47
1:K:46:ASP:O	1:K:73:PRO:HD2	2.14	0.47
1:K:52:ARG:NH2	1:K:85:ASP:O	2.37	0.47
1:L:73:PRO:HB3	1:L:114:GLN:HB3	1.96	0.47
1:M:27:TYR:HB3	4:M:208:HOH:O	2.14	0.47
1:N:50:LEU:O	1:N:76:LEU:HA	2.14	0.47
1:C:9:GLU:OE2	1:C:51:ASP:HB2	2.14	0.47
1:C:52:ARG:HG3	1:C:76:LEU:HD22	1.97	0.47
1:J:7:LEU:HD21	1:J:15:ALA:HB1	1.95	0.47
1:F:93:GLY:HA3	4:F:202:HOH:O	2.15	0.47
1:A:10:ASP:HB3	1:A:54:LEU:HD13	1.96	0.47
1:H:48:VAL:HG12	1:H:50:LEU:HD22	1.96	0.47
1:H:51:ASP:OD2	1:H:100:LYS:NZ	2.44	0.47
1:B:76:LEU:HG	4:B:328:HOH:O	2.14	0.46
1:D:90:LEU:CD1	1:D:97:TYR:HB2	2.43	0.46
1:F:11:ASP:OD1	1:F:12:LYS:N	2.47	0.46
1:M:51:ASP:O	1:M:59:SER:OG	2.19	0.46
1:M:57:GLY:N	4:M:219:HOH:O	2.47	0.46
1:F:98:LEU:HD13	1:F:110:ARG:HD2	1.97	0.46
1:G:70:LYS:NZ	4:G:225:HOH:O	2.36	0.46
1:H:63:LEU:HD11	4:H:235:HOH:O	2.14	0.46
1:L:32:VAL:HG13	1:L:37:ASP:HB2	1.97	0.46
1:M:34:ARG:O	1:M:38:VAL:HG23	2.15	0.46
1:M:77:LEU:HD21	1:M:102:PHE:HZ	1.79	0.46
1:N:63:LEU:HD11	1:N:67:LYS:NZ	2.30	0.46
1:G:87:VAL:HG22	1:H:106:GLU:HA	1.96	0.46
1:H:8:VAL:HG12	1:H:32:VAL:CG2	2.41	0.46
1:L:50:LEU:HB2	1:L:76:LEU:HD23	1.97	0.46
1:M:100:LYS:HG2	1:M:102:PHE:CE2	2.46	0.46
1:N:79:ALA:HB2	1:N:100:LYS:HE2	1.97	0.46
1:B:20:VAL:HG13	1:K:34:ARG:NH1	2.28	0.46
1:F:6:LEU:O	1:F:49:ILE:N	2.38	0.46
4:H:210:HOH:O	1:N:109:ALA:HB1	2.14	0.46
1:C:113:ALA:HB2	1:D:90:LEU:HB3	1.97	0.46
1:K:116:ARG:NH1	4:K:225:HOH:O	2.38	0.46
1:L:46:ASP:N	4:L:226:HOH:O	2.48	0.46
1:M:22:LEU:HG	1:M:23:GLU:N	2.31	0.46
1:M:34:ARG:HG2	1:M:35:ILE:H	1.80	0.46
1:M:52:ARG:N	1:M:78:THR:OG1	2.36	0.46
1:N:9:GLU:HG3	1:N:11:ASP:N	2.30	0.46
1:G:87:VAL:HG13	1:H:109:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:O	1:D:38:VAL:HG22	2.16	0.46
1:E:47:LEU:HD11	1:E:75:ILE:HD11	1.97	0.46
1:M:34:ARG:NH2	4:M:228:HOH:O	2.45	0.46
1:G:86:LYS:HE2	1:G:99:THR:HG22	1.97	0.46
1:E:48:VAL:HB	1:E:74:VAL:HG23	1.98	0.46
1:I:110:ARG:HB3	4:I:223:HOH:O	2.16	0.46
1:E:91:ASP:HA	4:E:302:HOH:O	2.16	0.45
1:I:110:ARG:NE	4:I:223:HOH:O	2.49	0.45
1:F:105:ALA:N	4:F:225:HOH:O	2.47	0.45
1:G:4:THR:O	1:G:5:LEU:HD23	2.16	0.45
1:F:28:GLU:N	4:F:213:HOH:O	2.47	0.45
1:M:5:LEU:HB2	1:M:29:CYS:SG	2.57	0.45
1:M:22:LEU:HD13	1:M:29:CYS:SG	2.55	0.45
1:D:26:GLY:HA3	4:D:204:HOH:O	2.16	0.45
1:E:42:TRP:CE2	1:E:66:TRP:HB3	2.51	0.45
1:F:18:LEU:O	1:F:22:LEU:HD12	2.16	0.45
1:I:52:ARG:HB3	1:I:78:THR:HG21	1.98	0.45
1:N:51:ASP:OD1	1:N:52:ARG:N	2.50	0.45
1:F:51:ASP:OD1	1:F:52:ARG:N	2.49	0.45
1:G:112:ARG:NH2	1:H:91:ASP:OD1	2.46	0.45
1:I:47:LEU:HD12	1:I:73:PRO:HB2	1.97	0.45
1:I:70:LYS:HG3	1:I:72:VAL:HG13	1.98	0.45
1:L:80:LEU:HB3	1:L:85:ASP:CG	2.35	0.45
1:M:34:ARG:N	4:M:227:HOH:O	2.48	0.45
1:A:96:ASP:OD2	4:A:312:HOH:O	2.21	0.45
1:D:68:LYS:HD3	1:D:68:LYS:HA	1.68	0.45
1:K:98:LEU:HD23	1:K:98:LEU:HA	1.80	0.45
1:G:59:SER:N	4:G:209:HOH:O	2.00	0.45
1:I:8:VAL:HG13	1:I:32:VAL:HG23	1.98	0.45
1:I:97:TYR:O	1:I:110:ARG:NH1	2.50	0.45
1:A:46:ASP:OD2	1:A:46:ASP:N	2.49	0.45
1:B:31:HIS:ND1	1:K:37:ASP:OD1	2.49	0.45
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.83	0.45
1:L:35:ILE:HG23	1:L:66:TRP:HH2	1.81	0.45
1:C:96:ASP:N	4:C:212:HOH:O	2.48	0.45
1:E:49:ILE:HG22	1:E:77:LEU:HB2	1.99	0.45
1:F:7:LEU:HA	1:F:49:ILE:HB	1.99	0.45
1:G:32:VAL:HG11	1:G:38:VAL:HG22	1.99	0.45
1:H:8:VAL:HG22	1:H:50:LEU:HA	1.99	0.45
1:H:26:GLY:O	4:H:207:HOH:O	2.20	0.45
1:I:47:LEU:HD21	1:I:75:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:60:VAL:HG23	1:M:92:SER:CB	2.38	0.45
1:C:40:PRO:N	4:C:201:HOH:O	2.50	0.44
1:G:10:ASP:OD1	1:G:11:ASP:N	2.46	0.44
1:G:12:LYS:NZ	4:G:208:HOH:O	1.99	0.44
1:G:102:PHE:HB2	4:G:207:HOH:O	2.16	0.44
1:M:22:LEU:HB2	1:M:27:TYR:HB2	1.99	0.44
1:C:9:GLU:OE2	1:C:51:ASP:CG	2.56	0.44
1:G:42:TRP:CZ3	1:G:48:VAL:HG11	2.53	0.44
1:H:86:LYS:O	1:H:90:LEU:HD23	2.17	0.44
1:H:101:PRO:HG3	1:N:112:ARG:HG3	2.00	0.44
1:E:4:THR:HA	1:E:28:GLU:O	2.18	0.44
1:H:6:LEU:HB3	1:H:48:VAL:HA	1.99	0.44
1:L:113:ALA:HA	1:L:116:ARG:HH22	1.82	0.44
1:A:52:ARG:HG2	1:A:60:VAL:HG23	2.00	0.44
1:F:112:ARG:NH1	4:F:226:HOH:O	2.50	0.44
1:G:98:LEU:HD12	1:G:99:THR:N	2.31	0.44
1:H:78:THR:OG1	1:H:79:ALA:N	2.51	0.44
1:H:90:LEU:HD21	1:H:97:TYR:HB2	1.99	0.44
1:H:95:ASN:HB2	4:H:216:HOH:O	2.18	0.44
1:I:41:GLN:HA	1:I:44:LYS:HE2	1.98	0.44
1:E:100:LYS:HG2	1:E:102:PHE:HD2	1.83	0.44
1:C:110:ARG:N	4:C:235:HOH:O	2.51	0.44
1:H:70:LYS:HG2	1:H:72:VAL:HG23	1.98	0.44
1:I:5:LEU:HD22	1:I:47:LEU:HB3	2.00	0.44
1:L:12:LYS:H	1:L:12:LYS:HG3	1.63	0.44
1:D:51:ASP:HA	1:D:77:LEU:O	2.18	0.44
1:H:38:VAL:HG12	4:H:213:HOH:O	2.17	0.44
1:K:9:GLU:HG2	1:K:15:ALA:HB2	2.00	0.44
1:M:77:LEU:O	1:M:77:LEU:CD1	2.65	0.44
1:N:43:LYS:HE2	1:N:43:LYS:HB2	1.79	0.44
1:D:98:LEU:HD12	1:D:98:LEU:HA	1.82	0.43
1:H:18:LEU:HG	1:H:22:LEU:HD11	2.00	0.43
1:E:32:VAL:HG12	4:E:313:HOH:O	2.18	0.43
1:E:49:ILE:HG21	1:E:77:LEU:HD12	2.00	0.43
1:E:50:LEU:O	1:E:76:LEU:HA	2.18	0.43
1:H:49:ILE:HD11	1:H:111:ILE:HD11	2.00	0.43
1:I:35:ILE:HG12	1:I:54:LEU:HD13	1.99	0.43
1:M:86:LYS:HA	4:M:220:HOH:O	2.18	0.43
1:N:58:ASP:OD2	1:N:60:VAL:HB	2.18	0.43
1:D:63:LEU:HG	1:D:93:GLY:HA3	1.99	0.43
1:J:116:ARG:NH2	4:J:222:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:ILE:O	1:M:38:VAL:HB	2.18	0.43
1:C:54:LEU:HB3	1:C:55:PRO:HD2	1.99	0.43
1:D:12:LYS:O	1:D:16:ASP:HB2	2.18	0.43
1:E:42:TRP:CZ2	1:E:66:TRP:HB3	2.54	0.43
1:H:35:ILE:H	1:H:56:ASP:CB	2.31	0.43
1:H:68:LYS:HA	1:H:68:LYS:HD3	1.71	0.43
1:I:52:ARG:HD3	1:I:80:LEU:HD12	1.99	0.43
1:K:5:LEU:HD23	1:K:47:LEU:HB3	2.00	0.43
1:I:78:THR:OG1	1:I:79:ALA:N	2.48	0.43
1:N:40:PRO:O	1:N:44:LYS:HE3	2.18	0.43
1:N:78:THR:OG1	1:N:79:ALA:N	2.52	0.43
1:C:29:CYS:SG	4:C:283:HOH:O	2.50	0.43
1:E:52:ARG:HB2	1:E:78:THR:CG2	2.49	0.43
1:G:47:LEU:CD1	1:G:73:PRO:HB2	2.49	0.43
1:L:7:LEU:N	1:L:30:LEU:O	2.32	0.43
1:B:10:ASP:OD2	1:B:10:ASP:N	2.45	0.43
1:C:20:VAL:O	1:C:24:GLN:N	2.48	0.43
1:E:84:LYS:NZ	4:E:317:HOH:O	2.38	0.43
1:I:61:GLN:HB2	4:I:210:HOH:O	2.19	0.43
1:J:49:ILE:O	4:J:206:HOH:O	2.21	0.43
1:M:12:LYS:NZ	4:M:201:HOH:O	1.88	0.43
1:C:10:ASP:HB3	1:C:54:LEU:HD22	2.00	0.43
1:C:52:ARG:HB2	1:C:78:THR:CB	2.48	0.43
1:E:7:LEU:O	1:E:32:VAL:N	2.48	0.43
1:E:87:VAL:O	1:E:91:ASP:HB2	2.19	0.43
1:N:44:LYS:NZ	4:N:218:HOH:O	2.52	0.43
1:A:52:ARG:HD3	1:A:78:THR:HG21	2.00	0.43
1:F:52:ARG:NH2	4:F:227:HOH:O	2.52	0.43
1:G:110:ARG:NH1	4:G:226:HOH:O	2.38	0.43
1:I:47:LEU:HA	4:I:213:HOH:O	2.18	0.43
1:I:58:ASP:O	4:I:210:HOH:O	2.22	0.43
1:M:77:LEU:O	1:M:77:LEU:HD13	2.19	0.43
1:D:22:LEU:HD21	1:D:111:ILE:HD13	2.01	0.42
1:E:6:LEU:HD23	1:E:48:VAL:HG13	2.01	0.42
1:F:86:LYS:HG2	1:F:97:TYR:CE1	2.54	0.42
1:G:96:ASP:OD1	1:H:110:ARG:NH2	2.52	0.42
1:H:82:THR:CG2	4:H:204:HOH:O	2.43	0.42
1:L:63:LEU:HD13	4:L:233:HOH:O	2.19	0.42
1:B:9:GLU:HG3	1:B:11:ASP:H	1.84	0.42
1:E:5:LEU:N	4:E:307:HOH:O	2.49	0.42
1:G:52:ARG:HA	4:G:209:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:LEU:HD13	1:J:30:LEU:HD12	1.99	0.42
1:L:24:GLN:HG3	1:L:25:ALA:N	2.34	0.42
1:N:42:TRP:NE1	1:N:66:TRP:O	2.52	0.42
1:G:81:VAL:CG1	1:G:99:THR:HB	2.48	0.42
1:K:47:LEU:HD13	1:K:111:ILE:HG23	2.01	0.42
1:M:89:GLY:HA2	1:M:92:SER:CB	2.47	0.42
1:C:12:LYS:HA	1:C:15:ALA:HB3	2.01	0.42
1:E:91:ASP:OD1	1:F:112:ARG:NH2	2.37	0.42
1:B:22:LEU:HA	1:B:108:PHE:HE1	1.85	0.42
1:G:20:VAL:HA	1:G:23:GLU:HB2	2.02	0.42
1:J:48:VAL:HG23	1:J:72:VAL:HG11	2.01	0.42
1:B:12:LYS:HA	1:B:12:LYS:HD2	1.87	0.42
1:F:47:LEU:HD12	1:F:73:PRO:HB2	2.01	0.42
1:B:77:LEU:HB3	4:B:325:HOH:O	2.18	0.42
1:C:12:LYS:O	1:C:16:ASP:N	2.52	0.42
1:E:116:ARG:H	1:E:116:ARG:HG2	1.53	0.42
1:B:22:LEU:HA	1:B:108:PHE:CE1	2.54	0.42
1:L:4:THR:OG1	1:L:45:ALA:HA	2.19	0.42
1:M:84:LYS:H	1:M:84:LYS:HG2	1.61	0.42
1:G:47:LEU:HD12	1:G:73:PRO:HB2	2.02	0.42
1:I:48:VAL:O	1:I:74:VAL:HG23	2.19	0.42
1:K:107:LEU:HD12	4:K:201:HOH:O	2.19	0.42
1:L:11:ASP:HB3	1:L:14:LEU:HG	2.02	0.42
1:N:117:ALA:O	4:N:205:HOH:O	2.22	0.42
1:F:8:VAL:HG22	1:F:32:VAL:HB	2.01	0.42
1:G:24:GLN:NE2	4:G:232:HOH:O	2.53	0.42
1:K:20:VAL:O	1:K:24:GLN:N	2.53	0.42
1:D:47:LEU:HB2	1:D:115:LEU:HD21	2.01	0.41
1:F:31:HIS:N	1:M:36:ALA:HB1	2.30	0.41
1:G:32:VAL:HG21	1:G:37:ASP:HB2	2.01	0.41
1:D:89:GLY:HA3	1:D:97:TYR:CE2	2.55	0.41
1:J:114:GLN:HG3	4:J:253:HOH:O	2.20	0.41
1:A:63:LEU:HD11	1:A:74:VAL:HG21	2.02	0.41
1:G:53:GLN:HB3	4:G:229:HOH:O	2.19	0.41
1:C:77:LEU:HA	1:C:98:LEU:O	2.20	0.41
1:D:63:LEU:HD23	1:D:92:SER:O	2.20	0.41
1:G:35:ILE:HG23	1:G:66:TRP:CH2	2.48	0.41
1:H:61:GLN:OE1	1:H:62:HIS:NE2	2.54	0.41
1:I:100:LYS:HE3	1:I:102:PHE:HE2	1.85	0.41
1:M:33:GLU:HB3	4:M:212:HOH:O	2.20	0.41
1:A:79:ALA:HB1	1:I:109:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASP:C	1:B:13:ASN:H	2.23	0.41
1:L:22:LEU:HB3	1:L:29:CYS:SG	2.60	0.41
1:N:6:LEU:O	4:N:204:HOH:O	2.21	0.41
1:B:16:ASP:OD1	1:K:34:ARG:NE	2.54	0.41
1:C:96:ASP:OD1	1:C:97:TYR:N	2.48	0.41
1:F:52:ARG:HH11	1:F:85:ASP:HB3	1.85	0.41
1:H:112:ARG:NE	4:H:221:HOH:O	2.35	0.41
1:I:85:ASP:N	4:I:207:HOH:O	2.53	0.41
1:M:35:ILE:HG23	1:M:66:TRP:CH2	2.55	0.41
1:N:33:GLU:HB2	4:N:232:HOH:O	2.21	0.41
1:N:52:ARG:HB3	4:N:234:HOH:O	2.19	0.41
1:N:6:LEU:HA	1:N:30:LEU:HB2	2.03	0.41
1:N:19:LEU:HD21	1:N:31:HIS:HB2	2.01	0.41
1:A:33:GLU:O	1:A:54:LEU:HD12	2.21	0.41
1:G:19:LEU:HD23	1:G:19:LEU:HA	1.87	0.41
1:K:58:ASP:HB3	1:K:61:GLN:HE21	1.85	0.41
1:N:14:LEU:HD11	1:N:102:PHE:CE1	2.51	0.41
1:N:63:LEU:HD11	1:N:67:LYS:HZ2	1.85	0.41
1:C:39:GLU:HB2	1:C:40:PRO:HD3	2.02	0.41
1:C:101:PRO:HD2	1:L:112:ARG:HH21	1.86	0.41
4:E:302:HOH:O	1:F:116:ARG:NH2	2.43	0.41
1:H:43:LYS:HE2	1:H:69:ILE:HG22	2.02	0.41
1:I:72:VAL:HB	4:I:213:HOH:O	2.20	0.41
1:J:106:GLU:HG3	1:J:110:ARG:HH11	1.86	0.41
1:L:70:LYS:HG3	1:L:72:VAL:HG13	2.03	0.41
4:B:305:HOH:O	1:C:62:HIS:CD2	2.73	0.41
1:H:96:ASP:HB2	4:H:216:HOH:O	2.20	0.41
1:I:68:LYS:N	1:I:68:LYS:HD2	2.36	0.41
1:M:70:LYS:HE2	1:M:70:LYS:HB3	1.83	0.41
1:J:98:LEU:HD23	1:J:107:LEU:HD13	2.03	0.40
1:K:75:ILE:HD11	4:K:232:HOH:O	2.21	0.40
1:L:5:LEU:HD22	1:L:22:LEU:HD12	2.03	0.40
1:N:98:LEU:HD12	1:N:98:LEU:HA	1.84	0.40
1:K:77:LEU:HD12	1:K:77:LEU:HA	1.87	0.40
1:M:50:LEU:HD12	1:M:74:VAL:HG11	2.03	0.40
1:B:50:LEU:HB3	1:B:76:LEU:HD23	2.03	0.40
1:L:49:ILE:HG22	4:L:235:HOH:O	2.20	0.40
1:L:57:GLY:HA3	4:L:215:HOH:O	2.21	0.40
1:N:63:LEU:HB3	4:N:206:HOH:O	2.20	0.40
1:E:106:GLU:O	1:E:110:ARG:HG3	2.22	0.40
1:F:81:VAL:O	4:F:210:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:ALA:N	4:G:207:HOH:O	2.11	0.40
1:N:10:ASP:OD1	1:N:55:PRO:HD3	2.21	0.40
1:B:7:LEU:O	1:B:31:HIS:HA	2.22	0.40
1:C:103:ALA:HB3	1:C:106:GLU:HB2	2.04	0.40
1:K:34:ARG:HH11	1:K:34:ARG:HD3	1.77	0.40
1:L:12:LYS:N	4:L:206:HOH:O	2.55	0.40
1:L:63:LEU:O	4:L:210:HOH:O	2.22	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:460:HOH:O	4:K:344:HOH:O[6_764]	2.03	0.17
4:I:275:HOH:O	4:J:335:HOH:O[6_764]	2.04	0.16
4:E:398:HOH:O	4:N:376:HOH:O[6_764]	2.05	0.15
4:G:237:HOH:O	4:H:271:HOH:O[6_654]	2.10	0.10
1:D:36:ALA:O	4:E:303:HOH:O[3_685]	2.14	0.06
4:D:446:HOH:O	4:G:411:HOH:O[3_685]	2.19	0.01
4:E:359:HOH:O	4:K:276:HOH:O[6_764]	2.19	0.01

## 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	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
1	B	113/117 (97%)	105 (93%)	8 (7%)	0	100	100
1	C	113/117 (97%)	106 (94%)	7 (6%)	0	100	100
1	D	113/117 (97%)	106 (94%)	7 (6%)	0	100	100
1	E	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
1	F	113/117 (97%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	113/117 (97%)	106 (94%)	7 (6%)	0	100	100
1	H	113/117 (97%)	104 (92%)	9 (8%)	0	100	100
1	I	113/117 (97%)	101 (89%)	12 (11%)	0	100	100
1	J	113/117 (97%)	105 (93%)	7 (6%)	1 (1%)	17	46
1	K	113/117 (97%)	99 (88%)	12 (11%)	2 (2%)	8	28
1	L	113/117 (97%)	106 (94%)	7 (6%)	0	100	100
1	M	113/117 (97%)	105 (93%)	8 (7%)	0	100	100
1	N	113/117 (97%)	102 (90%)	11 (10%)	0	100	100
All	All	1583/1638 (97%)	1471 (93%)	109 (7%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	83	VAL
1	J	93	GLY
1	K	81	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	99/100 (99%)	95 (96%)	4 (4%)	31	65
1	B	98/100 (98%)	98 (100%)	0	100	100
1	C	98/100 (98%)	95 (97%)	3 (3%)	40	74
1	D	98/100 (98%)	96 (98%)	2 (2%)	55	84
1	E	98/100 (98%)	96 (98%)	2 (2%)	55	84
1	F	98/100 (98%)	95 (97%)	3 (3%)	40	74
1	G	98/100 (98%)	97 (99%)	1 (1%)	76	93
1	H	98/100 (98%)	93 (95%)	5 (5%)	24	55
1	I	98/100 (98%)	91 (93%)	7 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	98/100 (98%)	97 (99%)	1 (1%)	76	93
1	K	98/100 (98%)	95 (97%)	3 (3%)	40	74
1	L	98/100 (98%)	94 (96%)	4 (4%)	30	64
1	M	98/100 (98%)	92 (94%)	6 (6%)	18	48
1	N	98/100 (98%)	94 (96%)	4 (4%)	30	64
All	All	1373/1400 (98%)	1328 (97%)	45 (3%)	38	72

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	46	ASP
1	A	97	TYR
1	A	98	LEU
1	C	50	LEU
1	C	77	LEU
1	C	100	LYS
1	D	18	LEU
1	D	39	GLU
1	E	13	ASN
1	E	77	LEU
1	F	22	LEU
1	F	76	LEU
1	F	92	SER
1	G	46	ASP
1	H	47	LEU
1	H	50	LEU
1	H	80	LEU
1	H	96	ASP
1	H	114	GLN
1	I	11	ASP
1	I	13	ASN
1	I	21	SER
1	I	34	ARG
1	I	56	ASP
1	I	68	LYS
1	I	108	PHE
1	J	96	ASP
1	K	34	ARG
1	K	90	LEU

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Mol	Chain	Res	Type
1	K	92	SER
1	L	19	LEU
1	L	44	LYS
1	L	53	GLN
1	L	58	ASP
1	M	12	LYS
1	M	22	LEU
1	M	28	GLU
1	M	47	LEU
1	M	97	TYR
1	M	112	ARG
1	N	28	GLU
1	N	29	CYS
1	N	34	ARG
1	N	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	GLN
1	D	114	GLN
1	E	24	GLN
1	G	24	GLN
1	H	114	GLN
1	J	53	GLN
1	K	53	GLN
1	L	114	GLN
1	M	24	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
2	BEF	B	201	-	0,3,3	-	-	-		
2	BEF	A	201	1	0,3,3	-	-	-		
2	BEF	E	201	-	0,3,3	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

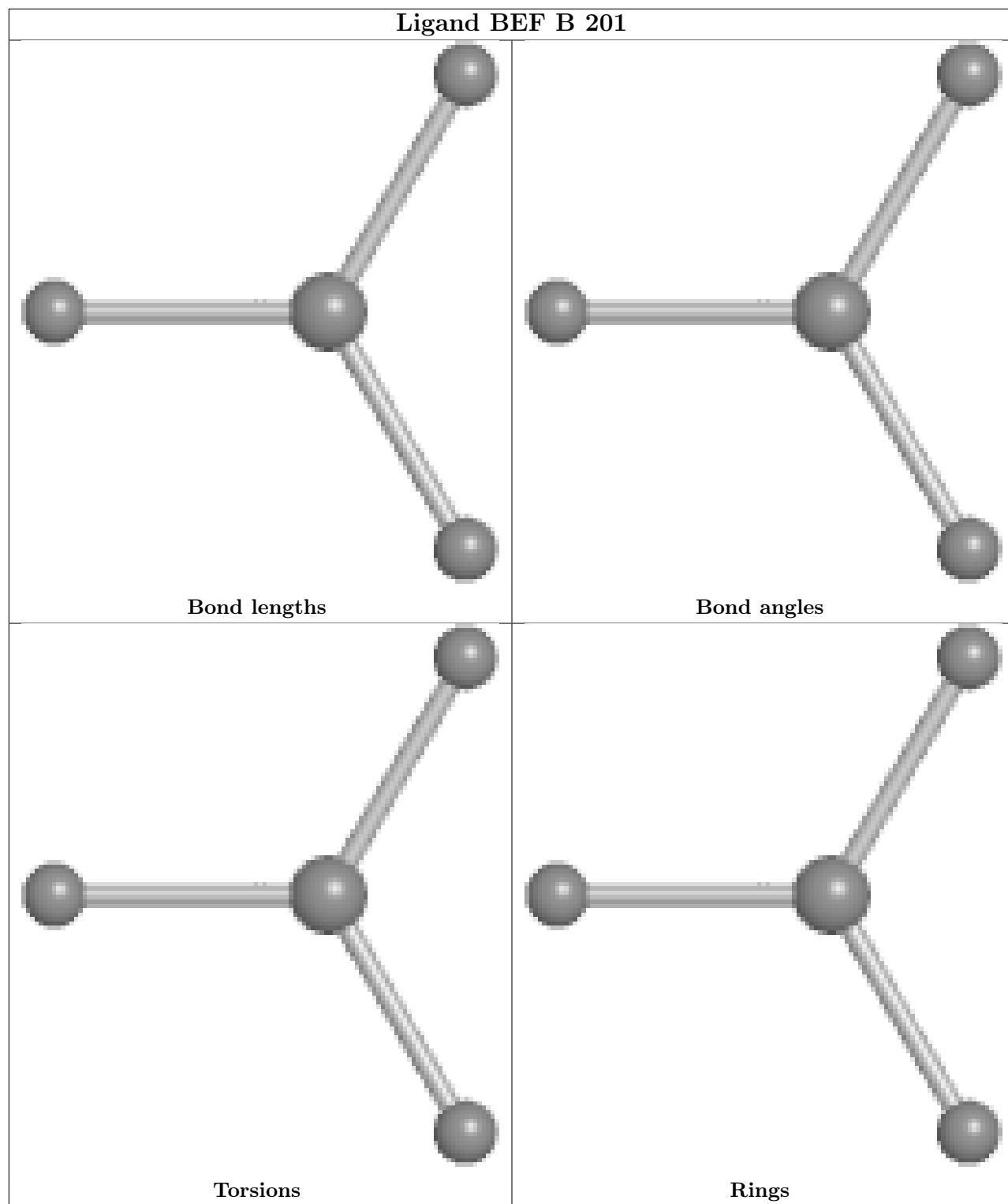
There are no torsion outliers.

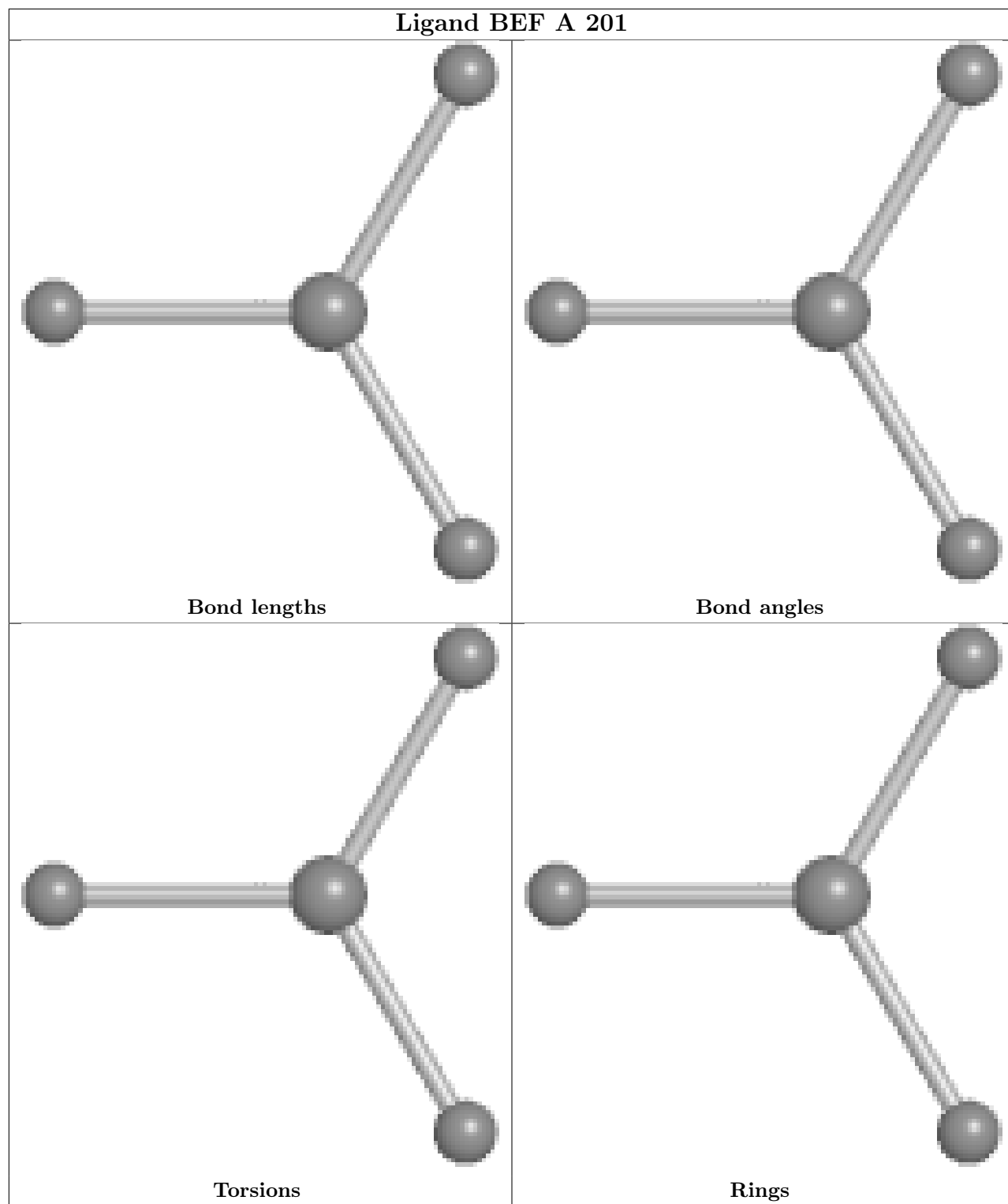
There are no ring outliers.

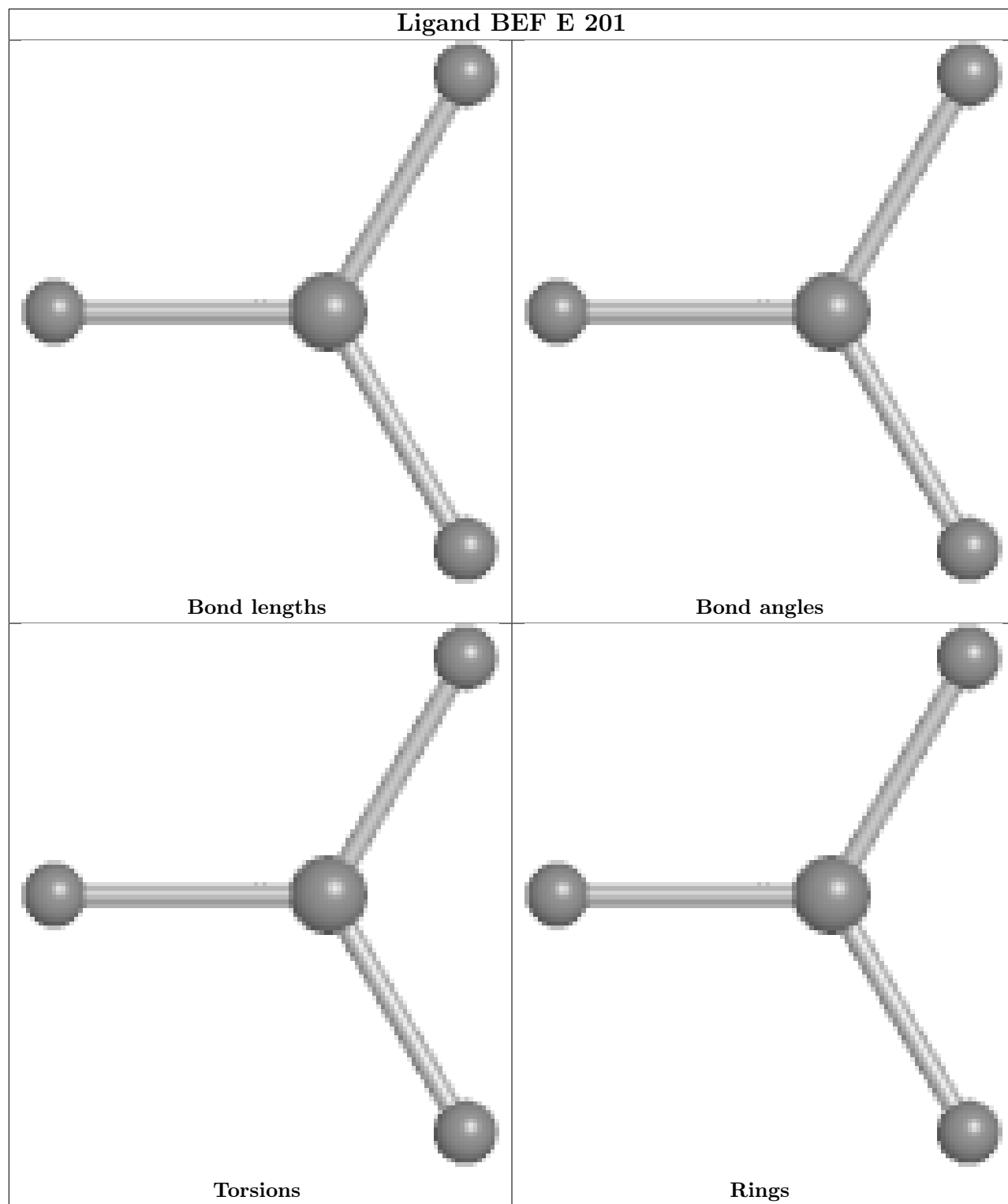
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	BEF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

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 [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, 95<sup>th</sup> 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(Å²)	Q<0.9	
1	A	116/117 (99%)	-0.75	0	100	100	12, 24, 39, 47	0
1	B	115/117 (98%)	-0.77	0	100	100	13, 23, 35, 44	0
1	C	115/117 (98%)	-0.58	0	100	100	17, 33, 48, 54	0
1	D	115/117 (98%)	-0.57	0	100	100	22, 32, 49, 54	0
1	E	115/117 (98%)	-0.57	0	100	100	26, 38, 48, 54	0
1	F	115/117 (98%)	-0.70	0	100	100	19, 32, 44, 52	0
1	G	115/117 (98%)	-0.41	0	100	100	31, 46, 59, 71	0
1	H	115/117 (98%)	-0.35	0	100	100	31, 46, 59, 64	0
1	I	115/117 (98%)	-0.68	0	100	100	22, 37, 56, 68	0
1	J	115/117 (98%)	-0.77	0	100	100	16, 28, 38, 45	0
1	K	115/117 (98%)	-0.60	1 (0%)	84	80	18, 35, 50, 80	0
1	L	115/117 (98%)	-0.49	0	100	100	31, 45, 57, 67	0
1	M	115/117 (98%)	-0.35	0	100	100	29, 48, 67, 72	0
1	N	115/117 (98%)	-0.35	0	100	100	33, 47, 59, 69	0
All	All	1611/1638 (98%)	-0.57	1 (0%)	95	95	12, 37, 56, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	117	ALA	3.6

### 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](#)

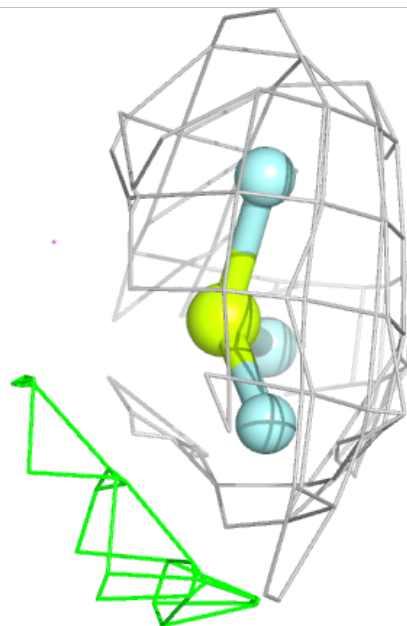
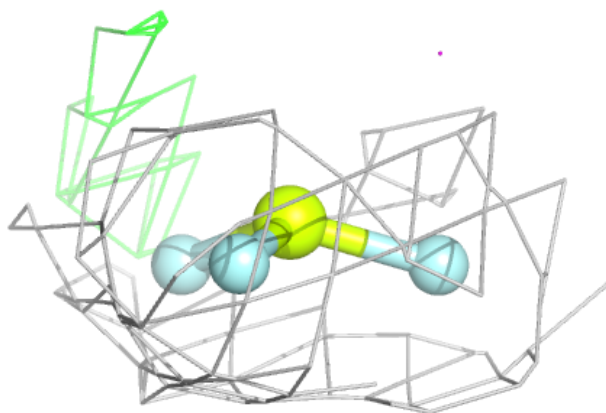
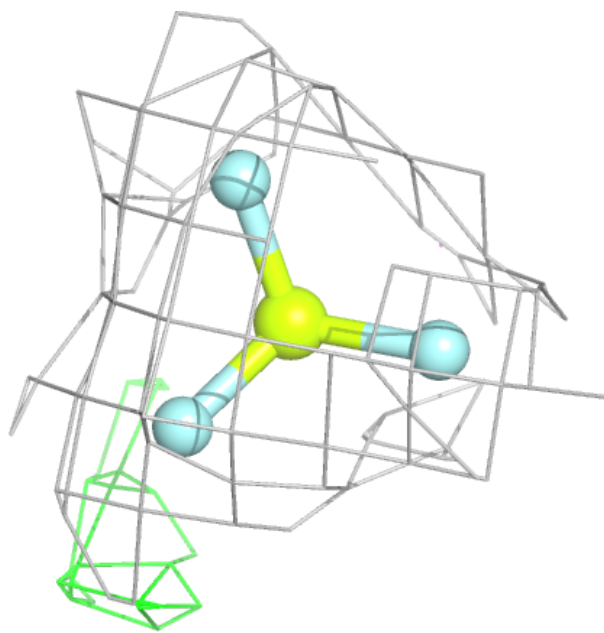
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BEF	A	201	4/4	0.96	0.07	18,23,28,35	0
2	BEF	B	201	4/4	0.97	0.10	13,18,26,26	0
3	MG	A	202	1/1	0.97	0.17	13,13,13,13	0
2	BEF	E	201	4/4	0.98	0.10	18,29,30,31	0
3	MG	B	202	1/1	0.98	0.11	14,14,14,14	0
3	MG	E	202	1/1	0.99	0.07	30,30,30,30	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.

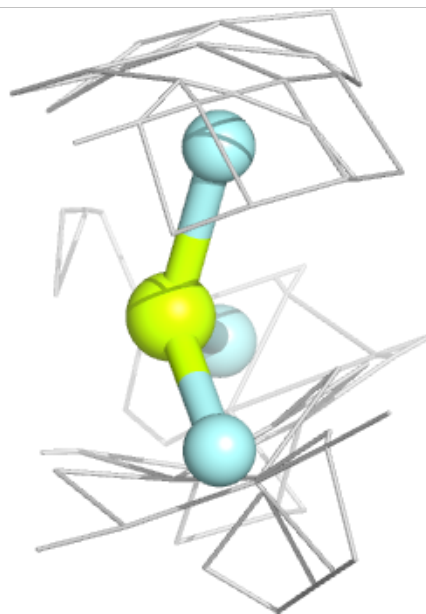
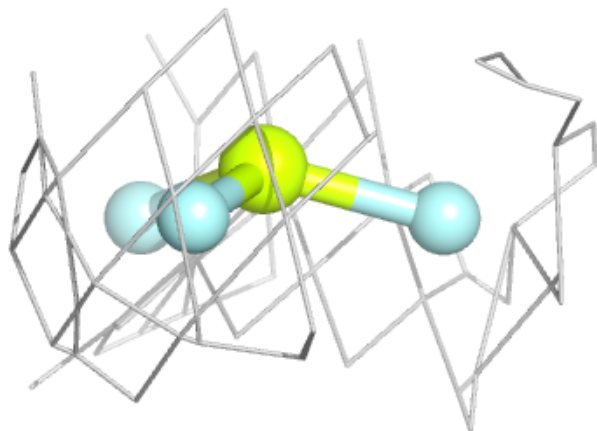
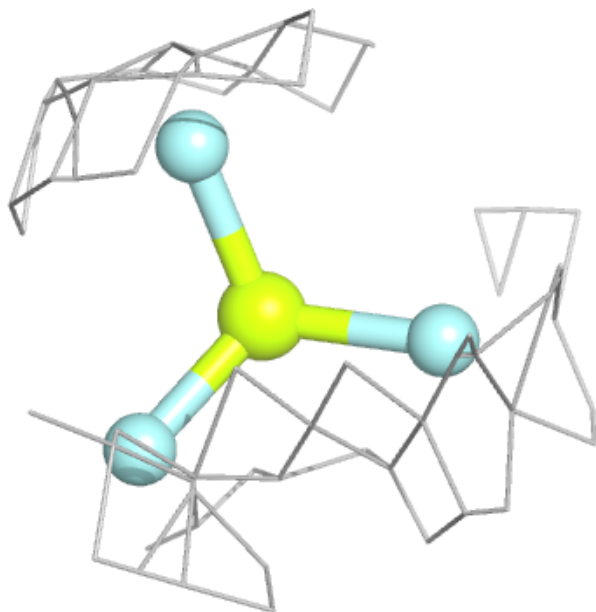
**Electron density around BEF A 201:**

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



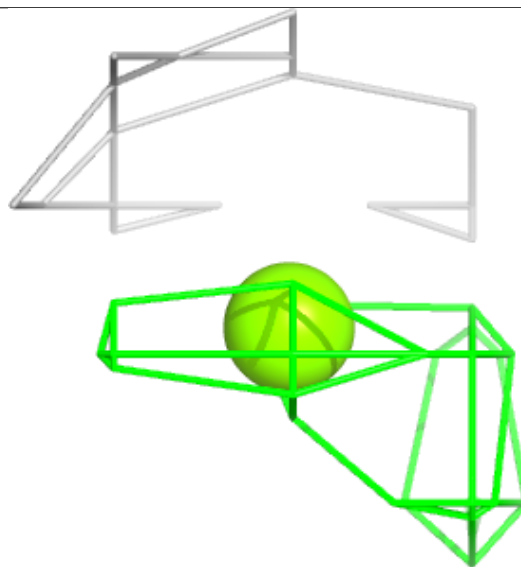
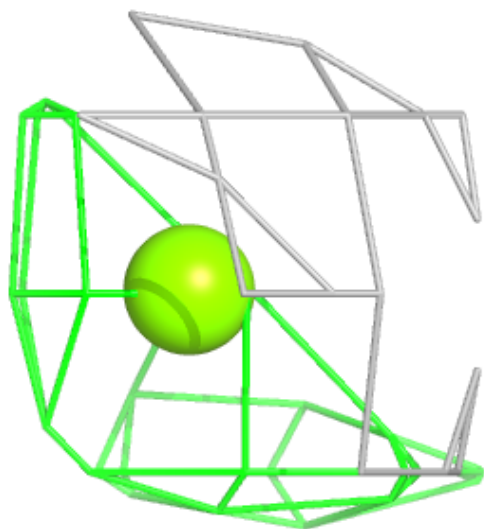
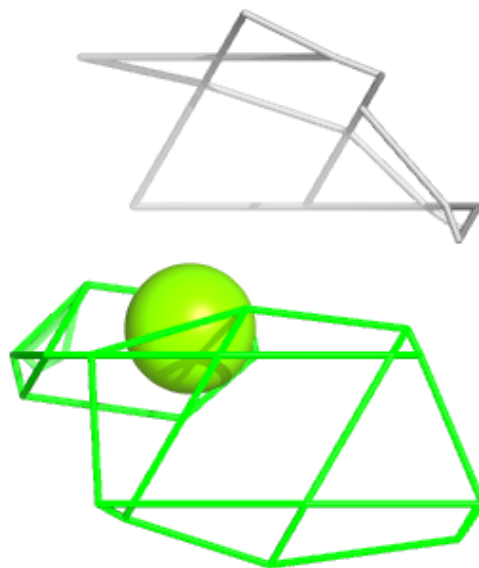
**Electron density around BEF B 201:**

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



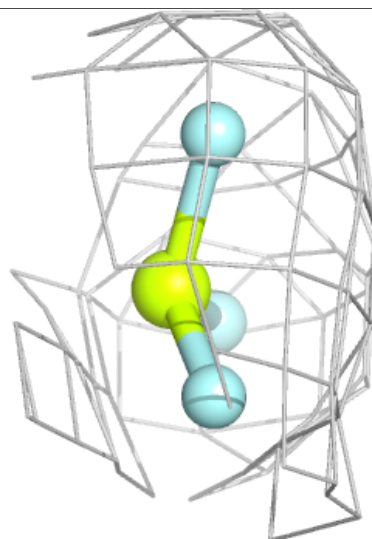
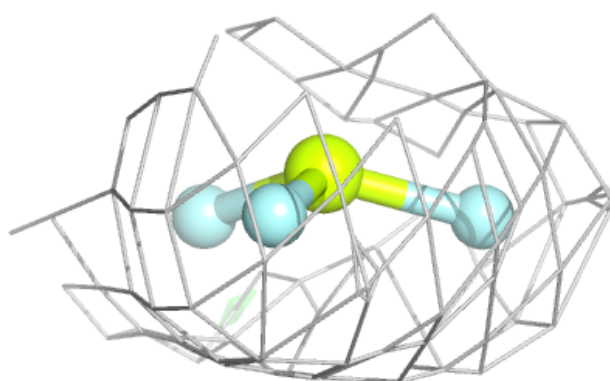
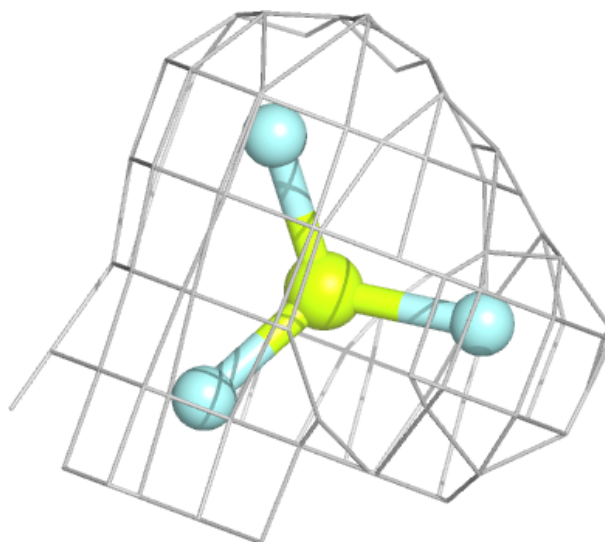
**Electron density around MG A 202:**

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



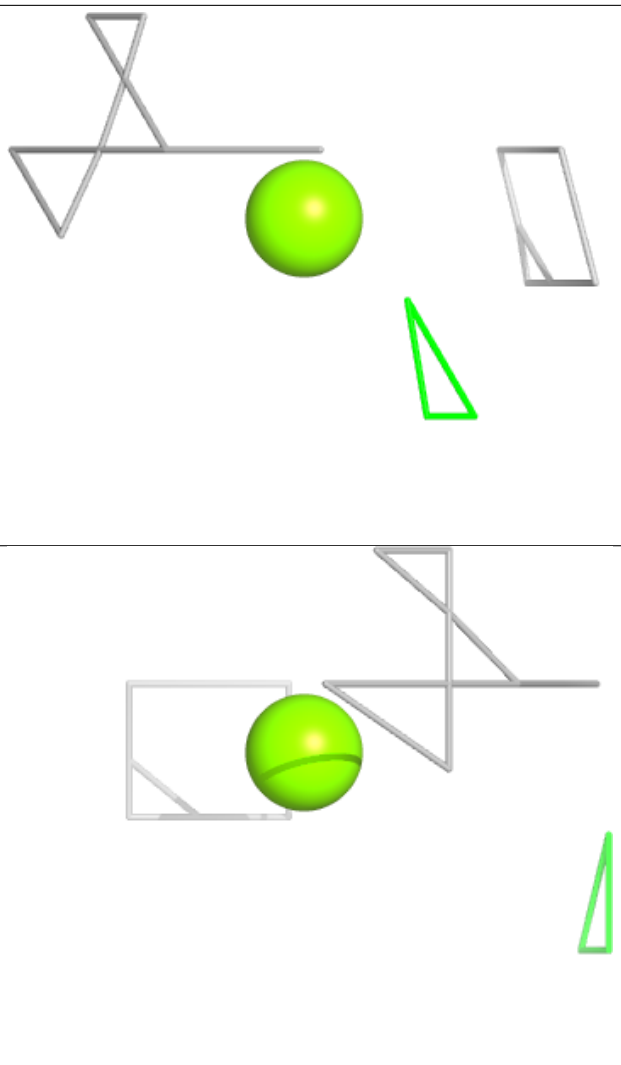
**Electron density around BEF E 201:**

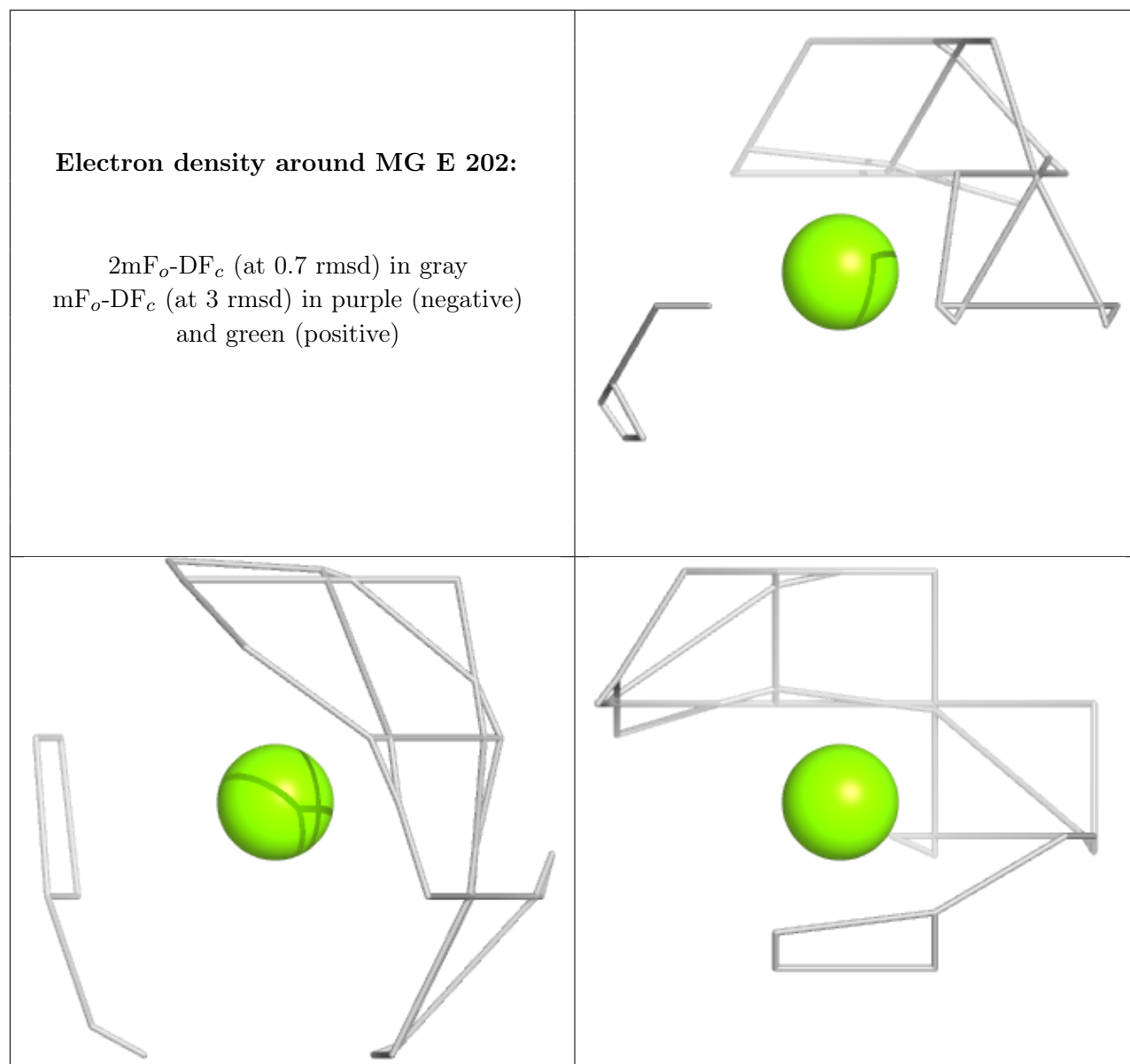
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG B 202:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.