



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:36 PM UTC

PDB ID : 3KR4 / pdb_00003kr4
Title : Structure of a protease 3
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

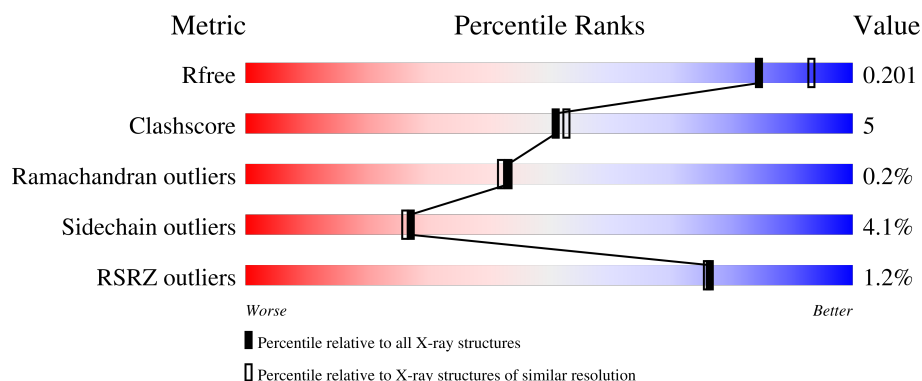
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



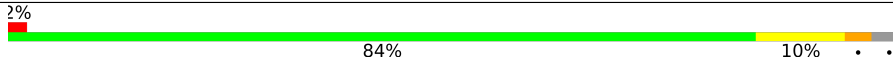
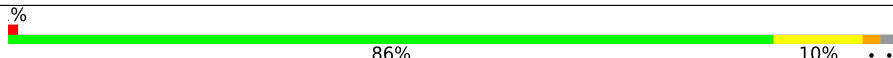
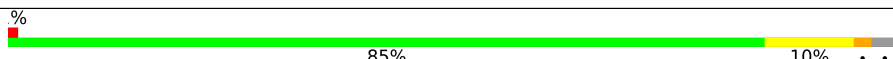
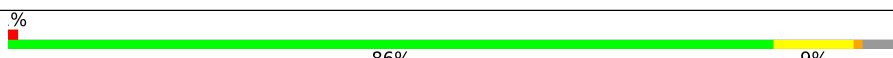
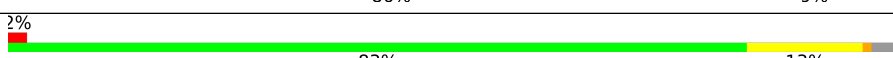
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	528	% 89% 8% .
1	B	528	2% 86% 10% ..
1	C	528	% 85% 12% ..
1	D	528	% 86% 10% ..
1	E	528	% 84% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	528	
1	G	528	
1	H	528	
1	I	528	
1	J	528	
1	K	528	
1	L	528	

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
6	SO4	L	25	-	-	X	-
7	1PE	B	61	-	-	X	-
7	1PE	B	62	-	-	-	X
7	1PE	L	612	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 53016 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	3	1	0
			3983	2558	639	766	20			
1	B	518	Total	C	N	O	S	0	0	0
			3936	2531	637	748	20			
1	C	518	Total	C	N	O	S	0	1	0
			3955	2545	638	753	19			
1	D	516	Total	C	N	O	S	0	0	0
			3946	2541	638	747	20			
1	E	510	Total	C	N	O	S	0	0	0
			3896	2509	626	743	18			
1	F	510	Total	C	N	O	S	0	0	0
			3873	2492	623	739	19			
1	G	516	Total	C	N	O	S	0	0	0
			3996	2564	650	762	20			
1	H	509	Total	C	N	O	S	0	1	0
			3943	2534	641	749	19			
1	I	518	Total	C	N	O	S	0	1	0
			4008	2570	652	767	19			
1	J	513	Total	C	N	O	S	0	1	0
			3963	2545	641	757	20			
1	K	509	Total	C	N	O	S	0	1	0
			3935	2528	638	750	19			
1	L	513	Total	C	N	O	S	0	1	0
			3944	2532	635	758	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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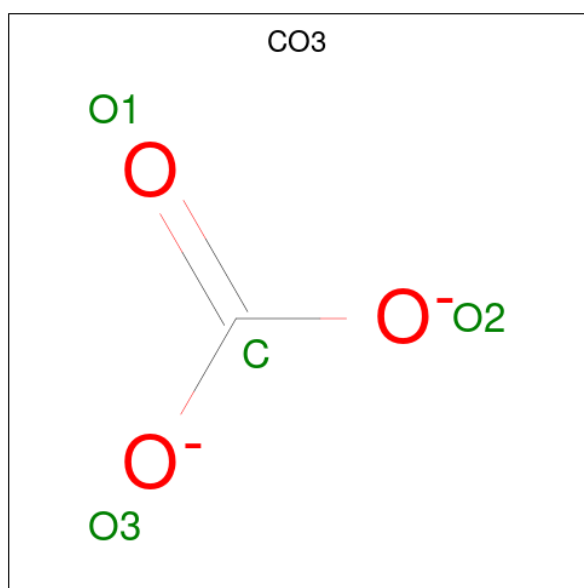
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0
2	E	1	Total C O 4 1 3	0	0
2	F	1	Total C O 4 1 3	0	0
2	G	1	Total C O 4 1 3	0	0
2	H	1	Total C O 4 1 3	0	0
2	I	1	Total C O 4 1 3	0	0
2	J	1	Total C O 4 1 3	0	0
2	K	1	Total C O 4 1 3	0	0
2	L	1	Total C O 4 1 3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

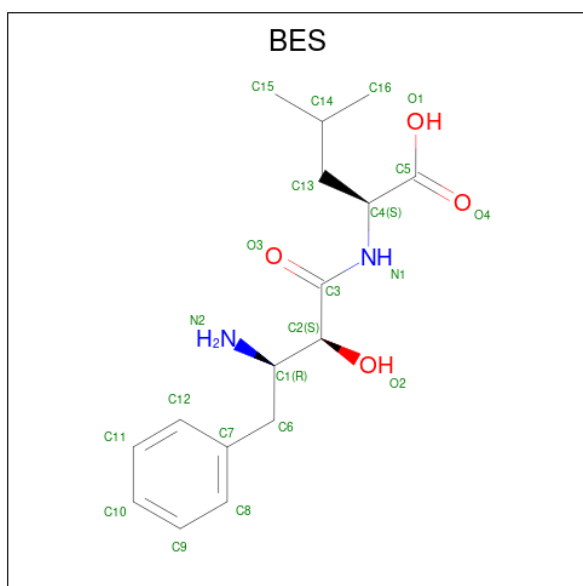
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (CCD ID: BES) (formula: $C_{16}H_{24}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	16	2	4		
4	B	1	Total	C	N	O	0	0
			22	16	2	4		
4	C	1	Total	C	N	O	0	0
			22	16	2	4		
4	D	1	Total	C	N	O	0	0
			22	16	2	4		
4	E	1	Total	C	N	O	0	0
			22	16	2	4		
4	F	1	Total	C	N	O	0	0
			22	16	2	4		
4	G	1	Total	C	N	O	0	0
			22	16	2	4		
4	H	1	Total	C	N	O	0	0
			22	16	2	4		

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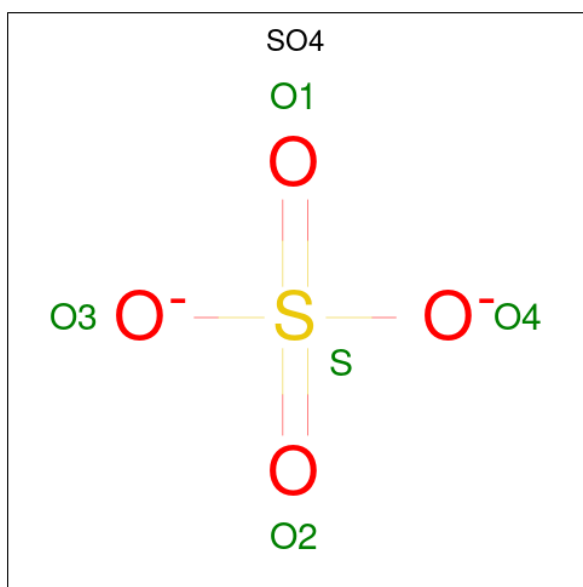
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	N	O	0	0
			22	16	2	4		
4	J	1	Total	C	N	O	0	0
			22	16	2	4		
4	K	1	Total	C	N	O	0	0
			22	16	2	4		
4	L	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

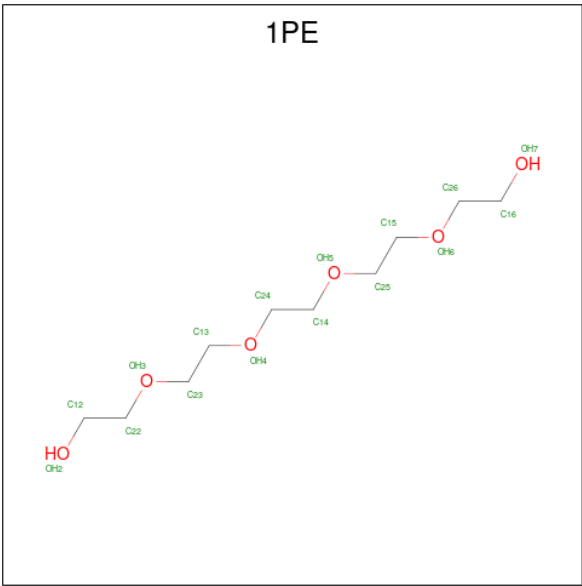
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	6	3		
7	A	1	Total	C	O	0	0
			12	8	4		
7	B	1	Total	C	O	0	0
			10	7	3		
7	B	1	Total	C	O	0	0
			10	7	3		
7	B	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			13	9	4		
7	C	1	Total	C	O	0	0
			9	6	3		
7	D	1	Total	C	O	0	0
			10	7	3		
7	D	1	Total	C	O	0	0
			11	8	3		
7	D	1	Total	C	O	0	0
			10	7	3		
7	D	1	Total	C	O	0	0
			7	5	2		
7	E	1	Total	C	O	0	0
			12	8	4		
7	E	1	Total	C	O	0	0
			12	8	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			8	5	3		
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			9	6	3		
7	G	1	Total	C	O	0	0
			7	4	3		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			15	10	5		
7	H	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		
7	I	1	Total	C	O	0	0
			15	10	5		
7	I	1	Total	C	O	0	0
			11	8	3		
7	I	1	Total	C	O	0	0
			7	5	2		
7	J	1	Total	C	O	0	0
			11	7	4		
7	J	1	Total	C	O	0	0
			10	6	4		
7	J	1	Total	C	O	0	0
			10	7	3		
7	K	1	Total	C	O	0	0
			12	8	4		
7	K	1	Total	C	O	0	0
			12	8	4		
7	K	1	Total	C	O	0	0
			11	7	4		
7	K	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	6	4		
7	L	1	Total	C	O	0	0
			12	8	4		
7	L	1	Total	C	O	0	0
			11	7	4		

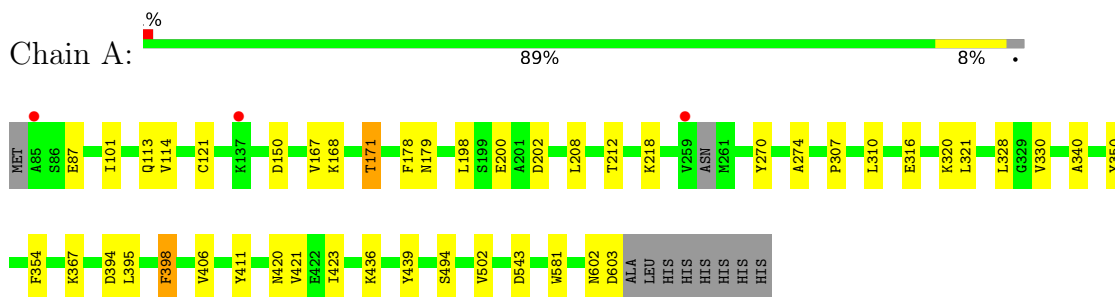
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	423	Total	O	0	0
			423	423		
8	B	361	Total	O	0	0
			361	361		
8	C	427	Total	O	0	0
			427	427		
8	D	411	Total	O	0	0
			411	411		
8	E	442	Total	O	0	0
			442	442		
8	F	373	Total	O	0	0
			373	373		
8	G	421	Total	O	0	0
			421	421		
8	H	389	Total	O	0	0
			389	389		
8	I	414	Total	O	0	0
			414	414		
8	J	403	Total	O	0	0
			403	403		
8	K	438	Total	O	0	0
			438	438		
8	L	356	Total	O	0	0
			356	356		

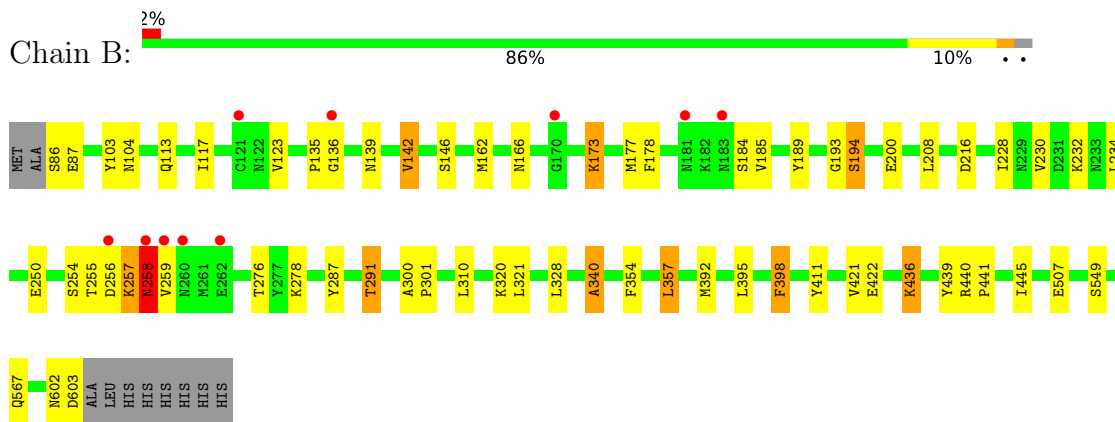
3 Residue-property plots [i](#)

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.

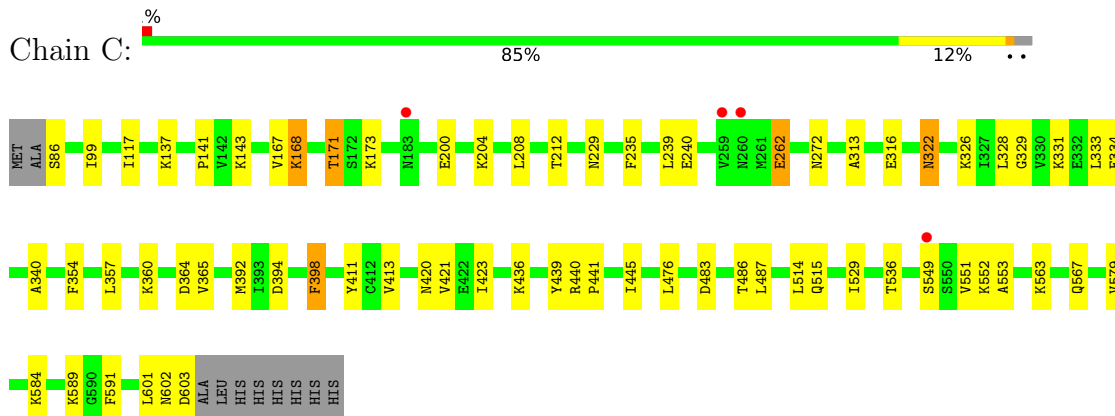
• Molecule 1: M17 leucyl aminopeptidase



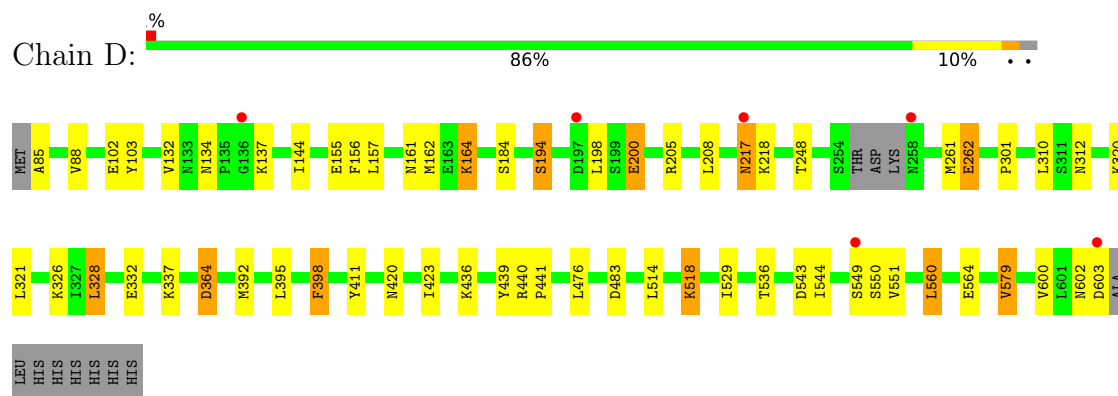
• Molecule 1: M17 leucyl aminopeptidase



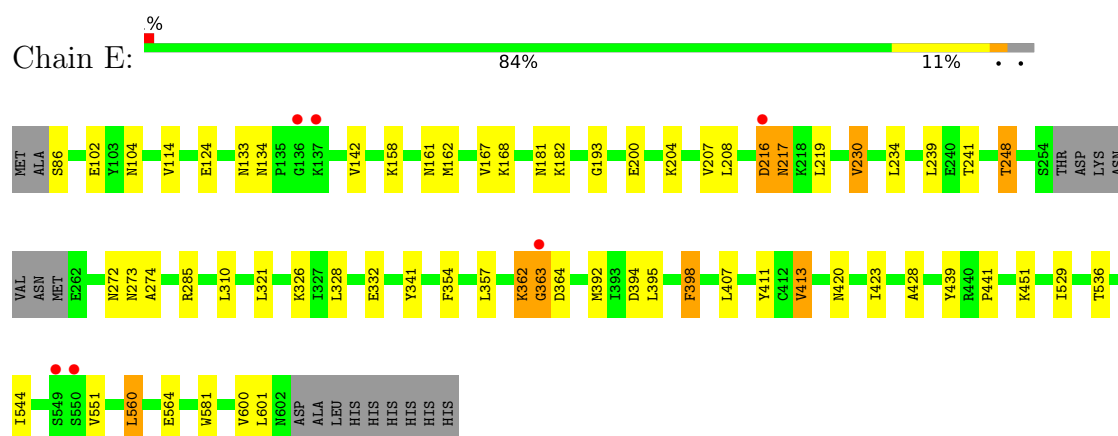
• Molecule 1: M17 leucyl aminopeptidase



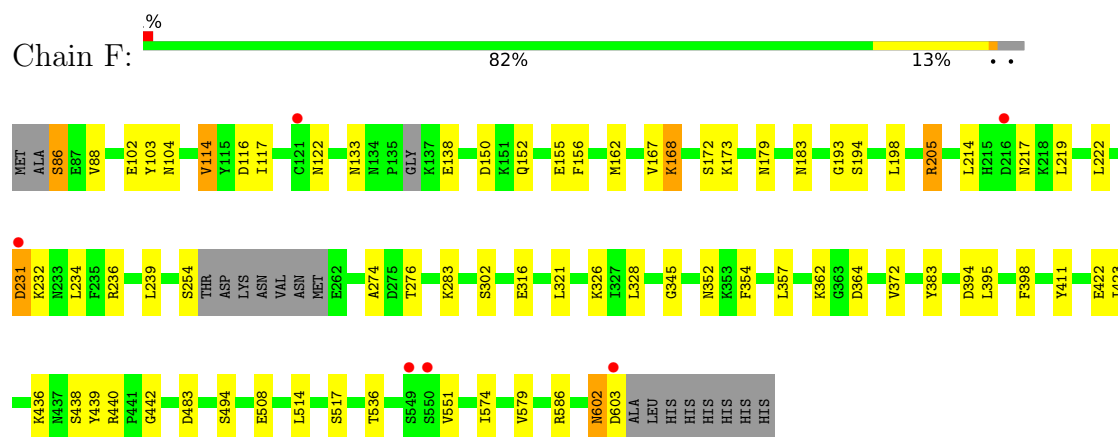
● Molecule 1: M17 leucyl aminopeptidase



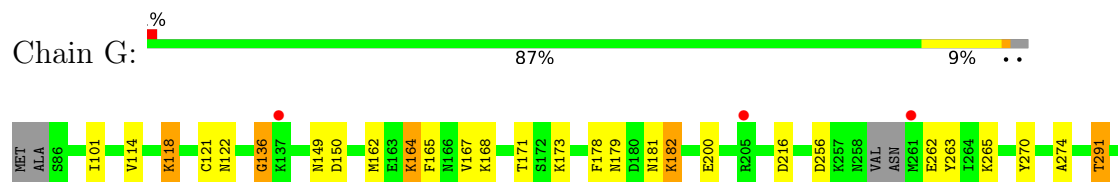
● Molecule 1: M17 leucyl aminopeptidase



● Molecule 1: M17 leucyl aminopeptidase

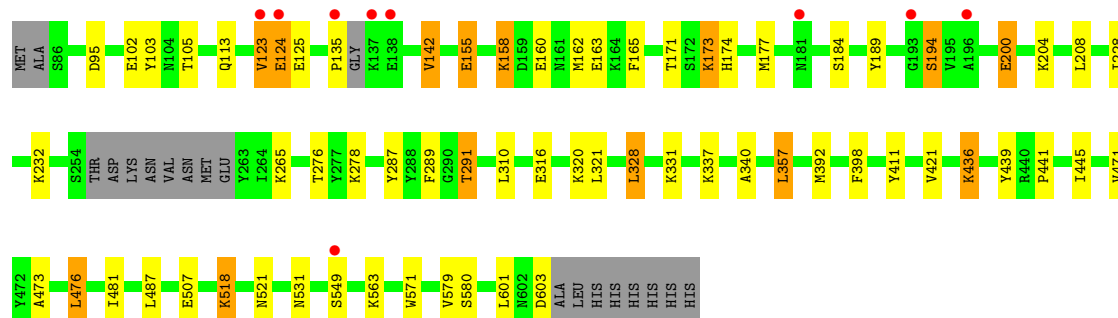
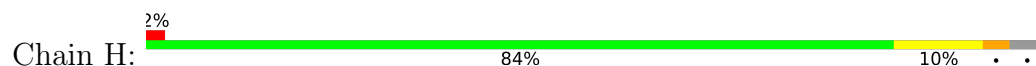


● Molecule 1: M17 leucyl aminopeptidase

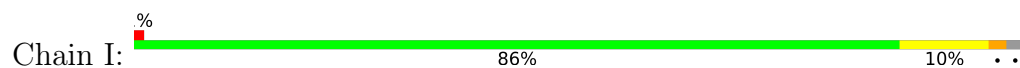




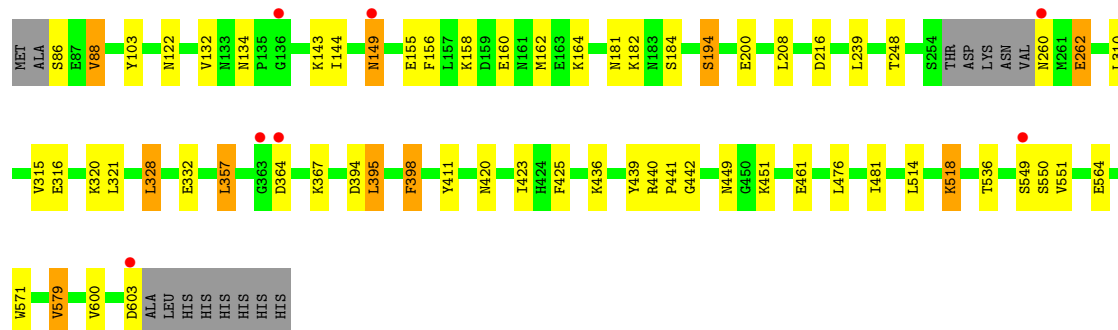
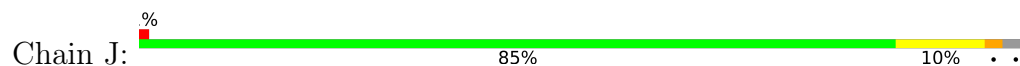
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

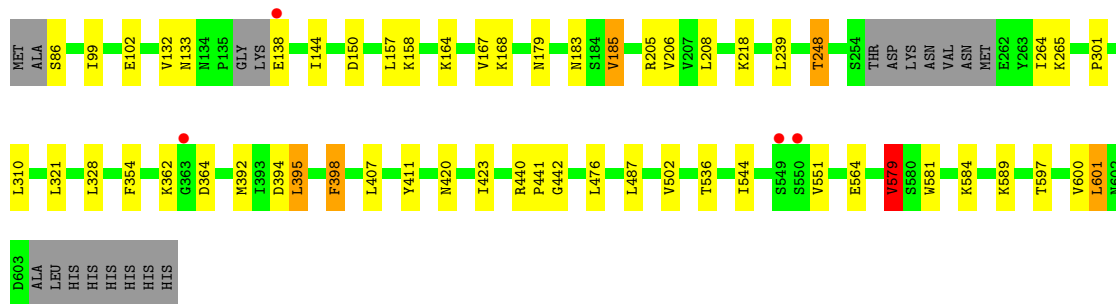


- Molecule 1: M17 leucyl aminopeptidase



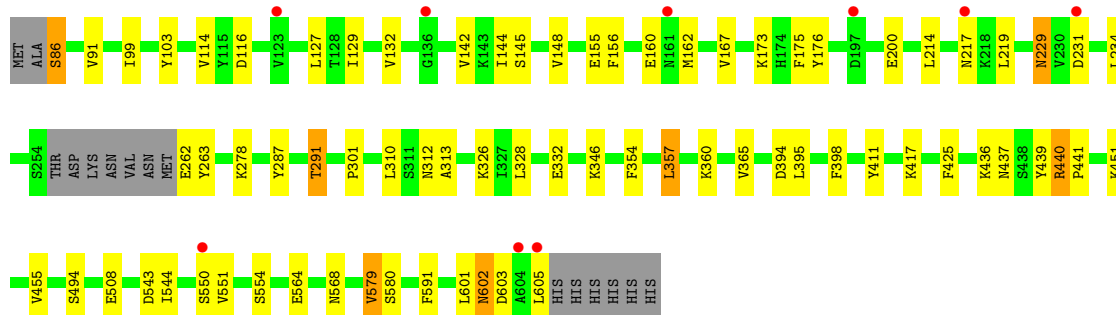
- Molecule 1: M17 leucyl aminopeptidase

Chain K:  86% 9% . .



• Molecule 1: M17 leucyl aminopeptidase

Chain L:  83% 13% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.56Å 178.12Å 230.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.00 43.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.15-2.00) 98.3 (43.15-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.192 , 0.242 (Not available) , 0.201	Depositor DCC
R_{free} test set	23578 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53016	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 47.00 % 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 1.0558e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO3, SO4, ZN, BES, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	4/4063 (0.1%)	0.97	2/5508 (0.0%)
1	B	0.98	5/4014 (0.1%)	1.01	4/5450 (0.1%)
1	C	1.01	3/4036 (0.1%)	0.97	7/5477 (0.1%)
1	D	1.02	1/4023 (0.0%)	1.00	3/5454 (0.1%)
1	E	1.04	2/3973 (0.1%)	1.00	3/5392 (0.1%)
1	F	1.00	2/3949 (0.1%)	1.03	3/5364 (0.1%)
1	G	1.01	2/4073 (0.0%)	0.98	4/5513 (0.1%)
1	H	0.96	1/4022 (0.0%)	1.01	10/5445 (0.2%)
1	I	0.99	3/4089 (0.1%)	0.98	6/5539 (0.1%)
1	J	1.03	2/4043 (0.0%)	1.01	8/5476 (0.1%)
1	K	1.05	2/4014 (0.0%)	1.02	10/5438 (0.2%)
1	L	1.02	4/4024 (0.1%)	1.04	8/5460 (0.1%)
All	All	1.01	31/48323 (0.1%)	1.00	68/65516 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	362	LYS	C-O	-6.71	1.15	1.24
1	B	421	VAL	C-O	-6.56	1.17	1.24
1	D	184	SER	C-O	-6.56	1.16	1.23
1	L	602	ASN	C-O	-6.50	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	123	VAL	C-O	-6.43	1.17	1.24
1	I	460	ALA	CA-CB	6.41	1.61	1.52
1	I	576	ILE	CA-CB	5.97	1.61	1.54
1	A	218	LYS	C-O	-5.94	1.16	1.23
1	E	413	VAL	CA-CB	5.89	1.62	1.54
1	J	315	VAL	CA-CB	5.76	1.61	1.54
1	I	432	ASN	N-CA	5.70	1.54	1.46
1	C	514	LEU	C-O	-5.69	1.17	1.24
1	A	502	VAL	CA-CB	5.66	1.61	1.54
1	L	313	ALA	CA-CB	-5.58	1.44	1.53
1	J	184	SER	C-O	-5.50	1.17	1.24
1	B	357	LEU	CG-CD2	-5.48	1.34	1.52
1	K	502	VAL	CA-CB	5.47	1.62	1.54
1	G	216	ASP	C-O	-5.44	1.16	1.23
1	F	183	ASN	C-O	-5.39	1.17	1.23
1	L	417	LYS	N-CA	5.32	1.50	1.46
1	F	574	ILE	CA-CB	5.19	1.60	1.53
1	L	455	VAL	CA-CB	5.17	1.60	1.54
1	A	406	VAL	CA-C	5.15	1.59	1.52
1	B	422	GLU	C-O	-5.13	1.18	1.24
1	G	263	TYR	C-O	-5.13	1.17	1.23
1	B	340	ALA	CA-CB	5.10	1.61	1.53
1	C	313	ALA	CA-CB	5.09	1.61	1.53
1	B	440	ARG	CZ-NH2	-5.08	1.26	1.33
1	K	264	ILE	CA-CB	5.08	1.59	1.54
1	A	340	ALA	CA-CB	5.05	1.61	1.53
1	C	486	THR	CA-CB	5.03	1.59	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	124	GLU	N-CA-C	9.21	130.43	110.80
1	G	136	GLY	CA-C-N	8.19	134.40	122.36
1	G	136	GLY	C-N-CA	8.19	134.40	122.36
1	D	579	VAL	N-CA-CB	-7.28	102.30	112.35
1	C	440	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	B	228	ILE	CA-C-N	-6.94	112.87	122.93
1	B	228	ILE	C-N-CA	-6.94	112.87	122.93
1	G	498	SER	CB-CA-C	6.93	120.25	109.03
1	B	440	ARG	CB-CG-CD	-6.68	95.94	111.30
1	F	602	ASN	N-CA-C	6.61	118.56	111.36
1	I	440	ARG	NE-CZ-NH2	-6.51	113.34	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	LEU	CD1-CG-CD2	-6.26	97.03	110.80
1	H	95	ASP	CA-C-N	6.17	126.12	119.76
1	H	95	ASP	C-N-CA	6.17	126.12	119.76
1	L	91	VAL	N-CA-C	-6.15	105.06	111.58
1	H	228	ILE	CA-C-N	-6.14	112.98	122.87
1	H	228	ILE	C-N-CA	-6.14	112.98	122.87
1	C	99	ILE	CA-C-N	-6.13	113.46	119.90
1	C	99	ILE	C-N-CA	-6.13	113.46	119.90
1	G	291	THR	OG1-CB-CG2	-6.06	97.18	109.30
1	K	310	LEU	CD1-CG-CD2	-6.04	97.51	110.80
1	H	471	VAL	CG1-CB-CG2	-5.91	97.79	110.80
1	I	586	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	J	149	ASN	N-CA-CB	-5.90	100.03	110.42
1	D	200	GLU	CA-CB-CG	5.87	125.84	114.10
1	A	420	ASN	N-CA-C	5.82	119.96	112.86
1	K	99	ILE	CA-C-N	-5.82	113.94	119.76
1	K	99	ILE	C-N-CA	-5.82	113.94	119.76
1	K	579	VAL	N-CA-CB	-5.80	104.35	112.35
1	K	185	VAL	CG1-CB-CG2	-5.78	98.08	110.80
1	L	551	VAL	N-CA-C	5.75	116.44	108.84
1	I	476	LEU	CD1-CG-CD2	-5.75	98.15	110.80
1	E	407	LEU	CD1-CG-CD2	-5.74	98.16	110.80
1	K	407	LEU	CD1-CG-CD2	-5.67	98.34	110.80
1	C	262	GLU	N-CA-C	-5.51	100.03	109.24
1	H	289	PHE	N-CA-CB	5.51	118.32	110.16
1	I	436	LYS	CD-CE-NZ	-5.51	94.27	111.90
1	H	357	LEU	CD1-CG-CD2	-5.48	98.74	110.80
1	L	440	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	F	440	ARG	NE-CZ-NH2	-5.44	114.31	119.20
1	A	310	LEU	CD1-CG-CD2	-5.41	98.89	110.80
1	K	476	LEU	CD1-CG-CD2	-5.41	98.90	110.80
1	F	362	LYS	N-CA-C	-5.38	102.91	110.50
1	J	310	LEU	CD1-CG-CD2	-5.33	99.08	110.80
1	K	440	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	J	476	LEU	CD1-CG-CD2	-5.29	99.17	110.80
1	L	554	SER	N-CA-C	5.27	117.03	111.28
1	K	206	VAL	CG1-CB-CG2	-5.27	99.20	110.80
1	I	392	MET	N-CA-C	5.25	118.68	111.54
1	D	476	LEU	CD1-CG-CD2	-5.23	99.29	110.80
1	L	99	ILE	CA-C-N	-5.23	114.53	119.76
1	L	99	ILE	C-N-CA	-5.23	114.53	119.76
1	L	145	SER	N-CA-C	5.20	117.75	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	461	GLU	CA-C-N	5.18	125.74	119.98
1	J	461	GLU	C-N-CA	5.18	125.74	119.98
1	C	436	LYS	CD-CE-NZ	-5.16	95.40	111.90
1	E	285	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	I	586	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	L	550	SER	N-CA-C	5.11	116.66	111.14
1	B	440	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	C	240	GLU	CB-CA-C	-5.08	102.91	110.88
1	H	228	ILE	N-CA-C	-5.08	100.57	108.95
1	J	88	VAL	N-CA-CB	5.08	115.66	110.23
1	J	88	VAL	CB-CA-C	5.07	115.66	110.94
1	H	580	SER	N-CA-C	5.06	116.88	111.36
1	J	579	VAL	N-CA-CB	-5.05	103.24	111.98
1	K	362	LYS	N-CA-C	-5.04	103.82	110.33
1	E	413	VAL	N-CA-CB	5.00	118.09	110.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	LYS	Peptide
1	G	136	GLY	Peptide

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	3983	0	3917	26	0
1	B	3936	0	3843	50	0
1	C	3955	0	3881	39	0
1	D	3946	0	3888	47	0
1	E	3896	0	3819	53	0
1	F	3873	0	3771	47	0
1	G	3996	0	3988	37	0
1	H	3943	0	3937	37	0
1	I	4008	0	3985	38	0
1	J	3963	0	3940	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3935	0	3907	42	0
1	L	3944	0	3874	45	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	22	0	22	1	0
4	B	22	0	22	3	0
4	C	22	0	22	4	0
4	D	22	0	22	3	0
4	E	22	0	22	4	0
4	F	22	0	22	0	0
4	G	22	0	22	0	0
4	H	22	0	22	3	0
4	I	22	0	22	2	0
4	J	22	0	22	2	0
4	K	22	0	22	5	0
4	L	22	0	22	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
6	D	10	0	0	1	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	G	10	0	0	0	0
6	J	10	0	0	1	0
6	K	5	0	0	0	0
6	L	5	0	0	2	0
7	A	21	0	22	2	0
7	B	30	0	30	7	0
7	C	22	0	24	5	0
7	D	38	0	38	6	0
7	E	32	0	36	3	0
7	F	30	0	39	3	0
7	G	43	0	47	5	0
7	H	20	0	20	4	0
7	I	33	0	37	8	0
7	J	31	0	36	10	0
7	K	41	0	44	1	0
7	L	33	0	40	11	0
8	A	423	0	0	3	0
8	B	361	0	0	8	0
8	C	427	0	0	9	0
8	D	411	0	0	13	0
8	E	442	0	0	13	0
8	F	373	0	0	12	0
8	G	421	0	0	5	0
8	H	389	0	0	5	0
8	I	414	0	0	11	0
8	J	403	0	0	12	0
8	K	438	0	0	10	0
8	L	356	0	0	7	0
All	All	53016	0	47427	497	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 5.

All (497) 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:104:ASN:HB2	8:B:3372:HOH:O	1.37	1.21
1:B:257:LYS:CB	1:B:258:ASN:HB3	1.71	1.18
1:F:316:GLU:HG3	7:F:32:1PE:H141	1.28	1.12
1:J:518:LYS:HE2	8:J:2650:HOH:O	1.50	1.08
1:D:320:LYS:HZ1	7:D:63:1PE:H142	1.16	1.06
1:G:164:LYS:HE3	8:J:3193:HOH:O	1.60	1.02
1:B:257:LYS:HB3	1:B:258:ASN:CB	1.88	1.01
1:D:161:ASN:HB2	8:D:4166:HOH:O	1.59	1.01
1:K:395:LEU:HD12	8:K:2124:HOH:O	1.58	1.00
1:L:395:LEU:HB2	8:L:2109:HOH:O	1.61	1.00
1:E:161:ASN:HB2	8:E:1724:HOH:O	1.61	0.99
1:B:320:LYS:HZ1	7:B:61:1PE:H132	1.25	0.98
1:I:567:GLN:HG2	8:I:1905:HOH:O	1.63	0.97
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.25	0.97
1:E:392:MET:HE3	4:E:1003:BES:H10	1.47	0.96
1:B:257:LYS:HB3	1:B:258:ASN:HB3	0.98	0.96
1:F:205:ARG:HG2	1:F:205:ARG:HH11	1.28	0.96
1:D:320:LYS:NZ	7:D:63:1PE:H142	1.80	0.96
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.31	0.95
1:B:257:LYS:HD3	8:B:4371:HOH:O	1.68	0.93
1:B:320:LYS:NZ	7:B:61:1PE:H132	1.82	0.92
1:B:436:LYS:HE2	8:B:3093:HOH:O	1.69	0.92
1:D:518:LYS:HE2	8:D:3930:HOH:O	1.69	0.92
1:B:320:LYS:HZ1	7:B:61:1PE:H142	1.36	0.91
1:F:122:ASN:HB3	8:F:5146:HOH:O	1.70	0.90
1:J:395:LEU:HB2	8:J:4608:HOH:O	1.69	0.90
1:F:603:ASP:HA	8:F:614:HOH:O	1.72	0.89
7:I:22:1PE:H252	8:I:4748:HOH:O	1.74	0.88
1:L:217:ASN:HB3	1:L:219:LEU:HD21	1.56	0.87
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.12	0.85
1:J:134:ASN:O	1:J:194:SER:HB3	1.76	0.84
1:E:392:MET:CE	4:E:1003:BES:H10	2.08	0.84
1:D:134:ASN:O	1:D:194:SER:HB3	1.76	0.83
1:E:395:LEU:HD12	8:E:1386:HOH:O	1.78	0.83
1:L:287:TYR:O	1:L:291:THR:HG23	1.79	0.82
1:E:133:ASN:HA	1:E:167:VAL:HG11	1.61	0.82
1:F:316:GLU:HG3	7:F:32:1PE:C14	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:ASN:HA	1:K:167:VAL:HG11	1.62	0.82
1:L:411:TYR:HE1	7:L:1:1PE:H261	1.44	0.81
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.14	0.81
1:L:451:LYS:HG2	7:L:612:1PE:H131	1.60	0.81
1:J:411:TYR:HE1	7:J:2:1PE:H151	1.45	0.81
1:H:204:LYS:HE3	8:H:2714:HOH:O	1.79	0.80
1:K:248:THR:HG23	8:K:2935:HOH:O	1.80	0.80
1:K:392:MET:CE	4:K:1003:BES:H10	2.11	0.80
1:H:155:GLU:O	1:H:158:LYS:HG2	1.83	0.79
1:I:331:LYS:HE2	1:I:334:GLU:OE1	1.83	0.79
1:D:217:ASN:CG	1:D:218:LYS:N	2.40	0.78
1:B:287:TYR:O	1:B:291:THR:HG23	1.82	0.78
1:B:257:LYS:CA	1:B:258:ASN:HB3	2.11	0.77
1:J:332:GLU:HG3	8:J:1169:HOH:O	1.84	0.76
1:H:232:LYS:HE2	1:H:276:THR:HB	1.68	0.75
7:C:18:1PE:H242	8:C:5189:HOH:O	1.84	0.75
1:E:451:LYS:HG2	7:E:43:1PE:H141	1.69	0.75
1:E:216:ASP:O	1:E:217:ASN:CG	2.30	0.74
1:J:451:LYS:HG3	7:J:45:1PE:H151	1.70	0.74
1:E:158:LYS:CB	8:E:3153:HOH:O	2.36	0.73
1:B:602:ASN:CB	8:B:3179:HOH:O	2.35	0.73
1:J:536:THR:HG21	1:J:551:VAL:HG23	1.71	0.73
1:I:320:LYS:NZ	7:I:21:1PE:H232	2.04	0.73
1:D:529:ILE:CG2	1:D:560:LEU:HD13	2.19	0.72
1:H:287:TYR:O	1:H:291:THR:HG23	1.89	0.72
7:I:22:1PE:H242	8:I:4748:HOH:O	1.90	0.71
1:I:392:MET:HE3	4:I:1003:BES:H10	1.72	0.71
1:J:332:GLU:HB3	8:J:1480:HOH:O	1.91	0.71
1:H:392:MET:CE	4:H:1003:BES:H10	2.21	0.71
1:G:122:ASN:ND2	1:G:149:ASN:HD22	1.89	0.71
1:B:87:GLU:CB	8:B:3048:HOH:O	2.37	0.71
1:B:232:LYS:HE2	1:B:276:THR:HB	1.74	0.70
1:I:230:VAL:HG22	1:I:234:LEU:HD23	1.74	0.70
1:F:232:LYS:HE3	1:F:276:THR:O	1.90	0.70
7:D:44:1PE:H242	8:E:3038:HOH:O	1.91	0.70
1:K:392:MET:HE3	4:K:1003:BES:H10	1.75	0.69
1:B:320:LYS:NZ	7:B:61:1PE:H142	2.08	0.69
1:D:536:THR:HG21	1:D:551:VAL:HG23	1.75	0.69
1:K:392:MET:HE1	4:K:1003:BES:H10	1.74	0.69
8:G:3958:HOH:O	1:H:436:LYS:HE2	1.91	0.69
1:E:248:THR:HG22	8:E:2449:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:411:TYR:HE1	7:I:22:1PE:H232	1.58	0.68
1:H:392:MET:HE3	4:H:1003:BES:H10	1.73	0.68
1:F:103:TYR:CD1	7:F:32:1PE:H161	2.29	0.68
1:J:398:PHE:HZ	4:J:1003:BES:H11	1.58	0.68
1:F:205:ARG:HG2	1:F:205:ARG:NH1	2.04	0.67
1:B:392:MET:HE3	4:B:1003:BES:H10	1.75	0.67
1:H:518:LYS:HB2	1:H:518:LYS:NZ	2.09	0.67
1:B:178:PHE:HZ	1:F:155:GLU:HG2	1.60	0.67
1:F:156:PHE:O	1:F:162:MET:HE3	1.95	0.67
1:C:411:TYR:HE1	7:C:18:1PE:H232	1.60	0.66
1:D:217:ASN:CG	1:D:218:LYS:H	2.00	0.66
1:B:392:MET:CE	4:B:1003:BES:H10	2.25	0.66
1:K:158:LYS:HD3	8:K:4267:HOH:O	1.95	0.66
1:C:331:LYS:HE2	1:C:334:GLU:OE1	1.95	0.66
1:D:262:GLU:HG3	8:D:637:HOH:O	1.95	0.66
1:L:114:VAL:HB	1:L:278:LYS:HD3	1.77	0.66
1:D:217:ASN:OD1	1:D:218:LYS:N	2.30	0.64
1:E:216:ASP:O	1:E:217:ASN:ND2	2.30	0.64
1:G:118:LYS:HE3	8:G:5157:HOH:O	1.97	0.64
1:H:518:LYS:HB2	1:H:518:LYS:HZ3	1.61	0.64
1:D:156:PHE:O	1:D:162:MET:HE3	1.96	0.64
1:B:178:PHE:CZ	1:F:155:GLU:HG2	2.32	0.64
1:J:156:PHE:O	1:J:162:MET:HE3	1.97	0.64
1:D:529:ILE:HG23	1:D:560:LEU:HD13	1.78	0.64
1:B:257:LYS:CB	1:B:258:ASN:CB	2.61	0.64
1:B:567:GLN:CG	8:B:2181:HOH:O	2.46	0.64
1:J:143:LYS:HE3	8:J:2375:HOH:O	1.96	0.63
1:E:217:ASN:O	1:E:219:LEU:HG	1.97	0.63
1:J:316:GLU:HG3	7:J:3:1PE:H241	1.81	0.63
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.32	0.63
7:G:12:1PE:C25	8:G:5126:HOH:O	2.44	0.63
1:A:421:VAL:HG21	1:A:423:ILE:HD11	1.80	0.62
1:E:207:VAL:HG11	1:E:241:THR:HG22	1.82	0.62
1:G:320:LYS:HZ3	7:G:58:1PE:H131	1.63	0.62
1:I:529:ILE:HG21	1:I:563:LYS:HE2	1.82	0.61
1:J:103:TYR:CD1	7:J:3:1PE:H161	2.35	0.61
1:L:602:ASN:O	1:L:605:LEU:HD23	2.00	0.61
1:E:181:ASN:O	1:E:182:LYS:HB2	2.00	0.61
7:C:18:1PE:H231	8:C:4932:HOH:O	2.00	0.61
1:C:392:MET:HE3	4:C:1003:BES:H10	1.81	0.61
1:D:603:ASP:CB	8:D:5023:HOH:O	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:ILE:CG2	1:E:560:LEU:HD13	2.31	0.61
1:J:320:LYS:HE2	7:J:3:1PE:H142	1.83	0.61
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.82	0.61
1:L:360:LYS:CD	8:L:1249:HOH:O	2.48	0.61
1:F:603:ASP:CB	8:F:3212:HOH:O	2.48	0.61
1:L:543:ASP:HB3	7:L:612:1PE:H222	1.81	0.61
1:C:602:ASN:CB	8:C:626:HOH:O	2.48	0.60
1:B:257:LYS:CA	1:B:258:ASN:CB	2.79	0.60
1:D:332:GLU:HG3	8:D:4864:HOH:O	2.01	0.60
1:D:218:LYS:HE3	8:D:3676:HOH:O	2.01	0.60
1:B:216:ASP:O	1:F:173:LYS:HE3	2.00	0.60
1:C:168:LYS:O	1:C:171:THR:HB	2.02	0.60
1:E:326:LYS:HD2	8:E:2964:HOH:O	2.01	0.59
1:J:449:ASN:O	7:J:45:1PE:H152	2.03	0.59
7:L:612:1PE:C12	8:L:3432:HOH:O	2.49	0.59
1:F:217:ASN:CB	1:F:219:LEU:HD21	2.33	0.59
1:L:440:ARG:NH2	8:L:4845:HOH:O	2.36	0.58
1:D:103:TYR:HB3	7:D:9:1PE:H241	1.85	0.58
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.84	0.58
1:F:114:VAL:HG23	1:F:274:ALA:HB1	1.85	0.58
1:K:579:VAL:O	1:K:589:LYS:HD2	2.04	0.58
1:F:104:ASN:HB3	8:F:2890:HOH:O	2.05	0.57
1:I:392:MET:CE	4:I:1003:BES:H10	2.33	0.57
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.85	0.57
1:K:536:THR:HG21	1:K:551:VAL:HG23	1.87	0.57
1:F:152:GLN:CB	8:F:4547:HOH:O	2.53	0.57
1:D:217:ASN:O	1:D:261:MET:HA	2.03	0.57
1:J:423:ILE:HD11	1:J:600:VAL:HG13	1.86	0.57
1:L:395:LEU:O	1:L:395:LEU:HG	2.03	0.57
1:E:332:GLU:HG3	8:E:4802:HOH:O	2.03	0.57
1:G:118:LYS:NZ	1:G:118:LYS:HB2	2.20	0.57
1:K:442:GLY:O	1:L:301:PRO:HB3	2.05	0.57
1:I:168:LYS:O	1:I:171:THR:HB	2.05	0.56
1:E:134:ASN:C	1:E:134:ASN:HD22	2.13	0.56
1:B:328:LEU:N	1:B:328:LEU:HD12	2.20	0.56
1:D:85:ALA:HA	1:D:312:ASN:OD1	2.06	0.56
7:I:22:1PE:H231	8:I:4748:HOH:O	2.05	0.56
1:B:123:VAL:HG12	1:B:123:VAL:O	2.06	0.55
1:G:181:ASN:O	1:G:182:LYS:HB2	2.06	0.55
1:L:217:ASN:CB	1:L:219:LEU:HD21	2.32	0.55
1:I:320:LYS:HZ3	7:I:21:1PE:H232	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ASN:HA	1:E:167:VAL:CG1	2.35	0.55
1:H:103:TYR:CD1	7:H:65:1PE:H222	2.42	0.55
1:K:597:THR:HG22	1:K:601:LEU:HD22	1.89	0.55
7:E:43:1PE:H142	1:F:254:SER:OG	2.06	0.55
1:K:133:ASN:HA	1:K:167:VAL:CG1	2.34	0.55
1:E:529:ILE:HG22	1:E:560:LEU:HD13	1.88	0.55
1:H:200:GLU:HG3	1:H:521:ASN:O	2.07	0.55
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.89	0.55
1:H:531:ASN:HB3	8:H:4401:HOH:O	2.06	0.54
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.88	0.54
1:A:421:VAL:CG2	1:A:423:ILE:HD11	2.37	0.54
1:I:261:MET:CB	8:I:4500:HOH:O	2.56	0.54
1:I:587:LYS:NZ	8:I:3619:HOH:O	2.38	0.54
1:H:316:GLU:CD	7:H:65:1PE:H242	2.33	0.54
1:J:181:ASN:O	1:J:182:LYS:HB2	2.07	0.54
1:L:411:TYR:CE1	7:L:1:1PE:H261	2.35	0.54
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.89	0.54
1:G:494:SER:HB3	1:L:494:SER:HB3	1.90	0.54
1:J:423:ILE:HD11	1:J:600:VAL:CG1	2.37	0.54
1:F:214:LEU:HD21	1:F:222:LEU:HD22	1.88	0.53
1:G:122:ASN:HD21	1:G:149:ASN:HD22	1.54	0.53
1:C:167:VAL:O	1:C:168:LYS:C	2.50	0.53
1:A:168:LYS:O	1:A:171:THR:HB	2.08	0.53
1:J:143:LYS:HE2	8:J:3169:HOH:O	2.08	0.53
1:G:316:GLU:HG3	7:G:58:1PE:H132	1.89	0.53
1:K:395:LEU:CD1	8:K:2124:HOH:O	2.32	0.53
1:L:103:TYR:N	6:L:25:SO4:O4	2.41	0.53
1:D:423:ILE:HD11	1:D:600:VAL:CG1	2.38	0.53
1:E:124:GLU:HG3	8:E:3953:HOH:O	2.09	0.53
1:K:364:ASP:O	1:K:420:ASN:HA	2.09	0.53
1:K:395:LEU:HD11	1:K:581:TRP:CD1	2.44	0.53
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.91	0.53
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.90	0.53
1:L:451:LYS:HZ3	7:L:612:1PE:H241	1.73	0.53
1:I:508:GLU:OE1	1:I:508:GLU:N	2.40	0.53
1:K:167:VAL:HG12	1:K:167:VAL:O	2.08	0.53
1:D:423:ILE:HD11	1:D:600:VAL:HG13	1.91	0.52
1:L:451:LYS:NZ	7:L:612:1PE:H241	2.24	0.52
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.91	0.52
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.90	0.52
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:VAL:HG12	1:E:167:VAL:O	2.07	0.52
1:E:395:LEU:HD11	1:E:581:TRP:CD1	2.45	0.52
1:F:602:ASN:CB	8:F:3410:HOH:O	2.58	0.52
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.91	0.52
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.44	0.52
1:G:316:GLU:HG3	7:G:58:1PE:C13	2.40	0.52
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.92	0.52
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.92	0.52
1:A:178:PHE:HZ	1:D:155:GLU:CG	2.15	0.52
1:F:205:ARG:HH11	1:F:205:ARG:CG	2.13	0.52
1:F:536:THR:HG21	1:F:551:VAL:HG23	1.91	0.52
1:J:423:ILE:CD1	1:J:600:VAL:HG11	2.40	0.52
1:A:316:GLU:HG2	1:A:320:LYS:HE2	1.91	0.51
1:B:320:LYS:HZ1	7:B:61:1PE:C14	2.15	0.51
1:F:102:GLU:CD	8:F:3843:HOH:O	2.52	0.51
1:L:451:LYS:NZ	7:L:612:1PE:H221	2.25	0.51
1:B:142:VAL:HG22	1:B:162:MET:HB3	1.93	0.51
1:B:173:LYS:HB2	1:B:189:TYR:CE1	2.45	0.51
1:I:113:GLN:NE2	8:I:3228:HOH:O	2.43	0.51
1:K:248:THR:HG22	8:K:1380:HOH:O	2.11	0.51
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.92	0.51
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.10	0.51
1:A:208:LEU:O	1:A:212:THR:HG23	2.11	0.51
1:E:423:ILE:HD11	1:E:600:VAL:CG1	2.41	0.51
1:I:218:LYS:HG3	1:K:164:LYS:HA	1.93	0.51
8:B:2359:HOH:O	1:E:551:VAL:HG13	2.11	0.51
7:E:43:1PE:C25	8:E:5443:HOH:O	2.59	0.50
1:L:262:GLU:HG3	1:L:263:TYR:H	1.76	0.50
1:L:508:GLU:CD	1:L:508:GLU:H	2.19	0.50
1:B:142:VAL:CG2	1:B:162:MET:HB3	2.42	0.50
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.93	0.50
1:I:238:PHE:HD2	1:I:239:LEU:HD12	1.77	0.50
1:D:328:LEU:HD12	1:D:328:LEU:N	2.26	0.50
1:J:143:LYS:CE	8:J:2375:HOH:O	2.54	0.50
1:L:231:ASP:HB3	1:L:234:LEU:H	1.77	0.50
1:L:579:VAL:HG13	1:L:591:PHE:CD1	2.46	0.50
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.94	0.50
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.94	0.50
1:J:320:LYS:CE	7:J:3:1PE:H142	2.42	0.50
1:C:262:GLU:CB	8:C:4548:HOH:O	2.60	0.50
1:C:398:PHE:HZ	4:C:1003:BES:H11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:GLU:C	1:F:423:ILE:HG13	2.36	0.49
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.95	0.49
1:B:254:SER:O	1:B:257:LYS:HE2	2.12	0.49
1:D:326:LYS:HD2	8:D:4349:HOH:O	2.11	0.49
8:G:3034:HOH:O	1:J:260:ASN:CB	2.60	0.49
1:L:326:LYS:HG2	1:L:328:LEU:CD1	2.42	0.49
1:C:411:TYR:CE1	7:C:18:1PE:H232	2.45	0.49
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.94	0.49
1:F:372:VAL:O	1:F:483:ASP:HA	2.12	0.49
1:A:543:ASP:HA	1:B:256:ASP:HB3	1.95	0.49
1:E:395:LEU:CD1	8:E:1386:HOH:O	2.48	0.49
1:J:328:LEU:N	1:J:328:LEU:HD12	2.27	0.49
1:D:602:ASN:CB	8:D:2182:HOH:O	2.59	0.49
1:F:236:ARG:HD2	1:F:283:LYS:HG2	1.94	0.49
1:H:320:LYS:HB3	7:H:64:1PE:H141	1.94	0.49
1:I:208:LEU:O	1:I:212:THR:HG23	2.13	0.49
1:K:248:THR:CG2	8:K:2935:HOH:O	2.46	0.49
1:H:473:ALA:O	1:H:476:LEU:HB2	2.12	0.49
1:E:364:ASP:O	1:E:420:ASN:HA	2.13	0.49
1:G:494:SER:CB	1:L:494:SER:HB3	2.43	0.49
1:E:423:ILE:CD1	1:E:600:VAL:HG11	2.42	0.48
1:H:135:PRO:HA	1:H:194:SER:O	2.13	0.48
1:H:328:LEU:N	1:H:328:LEU:HD12	2.27	0.48
1:F:326:LYS:HD2	8:F:4070:HOH:O	2.12	0.48
1:K:423:ILE:HD11	1:K:600:VAL:CG1	2.44	0.48
1:B:193:GLY:HA3	8:B:5092:HOH:O	2.13	0.48
1:I:167:VAL:O	1:I:168:LYS:C	2.57	0.48
1:I:367:LYS:HE3	1:I:603:ASP:OD1	2.14	0.48
1:K:487:LEU:O	4:K:1003:BES:H2	2.14	0.48
1:D:337:LYS:HE2	8:D:4137:HOH:O	2.13	0.48
1:D:514:LEU:O	1:D:518:LYS:HG2	2.13	0.48
1:C:529:ILE:HG21	1:C:563:LYS:HE2	1.94	0.47
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.96	0.47
7:I:22:1PE:H252	7:I:22:1PE:H242	1.70	0.47
1:K:544:ILE:CD1	1:K:564:GLU:HG3	2.44	0.47
1:C:235:PHE:O	1:C:239:LEU:HD13	2.14	0.47
1:J:411:TYR:CE1	7:J:2:1PE:H151	2.37	0.47
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.96	0.47
1:B:103:TYR:CD1	7:B:61:1PE:H131	2.48	0.47
1:C:487:LEU:O	4:C:1003:BES:H2	2.14	0.47
1:C:584:LYS:CG	8:C:4907:HOH:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:LYS:NZ	7:G:58:1PE:H222	2.29	0.47
1:B:254:SER:OG	1:B:255:THR:N	2.47	0.47
1:H:142:VAL:HG22	1:H:162:MET:HB3	1.96	0.47
1:J:158:LYS:HE3	1:J:160:GLU:OE1	2.15	0.47
1:G:256:ASP:O	1:G:256:ASP:CG	2.58	0.47
1:J:122:ASN:HA	1:J:149:ASN:HB2	1.96	0.47
1:B:320:LYS:CE	7:B:61:1PE:H142	2.45	0.47
1:D:543:ASP:CG	7:D:44:1PE:H241	2.38	0.47
1:E:395:LEU:HD11	1:E:581:TRP:CG	2.50	0.47
1:A:398:PHE:HZ	4:A:1003:BES:H11	1.79	0.47
1:B:123:VAL:O	1:B:185:VAL:HG11	2.15	0.47
1:E:167:VAL:O	1:E:168:LYS:C	2.58	0.47
1:H:287:TYR:O	1:H:291:THR:CG2	2.62	0.47
1:E:544:ILE:CD1	1:E:564:GLU:HG3	2.45	0.46
1:L:214:LEU:HD23	1:L:219:LEU:HD12	1.97	0.46
1:D:392:MET:CE	4:D:1003:BES:H10	2.46	0.46
1:D:398:PHE:C	1:D:398:PHE:CD2	2.92	0.46
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.15	0.46
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.98	0.46
1:K:395:LEU:HB2	8:K:2124:HOH:O	2.15	0.46
1:L:332:GLU:CB	8:L:3297:HOH:O	2.64	0.46
1:G:164:LYS:HE2	1:G:165:PHE:CZ	2.50	0.46
1:L:156:PHE:O	1:L:162:MET:HE3	2.15	0.46
1:J:549:SER:OG	1:J:550:SER:N	2.49	0.46
1:D:549:SER:OG	1:D:550:SER:N	2.49	0.46
1:G:316:GLU:HG2	1:G:320:LYS:HE2	1.96	0.46
1:J:320:LYS:NZ	7:J:3:1PE:H142	2.31	0.46
1:E:395:LEU:HB2	8:E:1386:HOH:O	2.16	0.46
7:K:42:1PE:C26	8:K:915:HOH:O	2.64	0.46
1:B:135:PRO:HA	1:B:194:SER:O	2.16	0.46
1:D:423:ILE:CD1	1:D:600:VAL:HG11	2.45	0.46
1:F:231:ASP:HB3	1:F:234:LEU:H	1.81	0.46
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.51	0.46
1:H:160:GLU:O	1:H:163:GLU:HG2	2.17	0.45
1:I:579:VAL:HG13	1:I:591:PHE:CD1	2.51	0.45
1:L:451:LYS:HZ1	7:L:612:1PE:H152	1.82	0.45
1:B:250:GLU:OE1	1:B:258:ASN:HB2	2.15	0.45
1:L:451:LYS:CG	7:L:612:1PE:H131	2.39	0.45
1:C:551:VAL:HG12	1:C:553:ALA:H	1.81	0.45
1:L:346:LYS:HB3	1:L:437:ASN:O	2.16	0.45
1:I:584:LYS:NZ	8:I:62:HOH:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:7:SO4:O2	1:F:436:LYS:HG2	2.15	0.45
1:I:137:LYS:CB	8:I:5069:HOH:O	2.63	0.45
1:I:320:LYS:HZ1	7:I:21:1PE:H232	1.77	0.45
1:I:584:LYS:HD3	1:I:584:LYS:N	2.32	0.45
1:H:142:VAL:CG2	1:H:162:MET:HB3	2.46	0.45
1:I:265:LYS:HE2	1:I:265:LYS:HB3	1.78	0.45
1:J:423:ILE:CD1	1:J:600:VAL:CG1	2.95	0.45
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.99	0.45
1:C:552:LYS:HG2	8:C:2589:HOH:O	2.15	0.45
1:E:363:GLY:N	8:E:1815:HOH:O	2.49	0.45
1:K:392:MET:HE3	4:K:1003:BES:C10	2.45	0.45
1:K:423:ILE:HD11	1:K:600:VAL:HG13	1.98	0.45
1:L:127:LEU:HD11	1:L:129:ILE:HD11	1.99	0.45
1:A:113:GLN:NE2	8:A:5301:HOH:O	2.50	0.45
1:G:121:CYS:HA	1:G:270:TYR:CE2	2.51	0.45
1:A:316:GLU:HG3	7:A:20:1PE:H131	1.98	0.45
1:I:235:PHE:O	1:I:239:LEU:HD13	2.17	0.45
1:C:117:ILE:HG22	1:C:272:ASN:HA	1.99	0.45
1:H:103:TYR:HD1	7:H:65:1PE:H222	1.81	0.45
1:A:320:LYS:HB3	7:A:19:1PE:H141	1.99	0.44
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.99	0.44
1:G:449:ASN:HD21	1:G:451:LYS:HE2	1.83	0.44
1:E:230:VAL:HG22	1:E:234:LEU:HD23	1.97	0.44
1:J:103:TYR:HB2	6:J:20:SO4:O2	2.17	0.44
1:B:256:ASP:O	1:B:256:ASP:CG	2.61	0.44
1:E:398:PHE:CD2	1:E:398:PHE:C	2.96	0.44
1:H:123:VAL:O	1:H:125:GLU:N	2.51	0.44
1:J:86:SER:N	8:J:1508:HOH:O	2.50	0.44
1:C:137:LYS:CB	8:C:2894:HOH:O	2.65	0.44
1:C:398:PHE:CD2	1:C:398:PHE:C	2.96	0.44
1:H:487:LEU:O	4:H:1003:BES:H2	2.17	0.44
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.99	0.44
1:J:364:ASP:O	1:J:420:ASN:HA	2.18	0.44
1:K:167:VAL:O	1:K:168:LYS:C	2.61	0.44
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.98	0.44
1:D:398:PHE:HZ	4:D:1003:BES:H11	1.83	0.44
1:E:341:TYR:CE1	1:E:428:ALA:HB1	2.53	0.44
1:F:172:SER:O	1:F:173:LYS:HG2	2.18	0.44
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.98	0.44
1:K:183:ASN:O	1:K:185:VAL:HG13	2.18	0.44
1:B:177:MET:O	1:B:184:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TYR:O	1:B:291:THR:CG2	2.58	0.44
1:C:208:LEU:O	1:C:212:THR:HG23	2.18	0.44
7:D:67:1PE:C15	8:D:5399:HOH:O	2.66	0.44
1:A:395:LEU:HD12	8:A:3005:HOH:O	2.17	0.43
1:J:262:GLU:HG3	8:J:1036:HOH:O	2.17	0.43
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.00	0.43
1:K:205:ARG:NH1	8:K:5087:HOH:O	2.50	0.43
1:A:167:VAL:O	1:A:168:LYS:C	2.62	0.43
1:C:567:GLN:CG	8:C:2276:HOH:O	2.66	0.43
1:E:272:ASN:O	1:E:273:ASN:HB2	2.18	0.43
1:H:165:PHE:HB3	1:H:189:TYR:OH	2.17	0.43
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.00	0.43
1:I:164:LYS:HG2	8:I:4415:HOH:O	2.17	0.43
1:I:364:ASP:O	1:I:420:ASN:HA	2.18	0.43
1:J:321:LEU:HD11	1:J:411:TYR:HA	2.01	0.43
1:K:441:PRO:HB2	1:L:394:ASP:HA	2.01	0.43
1:A:328:LEU:HB2	1:A:354:PHE:HB3	2.00	0.43
1:H:563:LYS:HE2	8:H:3025:HOH:O	2.19	0.43
1:C:392:MET:CE	4:C:1003:BES:H10	2.46	0.43
1:F:133:ASN:HB2	1:F:193:GLY:O	2.18	0.43
1:H:177:MET:O	1:H:184:SER:HA	2.17	0.43
1:C:413:VAL:HG11	1:C:423:ILE:HD13	2.01	0.43
1:D:392:MET:HE3	4:D:1003:BES:H10	2.01	0.43
1:E:392:MET:HE1	4:E:1003:BES:H10	1.96	0.43
1:G:395:LEU:HD11	1:G:581:TRP:CG	2.54	0.43
1:J:328:LEU:N	1:J:328:LEU:CD1	2.82	0.43
1:J:514:LEU:O	1:J:518:LYS:HG2	2.17	0.43
1:K:423:ILE:CD1	1:K:600:VAL:HG11	2.48	0.43
1:C:316:GLU:HG3	7:C:17:1PE:OH3	2.19	0.43
1:C:326:LYS:HG2	1:C:328:LEU:HD12	2.00	0.43
1:J:398:PHE:HZ	4:J:1003:BES:C11	2.30	0.43
1:L:86:SER:HB3	1:L:312:ASN:OD1	2.19	0.43
1:C:360:LYS:HE2	1:C:365:VAL:HG21	2.01	0.43
1:K:150:ASP:OD1	1:K:179:ASN:HB2	2.19	0.43
1:F:514:LEU:O	1:F:517:SER:HB3	2.19	0.42
1:J:451:LYS:HE3	1:J:564:GLU:O	2.19	0.42
1:K:321:LEU:HD11	1:K:411:TYR:HA	2.01	0.42
1:G:162:MET:HE2	1:G:162:MET:HA	2.02	0.42
1:G:173:LYS:HE2	1:J:216:ASP:OD2	2.19	0.42
1:G:302:SER:HB2	1:I:440:ARG:HD3	2.01	0.42
1:H:102:GLU:HG3	1:H:105:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:HIS:HB3	1:L:175:PHE:CD2	2.54	0.42
1:J:440:ARG:NH2	8:J:652:HOH:O	2.51	0.42
1:J:442:GLY:O	1:K:301:PRO:HB3	2.18	0.42
1:L:605:LEU:HD12	8:L:2621:HOH:O	2.19	0.42
1:B:117:ILE:HD11	1:B:146:SER:OG	2.19	0.42
1:J:481:ILE:O	1:J:571:TRP:HA	2.18	0.42
1:K:597:THR:HG22	1:K:601:LEU:CD2	2.48	0.42
1:C:536:THR:HG21	1:C:551:VAL:HG23	2.02	0.42
1:E:321:LEU:HD11	1:E:411:TYR:HA	2.02	0.42
1:F:328:LEU:HB2	1:F:354:PHE:HB3	2.00	0.42
1:I:218:LYS:HD3	1:I:262:GLU:CD	2.45	0.42
1:A:394:ASP:HA	1:C:441:PRO:HB2	2.01	0.42
1:G:291:THR:HG22	8:G:713:HOH:O	2.20	0.42
1:J:320:LYS:HZ3	7:J:3:1PE:H142	1.85	0.42
1:C:322:ASN:HB3	8:C:4013:HOH:O	2.19	0.42
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.02	0.42
1:F:345:GLY:HA3	1:F:352:ASN:OD1	2.20	0.42
1:G:167:VAL:O	1:G:168:LYS:C	2.63	0.42
1:G:367:LYS:HA	1:G:367:LYS:HD3	1.85	0.42
1:L:103:TYR:HB3	7:L:1:1PE:H252	2.02	0.42
1:C:329:GLY:O	1:C:333:LEU:HG	2.20	0.41
1:E:104:ASN:HB3	8:E:5393:HOH:O	2.19	0.41
1:I:117:ILE:HG22	1:I:272:ASN:HA	2.01	0.41
1:K:395:LEU:CB	8:K:2124:HOH:O	2.69	0.41
1:B:398:PHE:HZ	4:B:1003:BES:H11	1.85	0.41
1:D:440:ARG:NH2	8:D:625:HOH:O	2.53	0.41
1:E:200:GLU:O	1:E:204:LYS:HG3	2.19	0.41
1:J:357:LEU:HB2	1:J:425:PHE:HB2	2.02	0.41
1:K:133:ASN:CA	1:K:167:VAL:HG11	2.42	0.41
1:L:229:ASN:HA	8:L:3530:HOH:O	2.21	0.41
1:A:198:LEU:HD22	1:A:202:ASP:HB3	2.01	0.41
1:C:421:VAL:CG2	1:C:423:ILE:HD11	2.51	0.41
1:E:167:VAL:CG1	1:E:167:VAL:O	2.68	0.41
1:E:167:VAL:HG12	1:E:193:GLY:H	1.85	0.41
1:K:167:VAL:CG1	1:K:167:VAL:O	2.68	0.41
1:K:398:PHE:CD2	1:K:398:PHE:C	2.99	0.41
1:L:357:LEU:HB2	1:L:425:PHE:HB2	2.03	0.41
1:C:591:PHE:CD2	1:C:591:PHE:C	2.98	0.41
1:F:167:VAL:O	1:F:168:LYS:C	2.62	0.41
1:F:205:ARG:NH2	8:F:4961:HOH:O	2.53	0.41
1:F:383:TYR:HE2	1:F:438:SER:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:207:VAL:HG11	1:I:241:THR:HG22	2.02	0.41
1:I:326:LYS:HG2	1:I:328:LEU:HD12	2.01	0.41
1:K:395:LEU:HD23	1:K:398:PHE:CE2	2.56	0.41
1:B:230:VAL:HG12	1:B:234:LEU:HD23	2.02	0.41
1:E:133:ASN:CA	1:E:167:VAL:HG11	2.43	0.41
1:E:423:ILE:HD11	1:E:600:VAL:HG13	2.01	0.41
1:F:586:ARG:HD3	8:F:2842:HOH:O	2.20	0.41
1:L:217:ASN:HB3	1:L:219:LEU:CD2	2.38	0.41
1:L:544:ILE:CD1	1:L:564:GLU:HG3	2.51	0.41
1:G:505:ASN:OD1	1:G:505:ASN:C	2.64	0.41
1:I:279:GLU:HG2	8:I:4643:HOH:O	2.20	0.41
1:C:141:PRO:HG2	1:C:143:LYS:HE3	2.03	0.41
1:C:364:ASP:O	1:C:420:ASN:HA	2.20	0.41
1:D:164:LYS:HE2	8:D:2472:HOH:O	2.21	0.41
1:D:301:PRO:HB3	1:F:442:GLY:O	2.21	0.41
1:D:544:ILE:CD1	1:D:564:GLU:HG3	2.50	0.41
1:E:392:MET:HE3	4:E:1003:BES:C10	2.34	0.41
1:F:138:GLU:HA	1:F:194:SER:OG	2.21	0.41
1:F:150:ASP:OD1	1:F:179:ASN:HB2	2.20	0.41
1:G:265:LYS:HB3	1:G:265:LYS:HE2	1.93	0.41
1:H:337:LYS:HE2	8:H:4278:HOH:O	2.19	0.41
1:I:421:VAL:CG2	1:I:423:ILE:HD11	2.51	0.41
1:J:132:VAL:HG11	1:J:144:ILE:HD13	2.02	0.41
1:A:602:ASN:ND2	8:A:1683:HOH:O	2.54	0.41
1:H:171:THR:HG21	8:H:2774:HOH:O	2.21	0.41
1:I:579:VAL:HG13	1:I:591:PHE:CG	2.56	0.41
1:A:307:PRO:HD2	1:A:350:TYR:CB	2.51	0.40
1:C:515:GLN:OE1	1:C:515:GLN:HA	2.20	0.40
1:E:142:VAL:HG11	1:E:162:MET:HE3	2.03	0.40
1:E:423:ILE:HD11	1:E:600:VAL:HG11	2.02	0.40
1:B:139:ASN:O	1:B:166:ASN:HB2	2.21	0.40
1:B:300:ALA:HA	1:B:301:PRO:HD3	1.96	0.40
1:B:328:LEU:HB2	1:B:354:PHE:HB3	2.02	0.40
1:C:235:PHE:O	1:C:239:LEU:CD1	2.70	0.40
1:E:326:LYS:HG2	1:E:328:LEU:HD12	2.03	0.40
1:G:164:LYS:CE	8:J:3193:HOH:O	2.39	0.40
1:G:473:ALA:O	1:G:476:LEU:HB2	2.21	0.40
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.56	0.40
1:A:494:SER:HB3	1:F:494:SER:HB3	2.03	0.40
1:C:579:VAL:O	1:C:589:LYS:HD2	2.21	0.40
1:F:302:SER:HB2	8:F:629:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:LEU:N	1:D:328:LEU:CD1	2.85	0.40
1:D:364:ASP:O	1:D:420:ASN:HA	2.20	0.40
1:G:118:LYS:HB2	1:G:118:LYS:HZ2	1.86	0.40
1:H:265:LYS:HB2	1:H:265:LYS:HE2	1.85	0.40
1:D:102:GLU:CD	8:D:5170:HOH:O	2.64	0.40
1:F:86:SER:HB3	8:F:5276:HOH:O	2.22	0.40
1:F:205:ARG:NH1	1:F:205:ARG:CG	2.76	0.40
1:H:481:ILE:O	1:H:571:TRP:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/528 (98%)	503 (98%)	12 (2%)	0	100	100
1	B	516/528 (98%)	502 (97%)	11 (2%)	3 (1%)	21	17
1	C	517/528 (98%)	509 (98%)	8 (2%)	0	100	100
1	D	512/528 (97%)	492 (96%)	18 (4%)	2 (0%)	30	27
1	E	506/528 (96%)	493 (97%)	10 (2%)	3 (1%)	21	17
1	F	504/528 (96%)	487 (97%)	17 (3%)	0	100	100
1	G	512/528 (97%)	500 (98%)	11 (2%)	1 (0%)	43	42
1	H	504/528 (96%)	493 (98%)	10 (2%)	1 (0%)	43	42
1	I	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
1	J	510/528 (97%)	496 (97%)	14 (3%)	0	100	100
1	K	504/528 (96%)	495 (98%)	9 (2%)	0	100	100
1	L	510/528 (97%)	501 (98%)	9 (2%)	0	100	100
All	All	6127/6336 (97%)	5978 (98%)	139 (2%)	10 (0%)	43	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	124	GLU
1	B	136	GLY
1	B	258	ASN
1	B	259	VAL
1	E	362	LYS
1	E	363	GLY
1	E	217	ASN
1	G	386	LYS
1	D	137	LYS
1	D	364	ASP

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	427/455 (94%)	417 (98%)	10 (2%)	44	49
1	B	414/455 (91%)	395 (95%)	19 (5%)	24	22
1	C	419/455 (92%)	404 (96%)	15 (4%)	31	31
1	D	418/455 (92%)	398 (95%)	20 (5%)	23	21
1	E	413/455 (91%)	399 (97%)	14 (3%)	32	33
1	F	409/455 (90%)	392 (96%)	17 (4%)	26	25
1	G	437/455 (96%)	422 (97%)	15 (3%)	32	33
1	H	431/455 (95%)	406 (94%)	25 (6%)	18	15
1	I	437/455 (96%)	416 (95%)	21 (5%)	23	21
1	J	432/455 (95%)	414 (96%)	18 (4%)	26	25
1	K	428/455 (94%)	414 (97%)	14 (3%)	33	34
1	L	424/455 (93%)	402 (95%)	22 (5%)	21	18
All	All	5089/5460 (93%)	4879 (96%)	210 (4%)	27	26

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	101	ILE
1	A	171	THR
1	A	200	GLU
1	A	330	VAL
1	A	367	LYS
1	A	398	PHE
1	A	436	LYS
1	A	439	TYR
1	A	603	ASP
1	B	86	SER
1	B	113	GLN
1	B	142	VAL
1	B	173	LYS
1	B	194	SER
1	B	200	GLU
1	B	208	LEU
1	B	258	ASN
1	B	278	LYS
1	B	291	THR
1	B	310	LEU
1	B	357	LEU
1	B	395	LEU
1	B	398	PHE
1	B	436	LYS
1	B	439	TYR
1	B	507	GLU
1	B	549	SER
1	B	603	ASP
1	C	86	SER
1	C	168	LYS
1	C	171	THR
1	C	173	LYS
1	C	200	GLU
1	C	204	LYS
1	C	229	ASN
1	C	322	ASN
1	C	357	LEU
1	C	398	PHE
1	C	439	TYR
1	C	483	ASP
1	C	549	SER
1	C	601	LEU

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Mol	Chain	Res	Type
1	C	603	ASP
1	D	88	VAL
1	D	164	LYS
1	D	194	SER
1	D	198	LEU
1	D	200	GLU
1	D	205	ARG
1	D	208	LEU
1	D	217	ASN
1	D	248	THR
1	D	262	GLU
1	D	310	LEU
1	D	328	LEU
1	D	395	LEU
1	D	398	PHE
1	D	436	LYS
1	D	439	TYR
1	D	483	ASP
1	D	518	LYS
1	D	560	LEU
1	D	579	VAL
1	E	86	SER
1	E	102	GLU
1	E	208	LEU
1	E	216	ASP
1	E	230	VAL
1	E	239	LEU
1	E	248	THR
1	E	310	LEU
1	E	357	LEU
1	E	398	PHE
1	E	413	VAL
1	E	439	TYR
1	E	560	LEU
1	E	601	LEU
1	F	86	SER
1	F	88	VAL
1	F	114	VAL
1	F	116	ASP
1	F	117	ILE
1	F	168	LYS
1	F	198	LEU

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Mol	Chain	Res	Type
1	F	205	ARG
1	F	231	ASP
1	F	239	LEU
1	F	357	LEU
1	F	364	ASP
1	F	395	LEU
1	F	398	PHE
1	F	439	TYR
1	F	508	GLU
1	F	579	VAL
1	G	101	ILE
1	G	118	LYS
1	G	164	LYS
1	G	171	THR
1	G	182	LYS
1	G	200	GLU
1	G	262	GLU
1	G	310	LEU
1	G	398	PHE
1	G	421	VAL
1	G	436	LYS
1	G	439	TYR
1	G	476	LEU
1	G	498	SER
1	G	603	ASP
1	H	113	GLN
1	H	142	VAL
1	H	155	GLU
1	H	158	LYS
1	H	173	LYS
1	H	194	SER
1	H	200	GLU
1	H	208	LEU
1	H	278	LYS
1	H	291	THR
1	H	310	LEU
1	H	328	LEU
1	H	331	LYS
1	H	357	LEU
1	H	398	PHE
1	H	421	VAL
1	H	436	LYS

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Mol	Chain	Res	Type
1	H	439	TYR
1	H	476	LEU
1	H	507	GLU
1	H	518	LYS
1	H	549	SER
1	H	579	VAL
1	H	601	LEU
1	H	603	ASP
1	I	86	SER
1	I	168	LYS
1	I	171	THR
1	I	173	LYS
1	I	182	LYS
1	I	200	GLU
1	I	208	LEU
1	I	229	ASN
1	I	230	VAL
1	I	265	LYS
1	I	310	LEU
1	I	322	ASN
1	I	357	LEU
1	I	394	ASP
1	I	398	PHE
1	I	483	ASP
1	I	549	SER
1	I	579	VAL
1	I	584	LYS
1	I	601	LEU
1	I	603	ASP
1	J	88	VAL
1	J	164	LYS
1	J	194	SER
1	J	200	GLU
1	J	208	LEU
1	J	239	LEU
1	J	248	THR
1	J	262	GLU
1	J	328	LEU
1	J	357	LEU
1	J	367	LYS
1	J	395	LEU
1	J	398	PHE

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Mol	Chain	Res	Type
1	J	436	LYS
1	J	439	TYR
1	J	518	LYS
1	J	579	VAL
1	J	603	ASP
1	K	86	SER
1	K	102	GLU
1	K	132	VAL
1	K	138	GLU
1	K	208	LEU
1	K	218	LYS
1	K	239	LEU
1	K	248	THR
1	K	265	LYS
1	K	395	LEU
1	K	398	PHE
1	K	579	VAL
1	K	584	LYS
1	K	601	LEU
1	L	86	SER
1	L	116	ASP
1	L	144	ILE
1	L	148	VAL
1	L	155	GLU
1	L	160	GLU
1	L	167	VAL
1	L	173	LYS
1	L	200	GLU
1	L	229	ASN
1	L	291	THR
1	L	310	LEU
1	L	357	LEU
1	L	365	VAL
1	L	398	PHE
1	L	436	LYS
1	L	439	TYR
1	L	568	ASN
1	L	579	VAL
1	L	580	SER
1	L	601	LEU
1	L	603	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	420	ASN
1	A	545	ASN
1	B	113	GLN
1	B	139	ASN
1	B	420	ASN
1	B	545	ASN
1	C	273	ASN
1	C	322	ASN
1	D	183	ASN
1	D	215	HIS
1	D	420	ASN
1	E	134	ASN
1	E	229	ASN
1	E	602	ASN
1	F	104	ASN
1	F	272	ASN
1	F	521	ASN
1	G	149	ASN
1	H	139	ASN
1	H	183	ASN
1	H	545	ASN
1	I	113	GLN
1	I	139	ASN
1	I	181	ASN
1	I	183	ASN
1	I	602	ASN
1	J	113	GLN
1	J	183	ASN
1	J	420	ASN
1	K	113	GLN
1	K	229	ASN
1	L	161	ASN
1	L	181	ASN
1	L	183	ASN
1	L	217	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 99 ligands modelled in this entry, 24 are monoatomic - leaving 75 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	CO3	K	1002	-	3,3,3	0.43	0	2,3,3	0.94	0
7	1PE	E	43	-	7,7,15	0.54	0	6,6,14	0.29	0
4	BES	A	1003	3,5	22,22,22	0.87	0	26,29,29	1.58	4 (15%)
7	1PE	C	17	-	12,12,15	0.56	0	11,11,14	0.49	0
6	SO4	A	2	-	4,4,4	0.30	0	6,6,6	0.27	0
7	1PE	E	8	-	11,11,15	0.39	0	10,10,14	0.52	0
4	BES	B	1003	3,5	22,22,22	0.73	0	26,29,29	1.65	9 (34%)
7	1PE	E	7	-	11,11,15	0.54	0	10,10,14	0.43	0
4	BES	L	1003	3,5	22,22,22	0.80	0	26,29,29	1.53	6 (23%)
6	SO4	J	20	-	4,4,4	0.18	0	6,6,6	0.21	0
7	1PE	B	61	-	9,9,15	0.64	0	8,8,14	0.83	0
6	SO4	J	18	-	4,4,4	0.43	0	6,6,6	0.57	0
7	1PE	G	47	-	5,5,15	0.51	0	4,4,14	0.50	0
2	CO3	A	1002	-	3,3,3	0.48	0	2,3,3	1.39	0
7	1PE	L	1	-	9,9,15	0.32	0	8,8,14	0.52	0
7	1PE	L	612	-	11,11,15	0.45	0	10,10,14	0.50	0
6	SO4	G	23	-	4,4,4	0.30	0	6,6,6	0.32	0
7	1PE	F	31	-	9,9,15	0.37	0	8,8,14	0.61	0
7	1PE	G	30	-	6,6,15	0.49	0	5,5,14	0.32	0
4	BES	I	1003	3,5	22,22,22	0.97	0	26,29,29	1.72	6 (23%)
2	CO3	D	1002	-	3,3,3	1.35	1 (33%)	2,3,3	1.62	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1	-	4,4,4	0.29	0	6,6,6	0.35	0
6	SO4	E	22	-	4,4,4	0.23	0	6,6,6	0.23	0
7	1PE	K	50	-	5,5,15	0.61	0	4,4,14	0.33	0
4	BES	H	1003	3,5	22,22,22	0.79	0	26,29,29	1.45	4 (15%)
2	CO3	G	1002	-	3,3,3	0.80	0	2,3,3	0.76	0
7	1PE	D	67	-	6,6,15	0.50	0	5,5,14	0.29	0
4	BES	C	1003	3,5	22,22,22	0.91	0	26,29,29	1.47	2 (7%)
6	SO4	F	21	-	4,4,4	0.27	0	6,6,6	0.17	0
7	1PE	B	60	-	9,9,15	0.44	0	8,8,14	0.56	0
7	1PE	G	48	-	5,5,15	0.64	0	4,4,14	0.78	0
2	CO3	F	1002	-	3,3,3	1.25	0	2,3,3	1.55	0
6	SO4	D	5	-	4,4,4	0.20	0	6,6,6	0.23	0
7	1PE	D	63	-	9,9,15	0.75	0	8,8,14	0.80	0
4	BES	D	1003	3,5	22,22,22	0.85	0	26,29,29	1.14	3 (11%)
6	SO4	K	19	-	4,4,4	0.32	0	6,6,6	0.21	0
7	1PE	I	66	-	6,6,15	0.60	0	5,5,14	0.33	0
6	SO4	B	3	-	4,4,4	0.41	0	6,6,6	0.41	0
6	SO4	D	7	-	4,4,4	0.38	0	6,6,6	0.52	0
4	BES	E	1003	3,5	22,22,22	0.90	1 (4%)	26,29,29	1.42	2 (7%)
2	CO3	J	1002	-	3,3,3	0.67	0	2,3,3	1.64	0
7	1PE	B	62	-	9,9,15	0.61	0	8,8,14	0.40	0
4	BES	F	1003	3,5	22,22,22	0.81	0	26,29,29	1.60	5 (19%)
7	1PE	H	64	-	9,9,15	0.53	0	8,8,14	0.55	0
7	1PE	H	65	-	9,9,15	0.64	0	8,8,14	0.73	0
7	1PE	K	5	-	11,11,15	0.44	0	10,10,14	0.63	0
7	1PE	L	56	-	10,10,15	0.56	0	9,9,14	0.28	0
2	CO3	L	1002	-	3,3,3	0.38	0	2,3,3	1.34	0
4	BES	K	1003	3,5	22,22,22	0.92	0	26,29,29	1.61	4 (15%)
7	1PE	A	19	-	8,8,15	0.51	0	7,7,14	0.24	0
7	1PE	J	3	-	9,9,15	0.54	0	8,8,14	0.49	0
2	CO3	C	1002	-	3,3,3	0.90	0	2,3,3	1.14	0
7	1PE	G	58	-	14,14,15	0.71	0	13,13,14	0.54	0
4	BES	G	1003	3,5	22,22,22	0.99	2 (9%)	26,29,29	1.68	3 (11%)
4	BES	J	1003	3,5	22,22,22	0.97	1 (4%)	26,29,29	1.63	4 (15%)
7	1PE	C	18	-	8,8,15	0.54	0	7,7,14	0.41	0
6	SO4	A	24	-	4,4,4	0.29	0	6,6,6	0.14	0
7	1PE	D	9	-	9,9,15	0.46	0	8,8,14	0.30	0
7	1PE	D	44	-	10,10,15	0.73	0	9,9,14	0.65	0
2	CO3	I	1002	-	3,3,3	1.14	0	2,3,3	1.30	0
7	1PE	I	21	-	14,14,15	0.67	0	13,13,14	0.76	0
7	1PE	I	22	-	10,10,15	0.50	0	9,9,14	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1PE	J	2	-	10,10,15	0.41	0	9,9,14	0.58	0
7	1PE	K	4	-	11,11,15	0.57	0	10,10,14	0.37	0
6	SO4	L	25	-	4,4,4	0.31	0	6,6,6	0.34	0
2	CO3	H	1002	-	3,3,3	0.68	0	2,3,3	1.24	0
6	SO4	G	17	-	4,4,4	0.20	0	6,6,6	0.39	0
7	1PE	F	33	-	9,9,15	0.55	0	8,8,14	0.32	0
2	CO3	E	1002	-	3,3,3	0.97	0	2,3,3	0.94	0
7	1PE	A	20	-	11,11,15	0.62	0	10,10,14	0.53	0
7	1PE	F	32	-	9,9,15	0.57	0	8,8,14	0.39	0
7	1PE	J	45	-	9,9,15	0.52	0	8,8,14	0.36	0
7	1PE	K	42	-	10,10,15	0.58	0	9,9,14	0.40	0
2	CO3	B	1002	-	3,3,3	0.50	0	2,3,3	2.24	2 (100%)
7	1PE	G	12	-	8,8,15	0.58	0	7,7,14	0.38	0

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
7	1PE	E	43	-	-	2/5/5/13	-
4	BES	A	1003	3,5	-	2/24/24/24	0/1/1/1
7	1PE	C	17	-	-	2/10/10/13	-
7	1PE	E	8	-	-	0/9/9/13	-
4	BES	B	1003	3,5	-	5/24/24/24	0/1/1/1
7	1PE	E	7	-	-	3/9/9/13	-
4	BES	L	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	B	61	-	-	7/7/7/13	-
7	1PE	G	47	-	-	3/3/3/13	-
7	1PE	L	1	-	-	5/7/7/13	-
7	1PE	L	612	-	-	5/9/9/13	-
7	1PE	F	31	-	-	0/7/7/13	-
7	1PE	G	30	-	-	3/4/4/13	-
4	BES	I	1003	3,5	-	7/24/24/24	0/1/1/1
7	1PE	K	50	-	-	3/3/3/13	-
4	BES	H	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	D	67	-	-	3/4/4/13	-
4	BES	C	1003	3,5	-	7/24/24/24	0/1/1/1
7	1PE	B	60	-	-	3/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	G	48	-	-	2/3/3/13	-
7	1PE	D	63	-	-	3/7/7/13	-
4	BES	D	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	I	66	-	-	2/4/4/13	-
7	1PE	H	64	-	-	2/7/7/13	-
7	1PE	K	5	-	-	2/9/9/13	-
4	BES	E	1003	3,5	-	6/24/24/24	0/1/1/1
7	1PE	B	62	-	-	1/7/7/13	-
7	1PE	L	56	-	-	1/8/8/13	-
4	BES	F	1003	3,5	-	11/24/24/24	0/1/1/1
7	1PE	H	65	-	-	3/7/7/13	-
4	BES	K	1003	3,5	-	9/24/24/24	0/1/1/1
7	1PE	A	19	-	-	2/6/6/13	-
7	1PE	J	3	-	-	4/7/7/13	-
7	1PE	G	58	-	-	6/12/12/13	-
4	BES	G	1003	3,5	-	7/24/24/24	0/1/1/1
4	BES	J	1003	3,5	-	5/24/24/24	0/1/1/1
7	1PE	C	18	-	-	4/6/6/13	-
7	1PE	D	9	-	-	6/7/7/13	-
7	1PE	D	44	-	-	3/8/8/13	-
7	1PE	I	21	-	-	4/12/12/13	-
7	1PE	K	4	-	-	1/9/9/13	-
7	1PE	I	22	-	-	5/8/8/13	-
7	1PE	J	2	-	-	6/8/8/13	-
7	1PE	F	33	-	-	4/7/7/13	-
7	1PE	K	42	-	-	4/8/8/13	-
7	1PE	A	20	-	-	4/9/9/13	-
7	1PE	F	32	-	-	3/7/7/13	-
7	1PE	J	45	-	-	4/7/7/13	-
7	1PE	G	12	-	-	6/6/6/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1003	BES	O4-C5	2.19	1.28	1.22
4	E	1003	BES	C2-C3	-2.19	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1003	BES	O2-C2	2.16	1.46	1.42
2	D	1002	CO3	O1-C	2.12	1.33	1.25
4	G	1003	BES	C2-C1	2.10	1.56	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1003	BES	O2-C2-C1	5.53	121.01	109.64
4	G	1003	BES	O2-C2-C1	5.23	120.41	109.64
4	G	1003	BES	O2-C2-C3	-4.75	100.69	110.63
4	F	1003	BES	O2-C2-C1	4.75	119.42	109.64
4	K	1003	BES	O2-C2-C3	-4.57	101.08	110.63
4	I	1003	BES	O2-C2-C3	-4.55	101.11	110.63
4	A	1003	BES	O2-C2-C3	-4.27	101.70	110.63
4	A	1003	BES	O2-C2-C1	3.99	117.85	109.64
4	E	1003	BES	O2-C2-C3	-3.94	102.39	110.63
4	B	1003	BES	O2-C2-C1	3.89	117.64	109.64
4	C	1003	BES	O2-C2-C1	3.89	117.64	109.64
4	E	1003	BES	O2-C2-C1	3.73	117.32	109.64
4	I	1003	BES	C13-C4-N1	-3.71	102.22	110.58
4	L	1003	BES	O2-C2-C1	3.70	117.25	109.64
4	K	1003	BES	O2-C2-C1	3.61	117.06	109.64
4	H	1003	BES	O2-C2-C3	-3.59	103.11	110.63
4	J	1003	BES	C13-C4-N1	-3.56	102.54	110.58
4	L	1003	BES	O2-C2-C3	-3.47	103.38	110.63
4	C	1003	BES	O2-C2-C3	-3.38	103.57	110.63
4	D	1003	BES	O2-C2-C1	3.24	116.31	109.64
4	I	1003	BES	O2-C2-C1	3.10	116.02	109.64
4	H	1003	BES	O2-C2-C1	3.01	115.84	109.64
4	F	1003	BES	O2-C2-C3	-2.95	104.46	110.63
4	A	1003	BES	C7-C6-C1	2.77	119.38	113.48
4	D	1003	BES	O2-C2-C3	-2.75	104.88	110.63
4	B	1003	BES	C4-N1-C3	-2.68	115.88	121.65
4	K	1003	BES	C4-N1-C3	-2.67	115.92	121.65
4	K	1003	BES	C13-C4-N1	-2.65	104.60	110.58
4	B	1003	BES	O1-C5-O4	-2.63	118.11	124.08
4	B	1003	BES	C5-C4-N1	-2.50	104.76	110.57
4	H	1003	BES	C13-C4-N1	-2.50	104.94	110.58
4	F	1003	BES	C13-C4-N1	-2.49	104.95	110.58
4	L	1003	BES	C5-C4-N1	-2.48	104.82	110.57
4	B	1003	BES	C13-C4-N1	-2.47	105.00	110.58
4	A	1003	BES	C5-C4-N1	-2.45	104.88	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	BES	O1-C5-C4	2.43	121.73	113.51
2	B	1002	CO3	O3-C-O1	-2.40	113.53	119.68
4	F	1003	BES	C5-C4-N1	-2.39	105.03	110.57
4	I	1003	BES	C2-C3-N1	2.31	119.36	116.22
4	J	1003	BES	O2-C2-C3	-2.30	105.82	110.63
4	I	1003	BES	C4-N1-C3	-2.30	116.71	121.65
4	L	1003	BES	C4-N1-C3	-2.28	116.75	121.65
4	L	1003	BES	C13-C4-C5	2.25	117.05	110.28
4	F	1003	BES	C7-C6-C1	2.19	118.15	113.48
2	D	1002	CO3	O2-C-O1	2.15	125.18	119.68
4	B	1003	BES	O2-C2-C3	-2.12	106.21	110.63
4	L	1003	BES	C13-C4-N1	-2.12	105.80	110.58
4	H	1003	BES	C14-C13-C4	-2.10	109.75	115.40
4	J	1003	BES	O1-C5-C4	2.10	120.62	113.51
4	B	1003	BES	C12-C7-C8	2.08	121.33	118.23
2	B	1002	CO3	O2-C-O1	2.07	124.98	119.68
4	I	1003	BES	O1-C5-O4	-2.07	119.38	124.08
4	D	1003	BES	C13-C4-N1	-2.05	105.94	110.58
4	B	1003	BES	C14-C13-C4	-2.02	109.98	115.40
4	G	1003	BES	C5-C4-N1	-2.01	105.91	110.57

There are no chirality outliers.

All (198) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	BES	O2-C2-C3-O3
4	A	1003	BES	O2-C2-C3-N1
4	B	1003	BES	O2-C2-C3-O3
4	B	1003	BES	O2-C2-C3-N1
4	C	1003	BES	N2-C1-C2-C3
4	C	1003	BES	O2-C2-C3-O3
4	C	1003	BES	O2-C2-C3-N1
4	D	1003	BES	O2-C2-C3-O3
4	D	1003	BES	O2-C2-C3-N1
4	E	1003	BES	N2-C1-C2-C3
4	E	1003	BES	O2-C2-C3-N1
4	F	1003	BES	C2-C1-C6-C7
4	F	1003	BES	O2-C2-C3-O3
4	F	1003	BES	O2-C2-C3-N1
4	G	1003	BES	O2-C2-C3-O3
4	G	1003	BES	O2-C2-C3-N1
4	H	1003	BES	C2-C1-C6-C7

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Mol	Chain	Res	Type	Atoms
4	H	1003	BES	N2-C1-C2-C3
4	H	1003	BES	O2-C2-C3-O3
4	H	1003	BES	O2-C2-C3-N1
4	I	1003	BES	C2-C1-C6-C7
4	I	1003	BES	N2-C1-C2-C3
4	I	1003	BES	O2-C2-C3-O3
4	I	1003	BES	O2-C2-C3-N1
4	J	1003	BES	O2-C2-C3-O3
4	J	1003	BES	O2-C2-C3-N1
4	K	1003	BES	N2-C1-C2-C3
4	K	1003	BES	C6-C1-C2-C3
4	K	1003	BES	O2-C2-C3-O3
4	K	1003	BES	O2-C2-C3-N1
4	L	1003	BES	O2-C2-C3-N1
7	D	63	1PE	OH5-C14-C24-OH4
7	L	612	1PE	OH5-C14-C24-OH4
7	G	12	1PE	OH5-C14-C24-OH4
7	K	5	1PE	OH4-C13-C23-OH3
7	F	32	1PE	OH6-C15-C25-OH5
7	G	58	1PE	OH4-C13-C23-OH3
7	C	18	1PE	OH4-C13-C23-OH3
7	E	43	1PE	OH5-C14-C24-OH4
7	D	67	1PE	C14-C24-OH4-C13
7	D	9	1PE	OH5-C14-C24-OH4
7	L	1	1PE	OH6-C15-C25-OH5
7	B	60	1PE	OH5-C14-C24-OH4
7	B	61	1PE	C14-C24-OH4-C13
7	A	20	1PE	OH6-C15-C25-OH5
7	G	30	1PE	OH6-C15-C25-OH5
7	L	1	1PE	OH5-C14-C24-OH4
7	A	19	1PE	OH4-C13-C23-OH3
7	K	42	1PE	OH6-C15-C25-OH5
7	I	21	1PE	C12-C22-OH3-C23
7	K	50	1PE	C14-C24-OH4-C13
7	J	45	1PE	OH6-C15-C25-OH5
7	G	12	1PE	OH4-C13-C23-OH3
7	J	45	1PE	OH5-C14-C24-OH4
7	F	32	1PE	OH7-C16-C26-OH6
7	G	48	1PE	OH6-C15-C25-OH5
7	D	9	1PE	OH4-C13-C23-OH3
7	G	58	1PE	OH5-C14-C24-OH4
7	J	3	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
7	J	2	1PE	OH7-C16-C26-OH6
7	L	1	1PE	OH7-C16-C26-OH6
4	E	1003	BES	O2-C2-C3-O3
4	L	1003	BES	O2-C2-C3-O3
7	K	42	1PE	OH4-C13-C23-OH3
7	E	7	1PE	OH5-C14-C24-OH4
7	D	44	1PE	OH5-C14-C24-OH4
7	B	61	1PE	OH5-C14-C24-OH4
7	I	22	1PE	C24-C14-OH5-C25
4	E	1003	BES	N2-C1-C6-C7
4	H	1003	BES	N2-C1-C6-C7
4	K	1003	BES	N2-C1-C6-C7
4	L	1003	BES	N2-C1-C6-C7
7	B	60	1PE	OH4-C13-C23-OH3
4	F	1003	BES	N1-C4-C5-O4
7	K	50	1PE	OH5-C14-C24-OH4
7	G	48	1PE	C15-C25-OH5-C14
4	F	1003	BES	N1-C4-C5-O1
7	I	66	1PE	C15-C25-OH5-C14
7	H	65	1PE	C12-C22-OH3-C23
7	L	612	1PE	C12-C22-OH3-C23
7	I	22	1PE	C15-C25-OH5-C14
7	C	17	1PE	C12-C22-OH3-C23
7	G	12	1PE	C24-C14-OH5-C25
7	J	3	1PE	C15-C25-OH5-C14
7	E	43	1PE	C24-C14-OH5-C25
7	C	18	1PE	C12-C22-OH3-C23
7	I	21	1PE	OH6-C15-C25-OH5
7	G	12	1PE	C13-C23-OH3-C22
7	G	47	1PE	C24-C14-OH5-C25
4	K	1003	BES	C4-C13-C14-C16
7	A	20	1PE	C13-C23-OH3-C22
7	L	612	1PE	C24-C14-OH5-C25
7	D	9	1PE	C23-C13-OH4-C24
7	G	58	1PE	C16-C26-OH6-C15
7	I	21	1PE	C16-C26-OH6-C15
7	G	58	1PE	C14-C24-OH4-C13
4	C	1003	BES	N2-C1-C6-C7
4	D	1003	BES	N2-C1-C6-C7
4	F	1003	BES	N2-C1-C6-C7
4	G	1003	BES	N2-C1-C6-C7
4	I	1003	BES	N2-C1-C6-C7

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Mol	Chain	Res	Type	Atoms
7	C	18	1PE	OH5-C14-C24-OH4
7	J	3	1PE	OH7-C16-C26-OH6
7	B	61	1PE	C13-C23-OH3-C22
7	C	17	1PE	C13-C23-OH3-C22
7	F	33	1PE	C15-C25-OH5-C14
7	D	63	1PE	C13-C23-OH3-C22
7	L	1	1PE	C24-C14-OH5-C25
7	E	7	1PE	C15-C25-OH5-C14
7	J	2	1PE	C16-C26-OH6-C15
4	C	1003	BES	C2-C1-C6-C7
4	E	1003	BES	C2-C1-C6-C7
4	K	1003	BES	C2-C1-C6-C7
4	L	1003	BES	C2-C1-C6-C7
4	F	1003	BES	N2-C1-C2-C3
7	G	30	1PE	C15-C25-OH5-C14
4	D	1003	BES	N1-C4-C5-O1
4	B	1003	BES	C14-C13-C4-C5
7	D	67	1PE	OH5-C14-C24-OH4
7	B	61	1PE	C23-C13-OH4-C24
7	L	56	1PE	OH7-C16-C26-OH6
7	A	20	1PE	C23-C13-OH4-C24
7	H	65	1PE	OH5-C14-C24-OH4
7	A	19	1PE	C13-C23-OH3-C22
4	B	1003	BES	C13-C4-C5-O1
7	A	20	1PE	C25-C15-OH6-C26
4	C	1003	BES	C6-C1-C2-C3
4	E	1003	BES	C6-C1-C2-C3
4	F	1003	BES	C6-C1-C2-C3
4	G	1003	BES	C6-C1-C2-C3
4	H	1003	BES	C6-C1-C2-C3
4	I	1003	BES	C6-C1-C2-C3
4	L	1003	BES	C6-C1-C2-C3
4	F	1003	BES	C6-C1-C2-O2
7	L	1	1PE	C25-C15-OH6-C26
7	D	44	1PE	C16-C26-OH6-C15
7	G	12	1PE	C23-C13-OH4-C24
7	B	61	1PE	C12-C22-OH3-C23
7	D	9	1PE	C13-C23-OH3-C22
7	F	33	1PE	C25-C15-OH6-C26
7	K	42	1PE	C25-C15-OH6-C26
7	I	22	1PE	OH4-C13-C23-OH3
7	G	58	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
7	K	42	1PE	C14-C24-OH4-C13
4	B	1003	BES	C13-C4-C5-O4
4	K	1003	BES	C4-C13-C14-C15
7	D	63	1PE	C12-C22-OH3-C23
7	I	22	1PE	OH5-C14-C24-OH4
7	D	9	1PE	C12-C22-OH3-C23
7	F	33	1PE	C16-C26-OH6-C15
4	F	1003	BES	C13-C4-C5-O1
7	J	45	1PE	C14-C24-OH4-C13
7	I	66	1PE	C14-C24-OH4-C13
7	E	7	1PE	OH4-C13-C23-OH3
4	F	1003	BES	C13-C4-C5-O4
7	H	65	1PE	C23-C13-OH4-C24
7	B	61	1PE	C24-C14-OH5-C25
7	J	3	1PE	C16-C26-OH6-C15
7	K	50	1PE	C24-C14-OH5-C25
7	L	612	1PE	C23-C13-OH4-C24
7	H	64	1PE	C12-C22-OH3-C23
7	H	64	1PE	OH5-C14-C24-OH4
7	L	612	1PE	C15-C25-OH5-C14
7	J	2	1PE	C15-C25-OH5-C14
7	B	62	1PE	C14-C24-OH4-C13
4	J	1003	BES	N1-C4-C5-O4
7	B	61	1PE	OH4-C13-C23-OH3
7	K	5	1PE	C13-C23-OH3-C22
7	B	60	1PE	C24-C14-OH5-C25
7	K	4	1PE	C12-C22-OH3-C23
7	G	47	1PE	OH6-C15-C25-OH5
7	I	21	1PE	OH4-C13-C23-OH3
7	I	22	1PE	C12-C22-OH3-C23
7	D	67	1PE	C24-C14-OH5-C25
4	D	1003	BES	C2-C1-C6-C7
4	G	1003	BES	C2-C1-C6-C7
7	D	9	1PE	C24-C14-OH5-C25
7	J	2	1PE	C25-C15-OH6-C26
4	G	1003	BES	N2-C1-C2-C3
4	J	1003	BES	C4-C13-C14-C16
7	G	47	1PE	C15-C25-OH5-C14
4	L	1003	BES	N1-C4-C5-O4
7	G	12	1PE	C14-C24-OH4-C13
7	C	18	1PE	C23-C13-OH4-C24
4	I	1003	BES	C4-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
4	J	1003	BES	N1-C4-C5-O1
7	F	32	1PE	OH5-C14-C24-OH4
7	G	30	1PE	OH5-C14-C24-OH4
7	D	44	1PE	C23-C13-OH4-C24
4	D	1003	BES	N1-C4-C5-O4
7	J	2	1PE	OH6-C15-C25-OH5
7	J	45	1PE	C25-C15-OH6-C26
4	G	1003	BES	C14-C13-C4-C5
4	C	1003	BES	C6-C1-C2-O2
4	K	1003	BES	C6-C1-C2-O2
7	F	33	1PE	OH6-C15-C25-OH5
7	J	2	1PE	OH5-C14-C24-OH4
7	G	58	1PE	C12-C22-OH3-C23

There are no ring outliers.

35 monomers are involved in 96 short contacts:

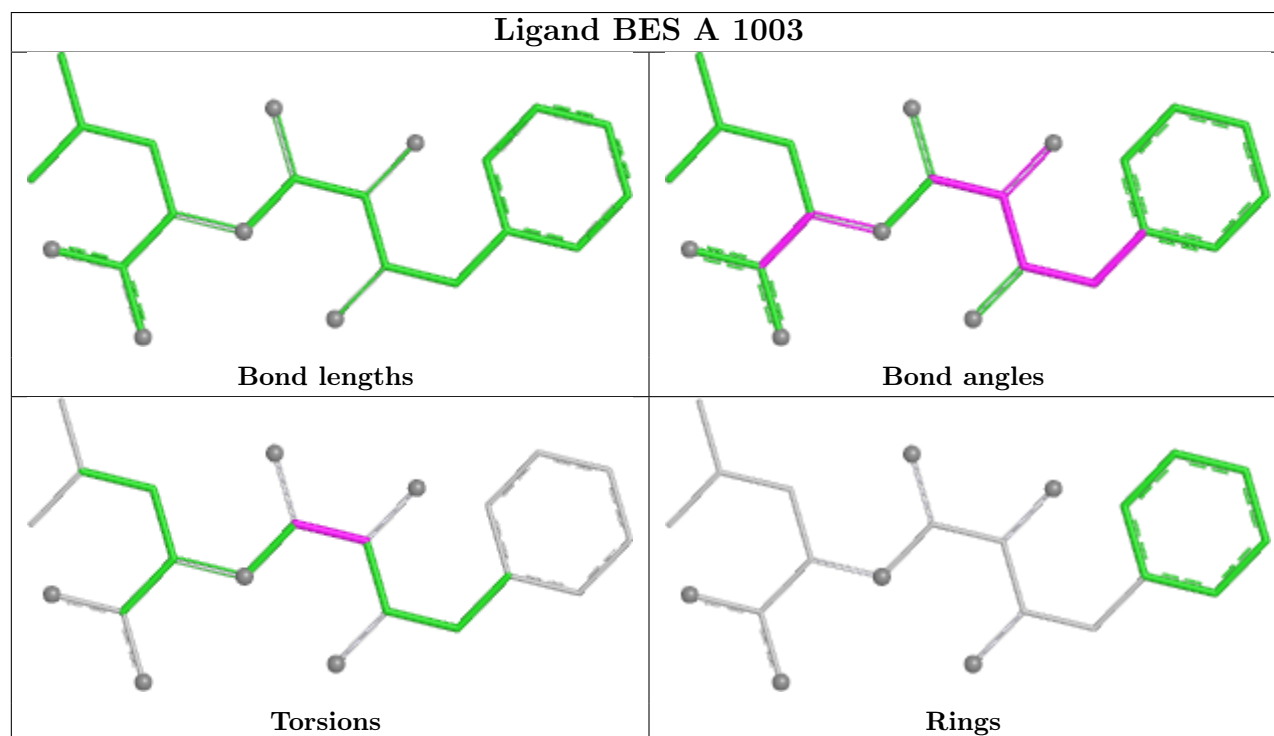
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	43	1PE	3	0
4	A	1003	BES	1	0
7	C	17	1PE	1	0
4	B	1003	BES	3	0
6	J	20	SO4	1	0
7	B	61	1PE	7	0
7	L	1	1PE	3	0
7	L	612	1PE	8	0
4	I	1003	BES	2	0
4	H	1003	BES	3	0
7	D	67	1PE	1	0
4	C	1003	BES	4	0
7	D	63	1PE	2	0
4	D	1003	BES	3	0
6	D	7	SO4	1	0
4	E	1003	BES	4	0
7	H	64	1PE	1	0
7	H	65	1PE	3	0
4	K	1003	BES	5	0
7	A	19	1PE	1	0
7	J	3	1PE	6	0
7	G	58	1PE	4	0
4	J	1003	BES	2	0
7	C	18	1PE	4	0

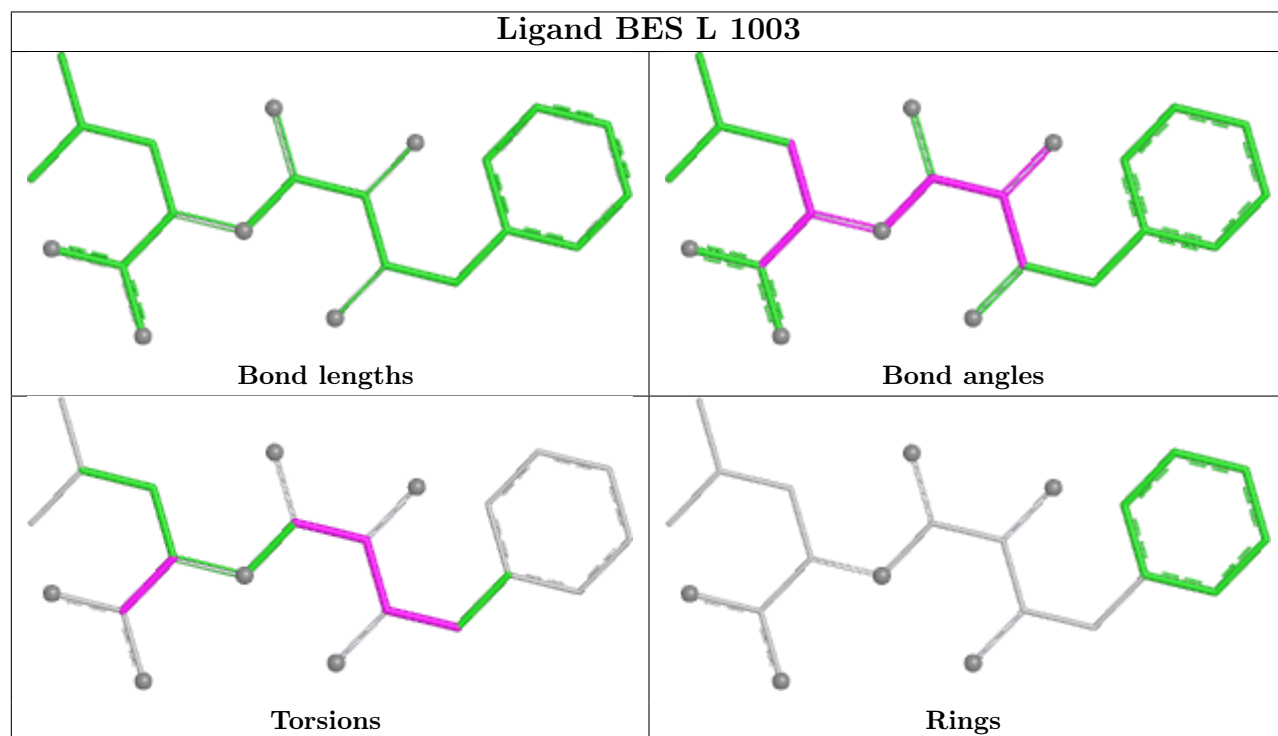
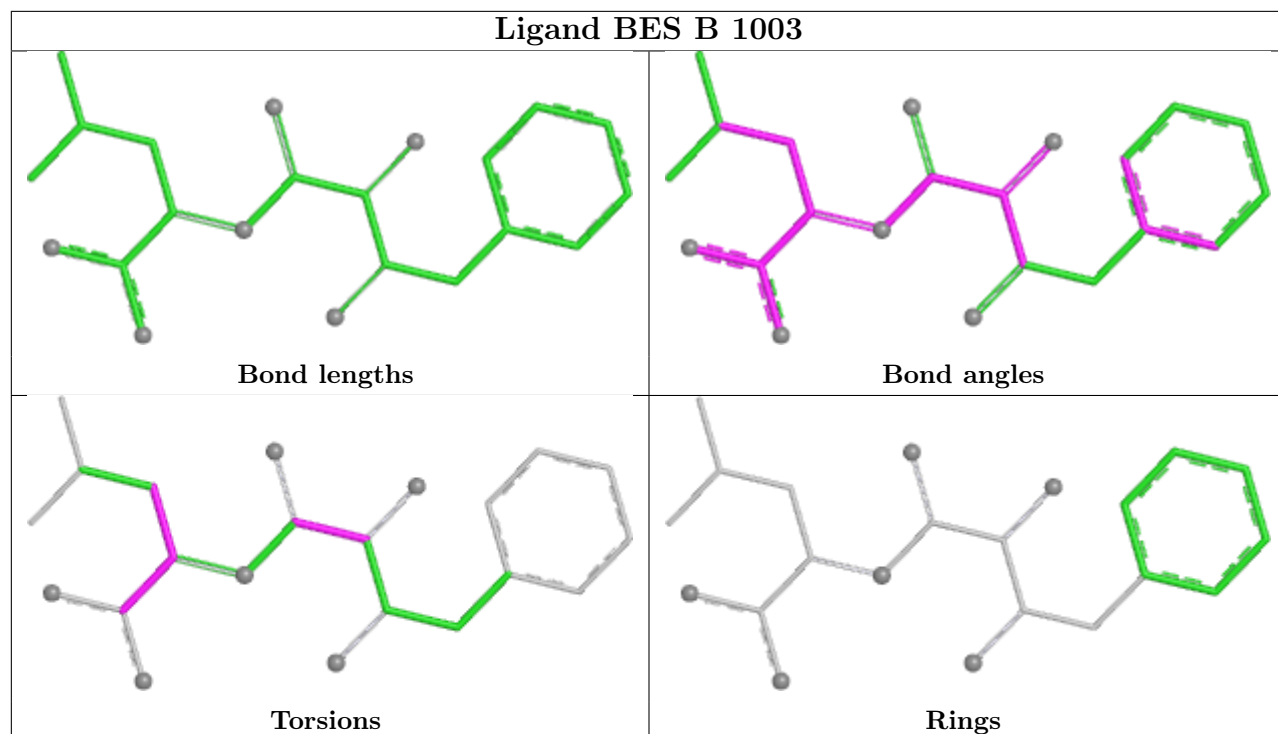
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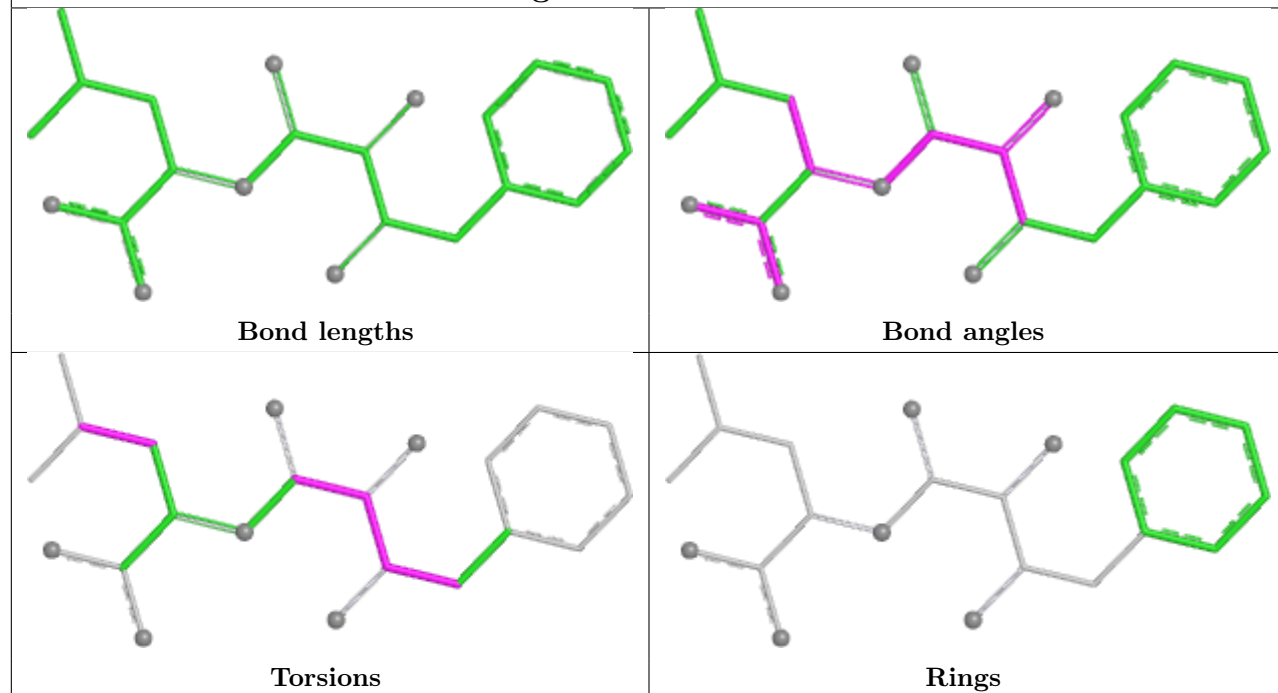
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	9	1PE	1	0
7	D	44	1PE	2	0
7	I	21	1PE	3	0
7	I	22	1PE	5	0
7	J	2	1PE	2	0
6	L	25	SO4	2	0
7	A	20	1PE	1	0
7	F	32	1PE	3	0
7	J	45	1PE	2	0
7	K	42	1PE	1	0
7	G	12	1PE	1	0

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

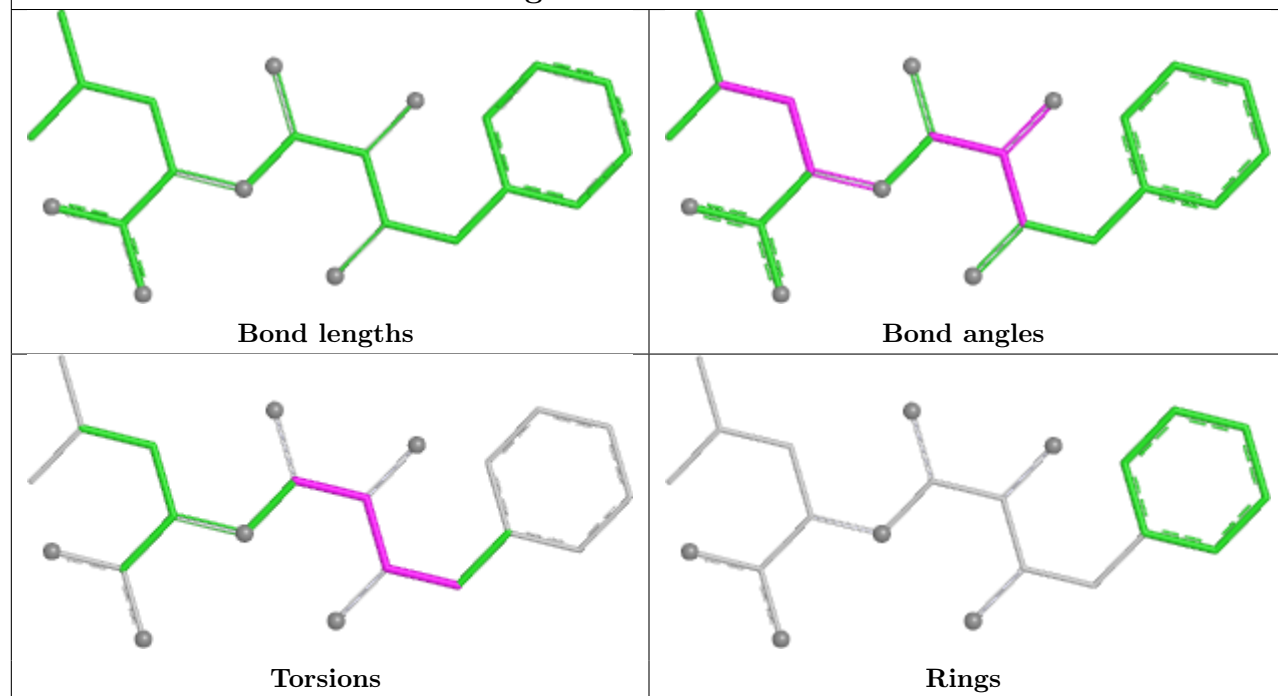




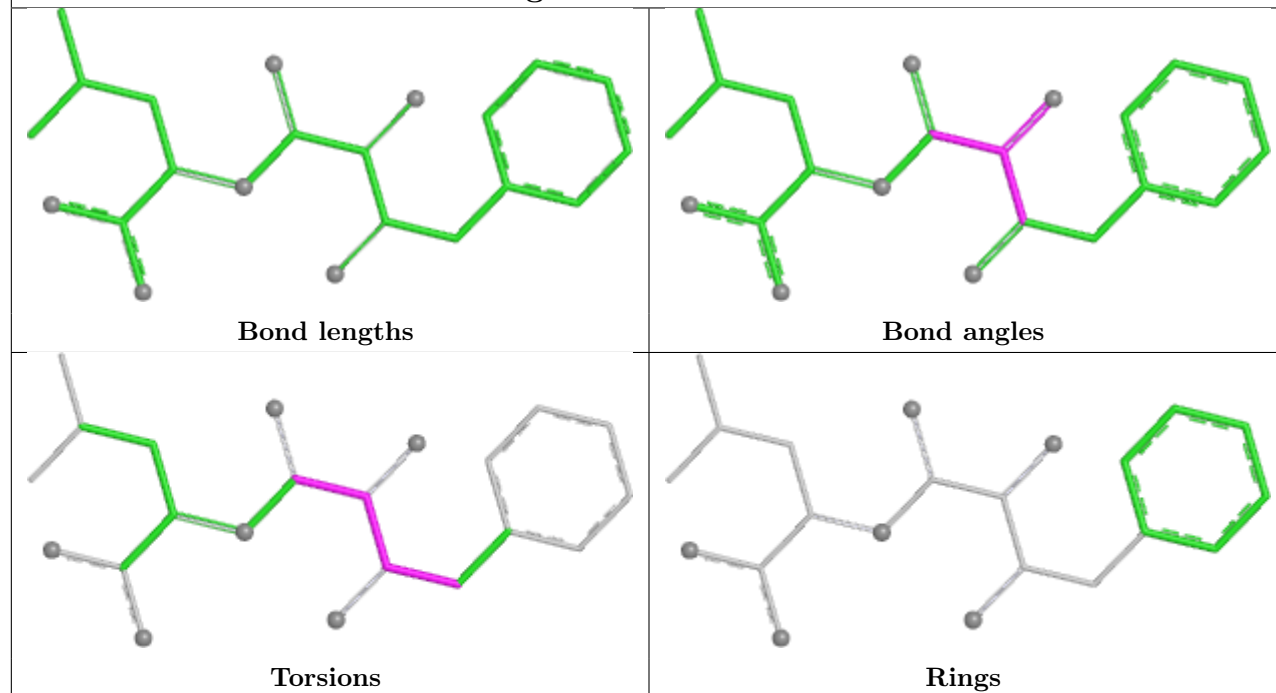
Ligand BES I 1003



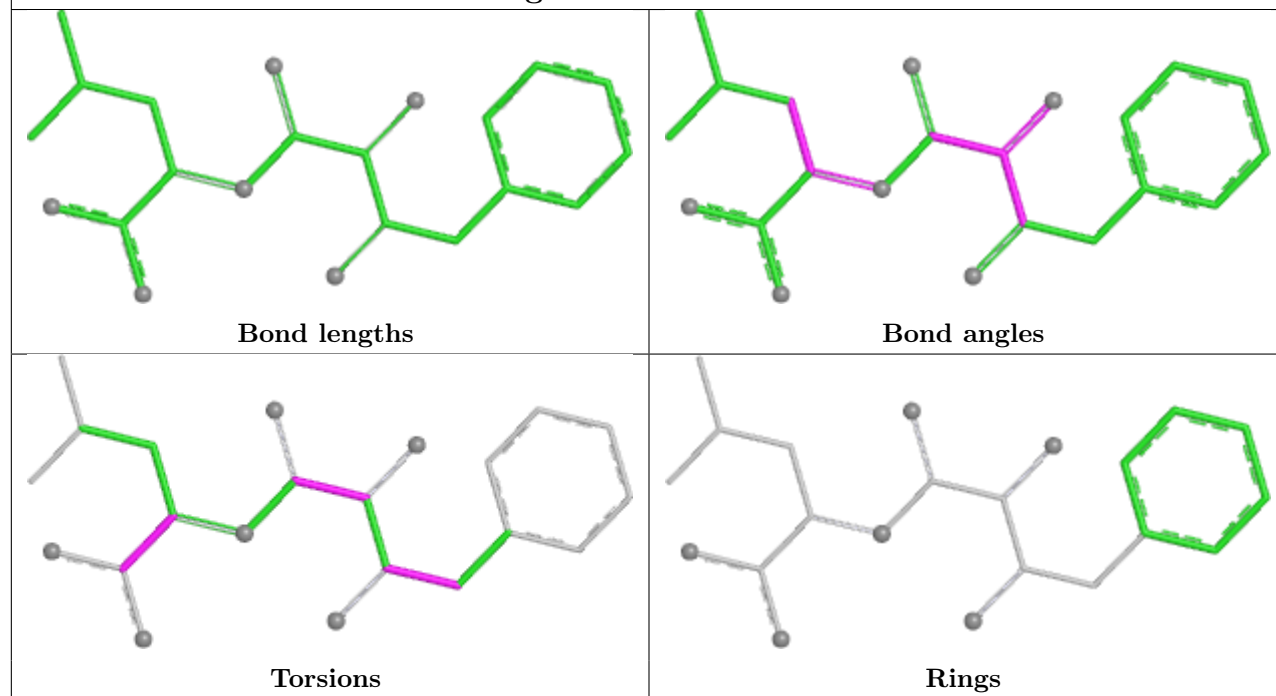
Ligand BES H 1003



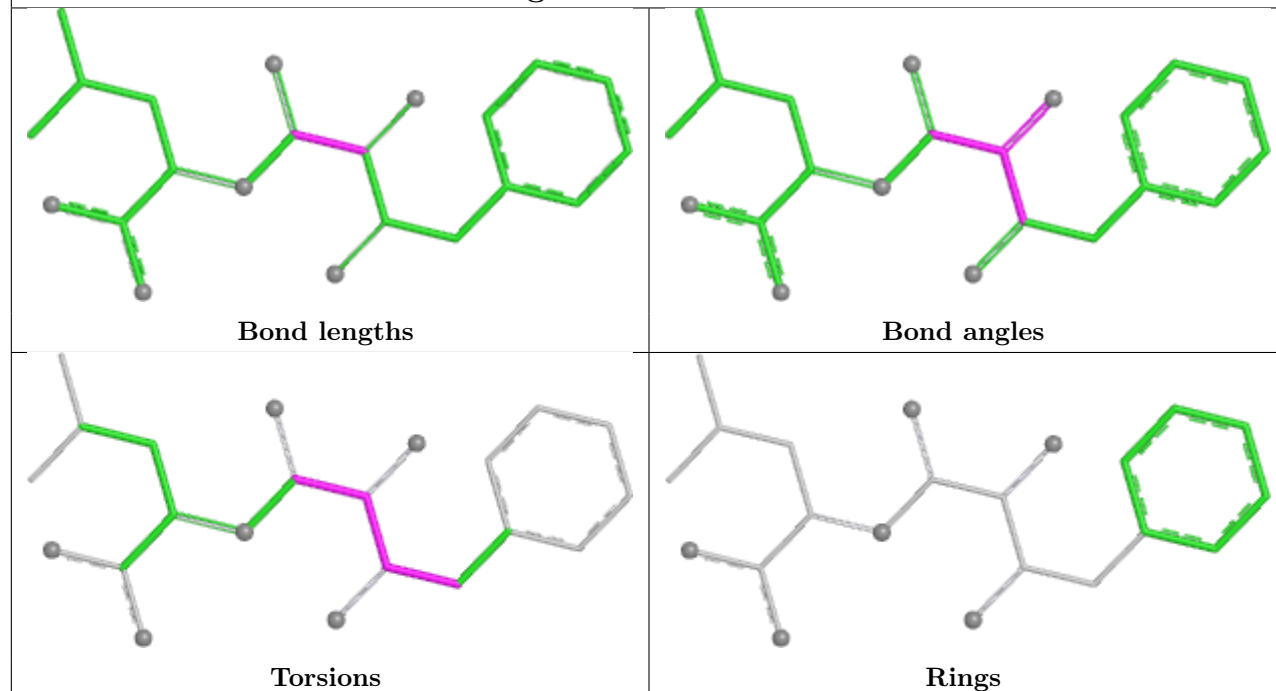
Ligand BES C 1003



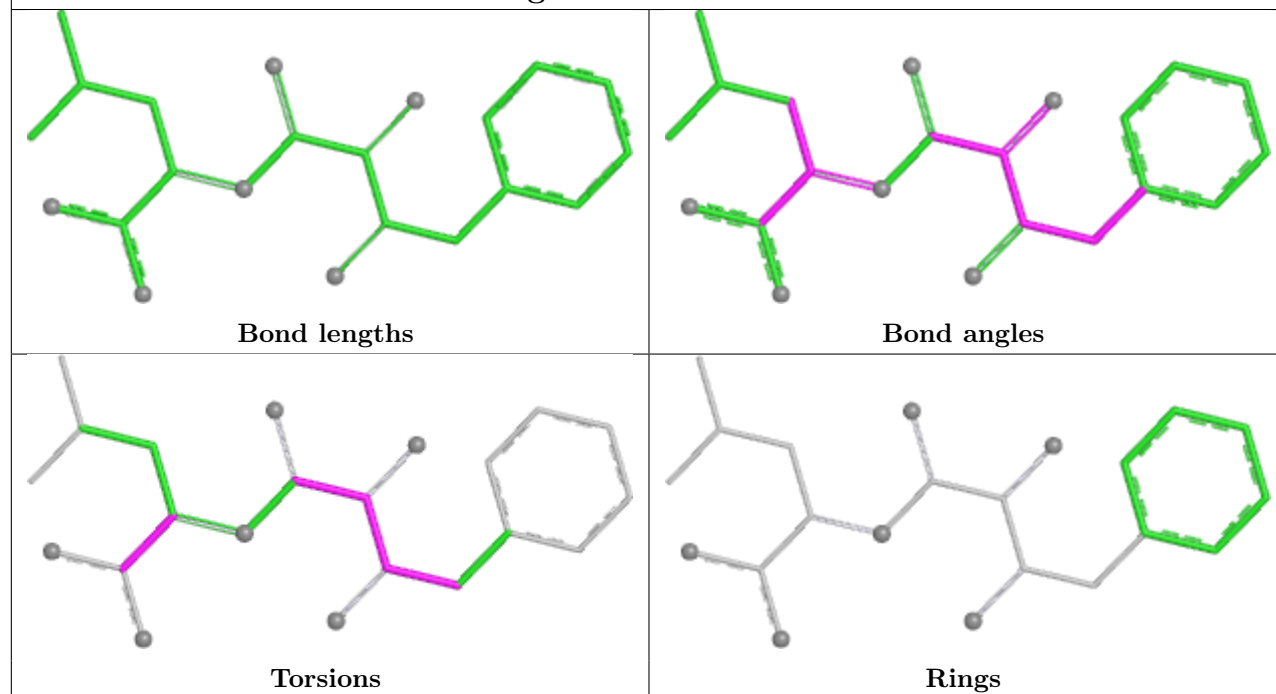
Ligand BES D 1003



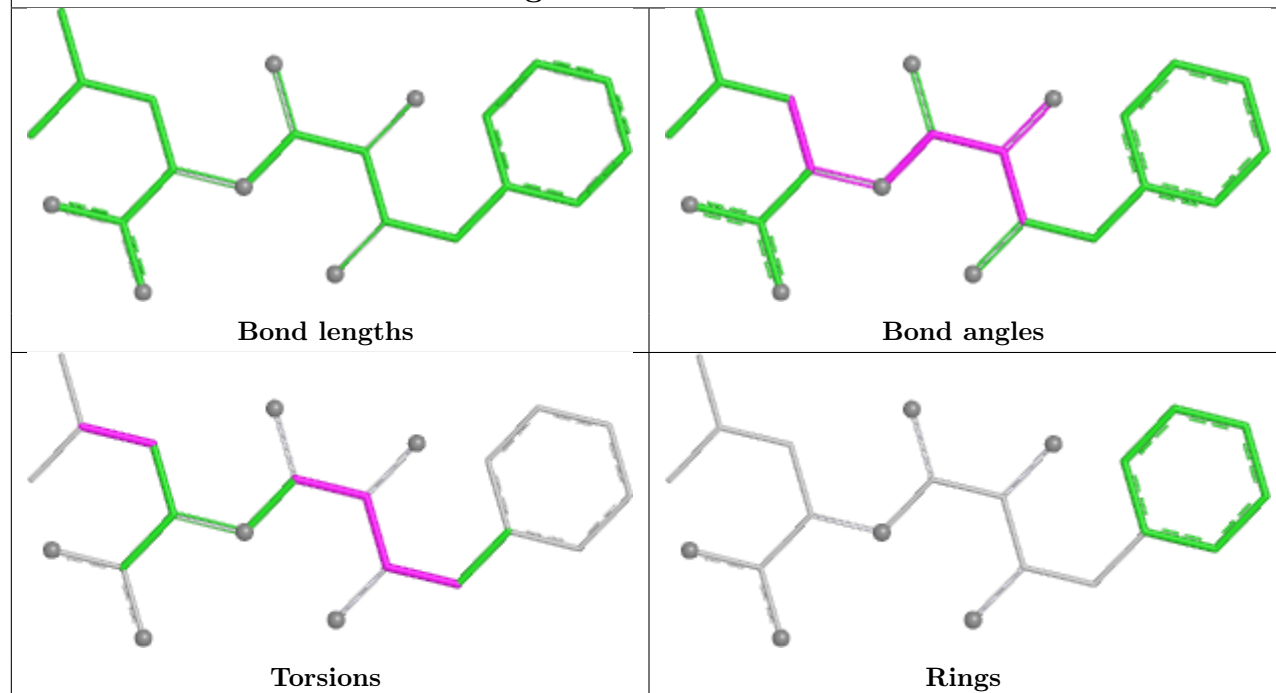
Ligand BES E 1003



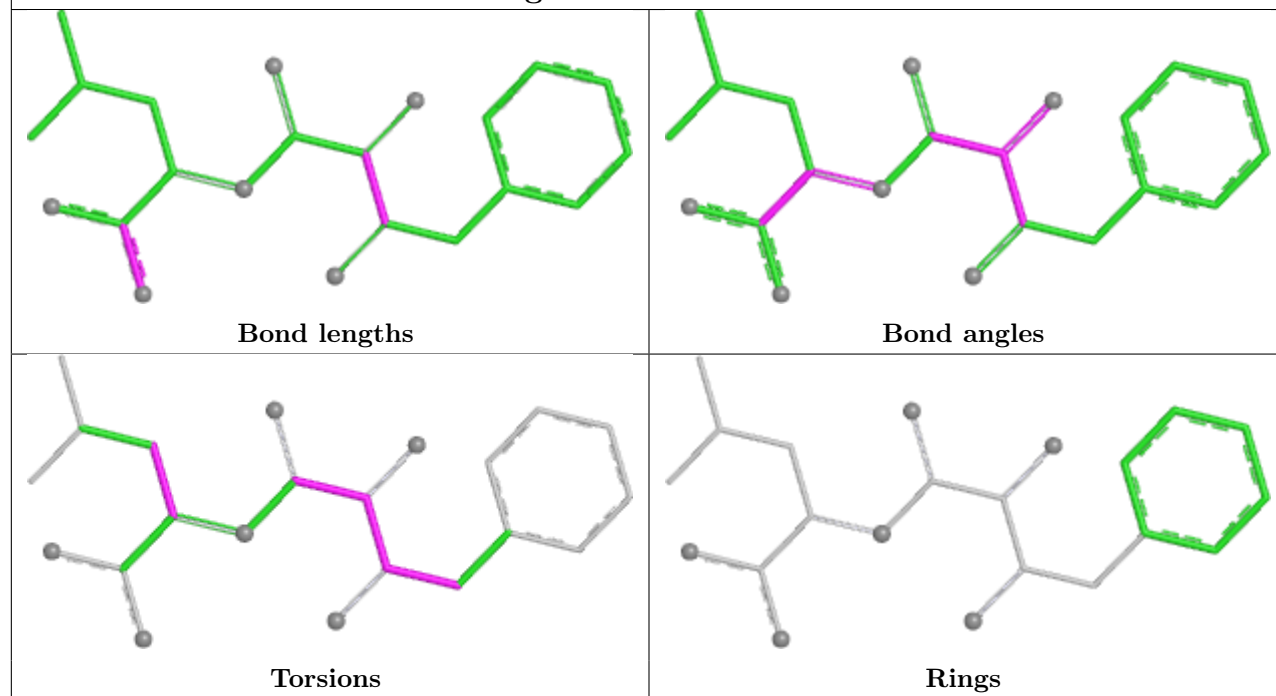
Ligand BES F 1003

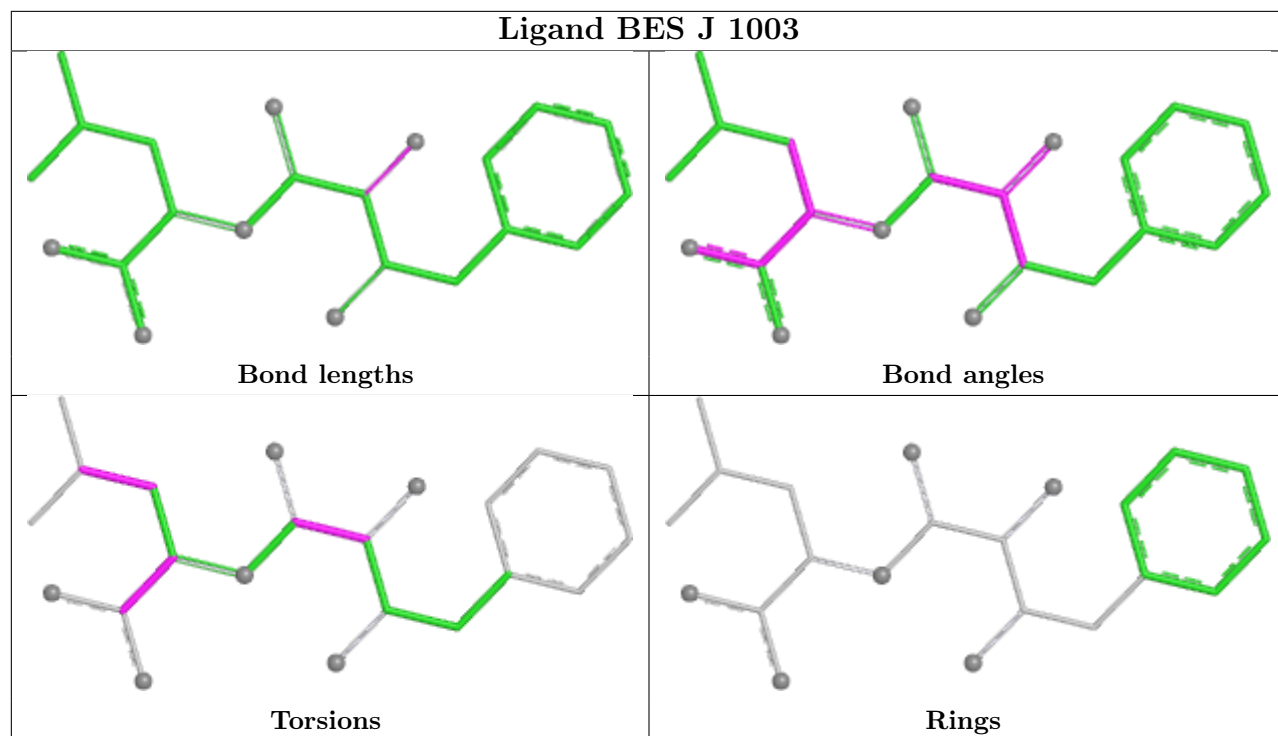


Ligand BES K 1003



Ligand BES G 1003





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	518/528 (98%)	-0.54	3 (0%) 85 85	5, 14, 29, 39	1 (0%)
1	B	518/528 (98%)	-0.30	10 (1%) 66 66	7, 16, 42, 51	0
1	C	518/528 (98%)	-0.50	4 (0%) 82 82	7, 15, 31, 42	1 (0%)
1	D	516/528 (97%)	-0.51	6 (1%) 76 76	8, 15, 29, 39	0
1	E	510/528 (96%)	-0.57	6 (1%) 76 76	8, 14, 25, 37	0
1	F	510/528 (96%)	-0.36	6 (1%) 76 76	8, 17, 37, 46	0
1	G	516/528 (97%)	-0.52	4 (0%) 82 82	7, 14, 28, 40	0
1	H	509/528 (96%)	-0.32	9 (1%) 67 67	7, 16, 42, 52	1 (0%)
1	I	518/528 (98%)	-0.49	3 (0%) 85 85	7, 14, 31, 41	1 (0%)
1	J	513/528 (97%)	-0.51	7 (1%) 73 73	8, 15, 29, 40	1 (0%)
1	K	509/528 (96%)	-0.56	4 (0%) 82 82	8, 14, 25, 38	1 (0%)
1	L	513/528 (97%)	-0.37	9 (1%) 67 67	8, 16, 40, 46	1 (0%)
All	All	6168/6336 (97%)	-0.46	71 (1%) 76 76	5, 15, 34, 52	7 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	ASN	4.8
1	E	216	ASP	4.8
1	D	136	GLY	4.7
1	J	136	GLY	4.4
1	B	136	GLY	4.4
1	B	256	ASP	4.1
1	L	605	LEU	4.1
1	B	259	VAL	3.9
1	F	603	ASP	3.9
1	B	121	CYS	3.8
1	B	258	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	261	MET	3.8
1	E	136	GLY	3.3
1	L	217	ASN	3.3
1	F	121	CYS	3.1
1	D	603	ASP	3.0
1	B	260	ASN	3.0
1	K	550	SER	3.0
1	J	603	ASP	2.9
1	H	124	GLU	2.8
1	A	85	ALA	2.8
1	B	183	ASN	2.7
1	K	549	SER	2.7
1	C	183	ASN	2.7
1	I	259	VAL	2.7
1	F	550	SER	2.6
1	F	216	ASP	2.6
1	H	138	GLU	2.6
1	G	549	SER	2.6
1	I	508	GLU	2.6
1	K	363	GLY	2.6
1	C	260	ASN	2.5
1	L	136	GLY	2.5
1	H	181	ASN	2.5
1	C	549	SER	2.4
1	J	149	ASN	2.4
1	J	549	SER	2.4
1	H	196	ALA	2.4
1	E	363	GLY	2.4
1	F	549	SER	2.4
1	J	364	ASP	2.3
1	H	137	LYS	2.3
1	H	123	VAL	2.3
1	B	181	ASN	2.3
1	D	258	ASN	2.3
1	D	197	ASP	2.3
1	L	123	VAL	2.3
1	J	260	ASN	2.3
1	L	604	ALA	2.3
1	L	197	ASP	2.3
1	D	549	SER	2.3
1	E	549	SER	2.3
1	A	259	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	138	GLU	2.2
1	G	205	ARG	2.2
1	H	549	SER	2.2
1	H	135	PRO	2.2
1	L	231	ASP	2.2
1	I	395	LEU	2.2
1	E	550	SER	2.2
1	E	137	LYS	2.2
1	B	262	GLU	2.1
1	C	259	VAL	2.1
1	F	231	ASP	2.1
1	L	161	ASN	2.1
1	J	363	GLY	2.1
1	L	550	SER	2.1
1	H	193	GLY	2.1
1	G	137	LYS	2.1
1	A	137	LYS	2.0
1	B	170	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
7	1PE	B	62	10/16	0.28	0.44	91,95,97,98	0
7	1PE	K	50	6/16	0.66	0.20	37,40,45,46	0
7	1PE	D	44	11/16	0.70	0.19	36,38,43,44	0
7	1PE	D	63	10/16	0.75	0.17	22,30,33,36	0
7	1PE	B	61	10/16	0.75	0.16	38,40,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	1PE	I	66	7/16	0.78	0.16	30,32,34,34	0
7	1PE	H	65	10/16	0.78	0.15	32,40,41,41	0
7	1PE	A	20	12/16	0.79	0.19	40,43,46,47	0
7	1PE	J	45	10/16	0.81	0.18	44,48,51,51	0
5	MG	D	1004	1/1	0.82	0.35	28,28,28,28	0
7	1PE	C	17	13/16	0.82	0.13	22,36,38,38	0
7	1PE	D	67	7/16	0.82	0.17	29,33,41,41	0
7	1PE	G	58	15/16	0.82	0.17	37,42,52,53	0
7	1PE	K	42	11/16	0.83	0.14	33,42,47,47	0
7	1PE	L	56	11/16	0.83	0.14	43,45,48,50	0
7	1PE	K	4	12/16	0.84	0.12	31,32,34,35	0
7	1PE	E	43	8/16	0.84	0.13	33,35,35,39	0
7	1PE	E	7	12/16	0.85	0.13	32,34,36,36	0
6	SO4	A	24	5/5	0.85	0.13	52,55,56,57	0
7	1PE	I	21	15/16	0.85	0.13	26,33,46,47	0
5	MG	L	1004	1/1	0.86	0.28	33,33,33,33	0
5	MG	A	1004	1/1	0.86	0.34	24,24,24,24	0
7	1PE	J	3	10/16	0.87	0.13	36,37,40,41	0
7	1PE	G	12	9/16	0.87	0.12	27,28,32,32	0
4	BES	B	1003	22/22	0.88	0.12	17,30,39,45	0
7	1PE	L	612	12/16	0.88	0.11	22,36,39,40	0
5	MG	J	1004	1/1	0.88	0.48	22,22,22,22	0
5	MG	H	1004	1/1	0.89	0.34	40,40,40,40	0
7	1PE	F	32	10/16	0.89	0.11	37,39,39,39	0
7	1PE	D	9	10/16	0.89	0.12	21,25,35,37	0
6	SO4	L	25	5/5	0.89	0.13	56,59,59,60	0
4	BES	F	1003	22/22	0.89	0.12	13,27,36,40	0
4	BES	G	1003	22/22	0.89	0.12	13,28,34,39	0
6	SO4	A	2	5/5	0.89	0.13	45,46,50,51	0
4	BES	H	1003	22/22	0.90	0.11	15,25,34,37	0
4	BES	I	1003	22/22	0.90	0.10	11,27,30,32	0
7	1PE	J	2	11/16	0.90	0.10	23,26,37,42	0
4	BES	K	1003	22/22	0.90	0.11	16,26,32,39	0
4	BES	A	1003	22/22	0.90	0.11	20,29,35,40	0
5	MG	C	1004	1/1	0.90	0.26	27,27,27,27	0
7	1PE	G	30	7/16	0.90	0.11	35,38,42,43	0
7	1PE	G	48	6/16	0.90	0.12	25,31,33,36	0
4	BES	C	1003	22/22	0.90	0.11	22,27,36,36	0
7	1PE	A	19	9/16	0.90	0.10	20,24,28,31	0
4	BES	E	1003	22/22	0.91	0.10	19,29,35,39	0
7	1PE	G	47	6/16	0.91	0.10	30,31,32,35	0
7	1PE	I	22	11/16	0.91	0.10	18,23,36,38	0

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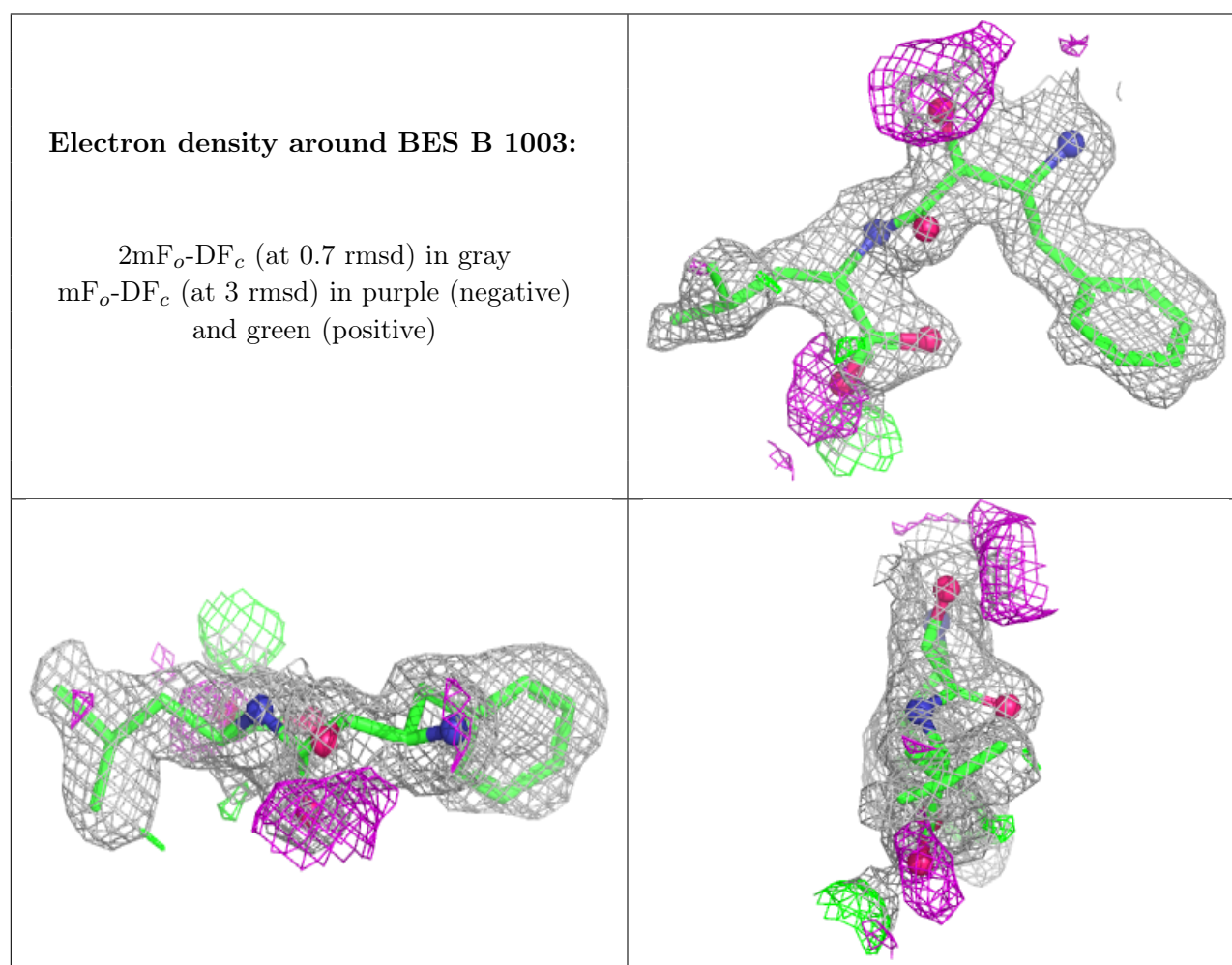
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	1PE	F	33	10/16	0.91	0.10	21,29,31,34	0
4	BES	D	1003	22/22	0.91	0.10	13,28,32,33	0
7	1PE	H	64	10/16	0.91	0.10	19,26,34,35	0
5	MG	F	1004	1/1	0.92	0.23	37,37,37,37	0
7	1PE	B	60	10/16	0.92	0.10	23,28,33,35	0
5	MG	B	1004	1/1	0.92	0.40	16,16,16,16	0
6	SO4	E	22	5/5	0.92	0.20	44,45,47,48	0
7	1PE	K	5	12/16	0.92	0.10	25,27,38,38	0
6	SO4	J	20	5/5	0.92	0.11	60,62,62,62	0
7	1PE	C	18	9/16	0.92	0.09	20,21,26,29	0
4	BES	L	1003	22/22	0.92	0.09	12,26,33,34	0
4	BES	J	1003	22/22	0.92	0.11	11,28,37,40	0
6	SO4	K	19	5/5	0.93	0.10	52,53,54,54	0
5	MG	E	1004	1/1	0.93	0.30	26,26,26,26	0
6	SO4	D	5	5/5	0.93	0.11	53,53,56,56	0
6	SO4	A	1	5/5	0.93	0.15	50,51,53,53	0
6	SO4	G	23	5/5	0.93	0.17	46,49,50,50	0
2	CO3	A	1002	4/4	0.93	0.10	13,14,14,17	0
5	MG	I	1004	1/1	0.94	0.37	15,15,15,15	0
7	1PE	E	8	12/16	0.94	0.09	20,23,35,35	0
5	MG	G	1004	1/1	0.94	0.22	23,23,23,23	0
7	1PE	L	1	10/16	0.94	0.08	25,27,32,38	0
7	1PE	F	31	10/16	0.94	0.08	26,27,29,29	0
6	SO4	F	21	5/5	0.94	0.10	56,59,59,59	0
2	CO3	B	1002	4/4	0.95	0.06	11,12,12,16	0
2	CO3	J	1002	4/4	0.95	0.06	12,14,15,16	0
5	MG	K	1004	1/1	0.95	0.26	23,23,23,23	0
2	CO3	E	1002	4/4	0.96	0.07	16,17,18,19	0
2	CO3	G	1002	4/4	0.97	0.05	11,12,12,15	0
2	CO3	H	1002	4/4	0.97	0.04	10,10,11,14	0
2	CO3	I	1002	4/4	0.97	0.05	14,15,15,18	0
2	CO3	C	1002	4/4	0.97	0.05	12,13,13,16	0
2	CO3	K	1002	4/4	0.97	0.05	13,14,14,18	0
2	CO3	L	1002	4/4	0.97	0.05	14,15,15,16	0
2	CO3	F	1002	4/4	0.97	0.05	12,12,13,15	0
3	ZN	F	1001	1/1	0.98	0.09	40,40,40,40	0
2	CO3	D	1002	4/4	0.98	0.05	11,12,12,16	0
3	ZN	I	1001	1/1	0.99	0.10	36,36,36,36	0
3	ZN	J	1001	1/1	0.99	0.07	38,38,38,38	0
3	ZN	K	1001	1/1	0.99	0.11	37,37,37,37	0
3	ZN	L	1001	1/1	0.99	0.10	37,37,37,37	0
6	SO4	B	3	5/5	0.99	0.03	8,9,10,10	0

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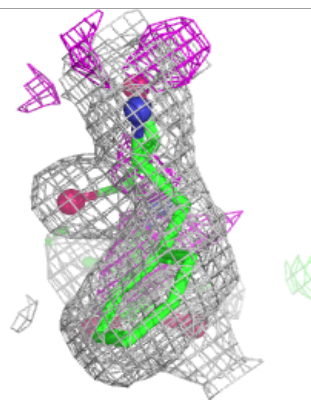
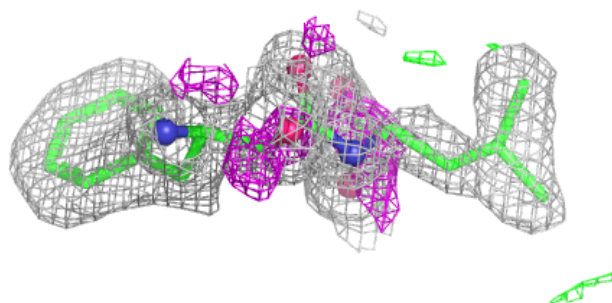
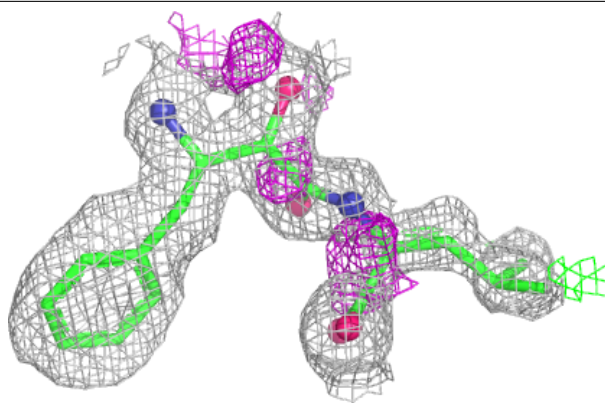
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	1001	1/1	0.99	0.10	37,37,37,37	0
6	SO4	D	7	5/5	0.99	0.03	8,11,11,12	0
3	ZN	C	1001	1/1	0.99	0.11	39,39,39,39	0
3	ZN	E	1001	1/1	0.99	0.07	38,38,38,38	0
6	SO4	G	17	5/5	0.99	0.03	10,11,13,14	0
3	ZN	A	1001	1/1	0.99	0.09	39,39,39,39	0
6	SO4	J	18	5/5	0.99	0.03	11,11,12,14	0
3	ZN	G	1001	1/1	0.99	0.09	38,38,38,38	0
3	ZN	H	1001	1/1	1.00	0.11	34,34,34,34	0
3	ZN	D	1001	1/1	1.00	0.07	34,34,34,34	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.

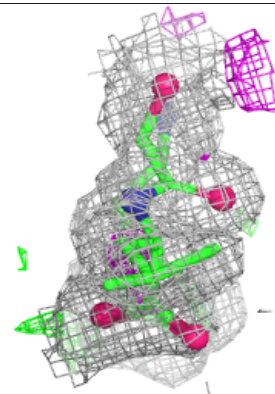
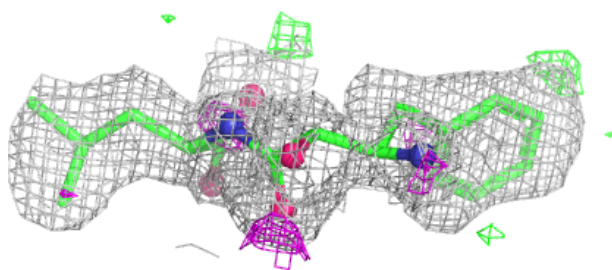
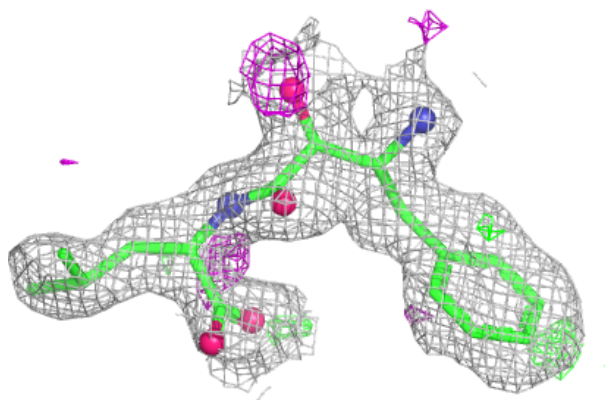


Electron density around BES F 1003:

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

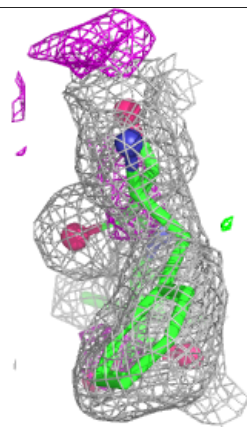
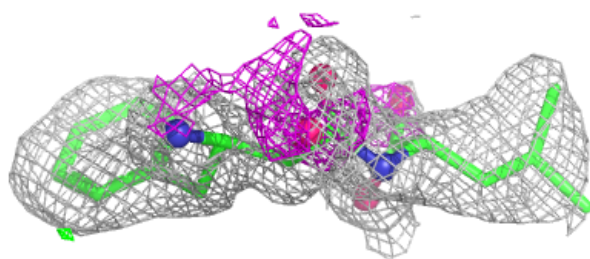
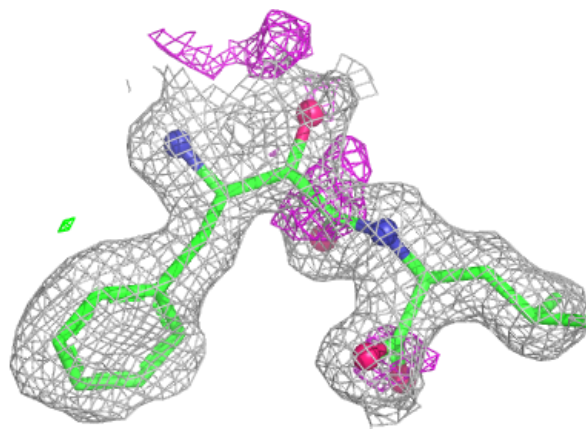
**Electron density around BES G 1003:**

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



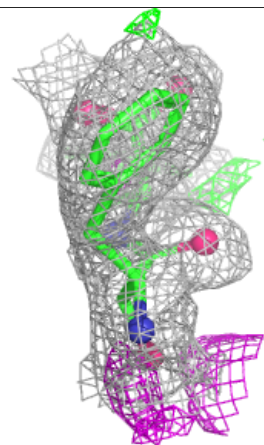
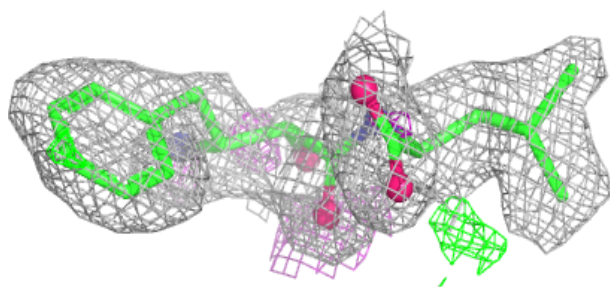
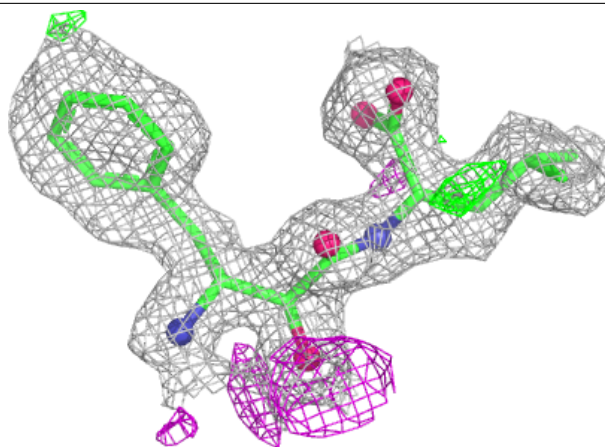
Electron density around BES H 1003:

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



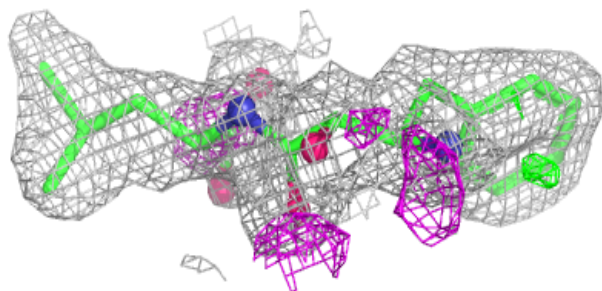
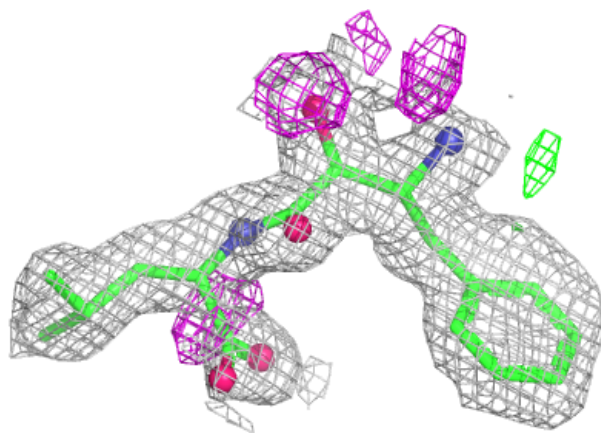
Electron density around BES I 1003:

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



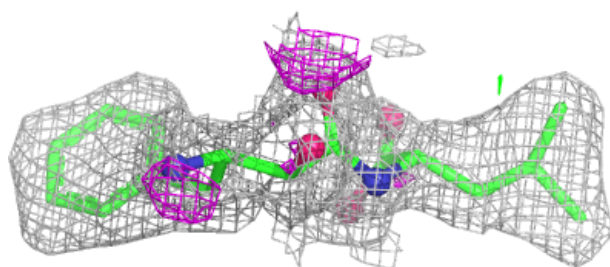
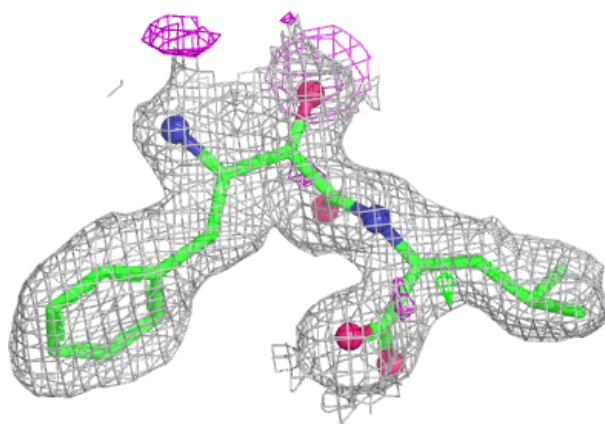
Electron density around BES K 1003:

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



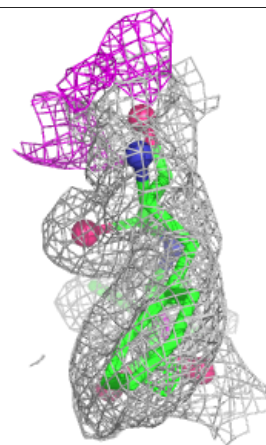
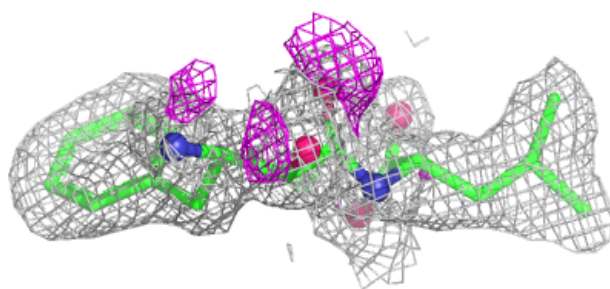
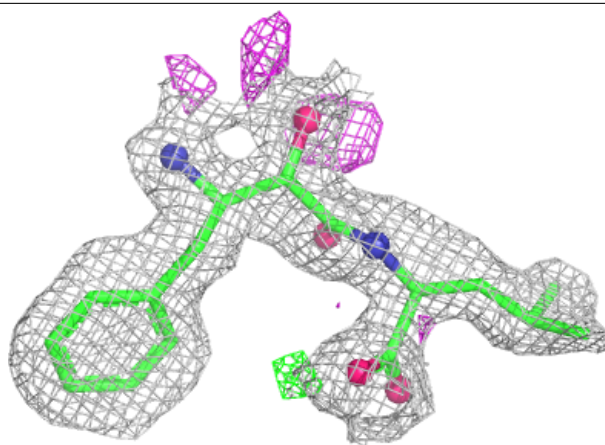
Electron density around BES A 1003:

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



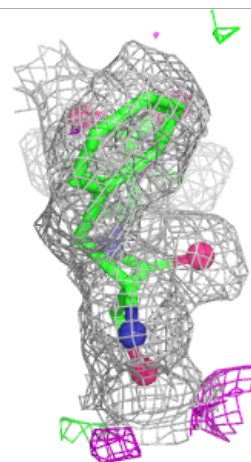
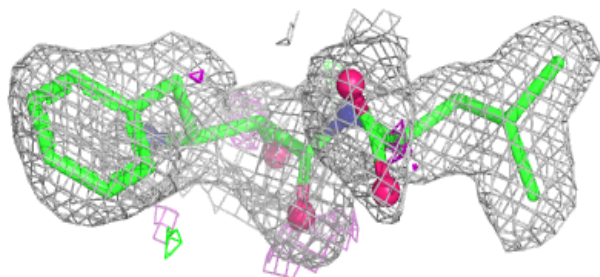
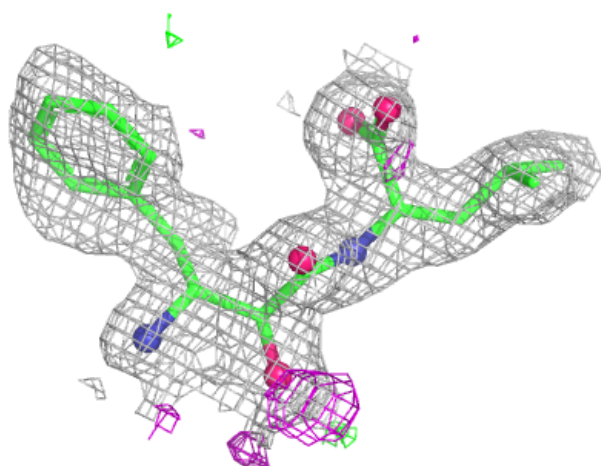
Electron density around BES C 1003:

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



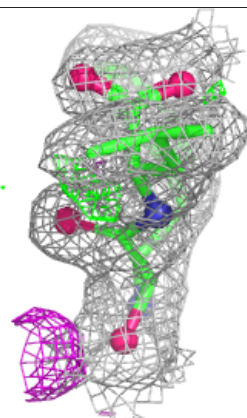
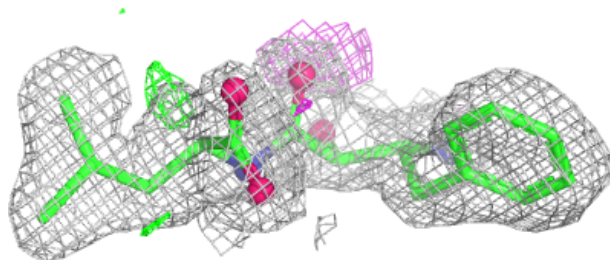
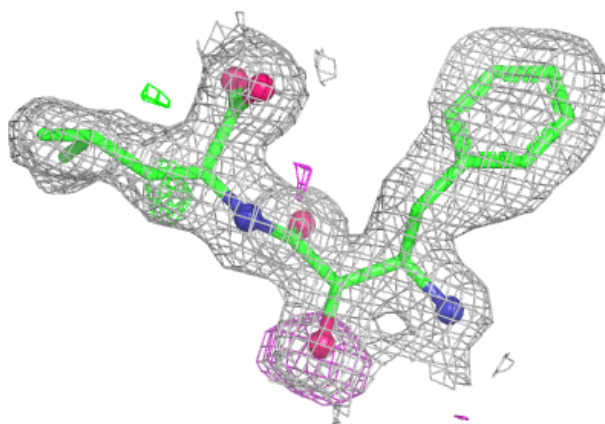
Electron density around BES E 1003:

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

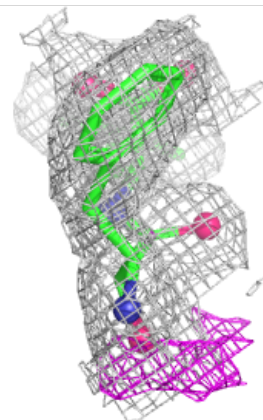
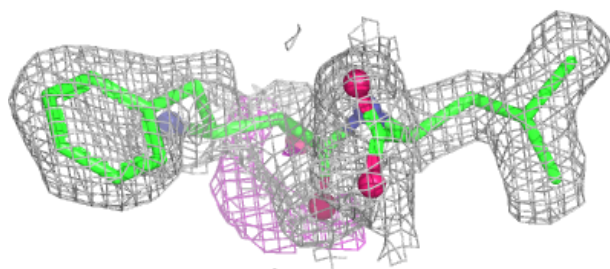
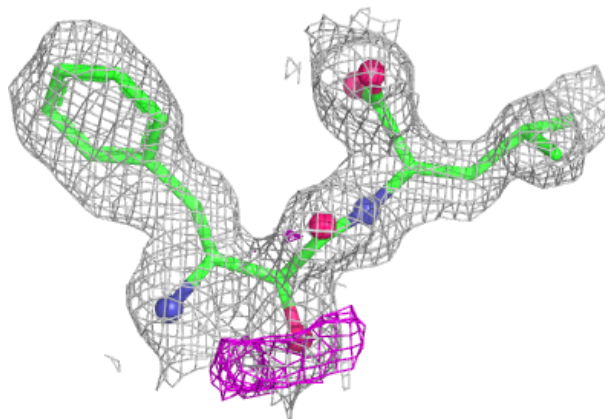


Electron density around BES D 1003:

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

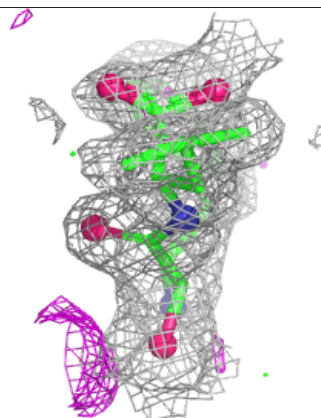
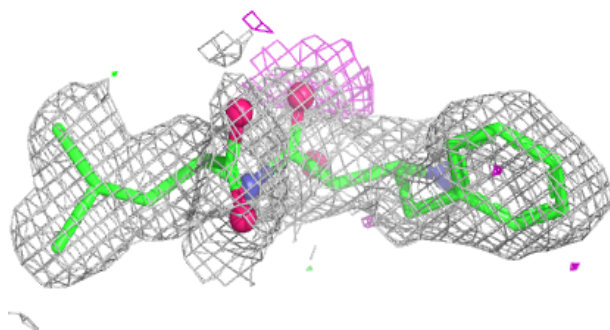
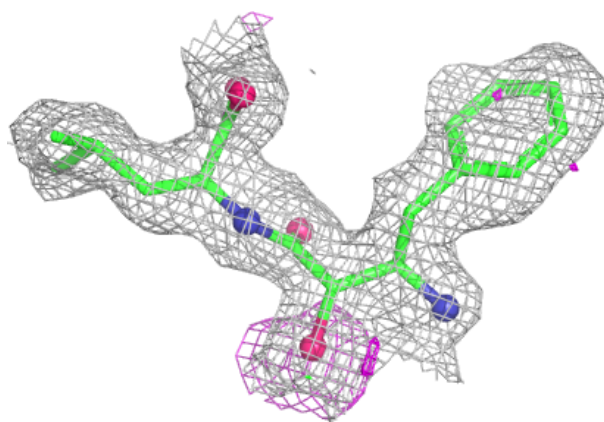
**Electron density around BES L 1003:**

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



Electron density around BES J 1003:

$2mF_o-DF_c$ (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.