



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2021 – 03:21 PM EDT

PDB ID : 3KR5  
Title : Structure of a protease 4  
Authors : McGowan, S.; Whisstock, J.C.  
Deposited on : 2009-11-17  
Resolution : 2.56 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.2  
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) : 2.23.2

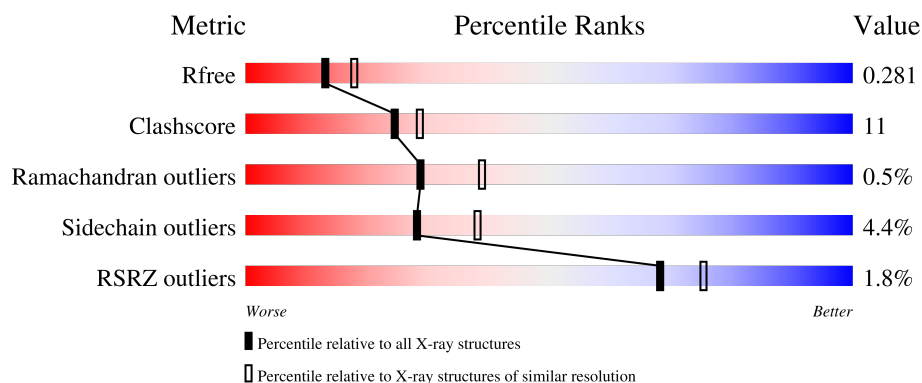
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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.



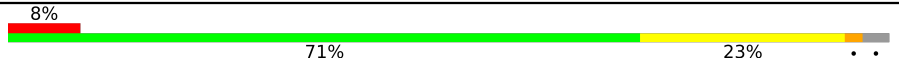
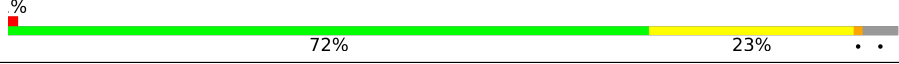
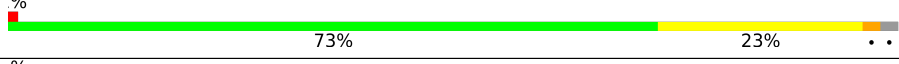

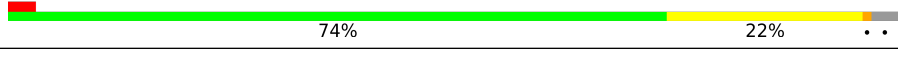
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	528	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	B	528	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	C	528	<div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	D	528	<div> <div>%</div> <div>74%</div> <div>20%</div> <div>..</div> </div>
1	E	528	<div> <div>%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>

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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
2	CO3	D	1002	-	-	X	-
2	CO3	K	1002	-	-	X	-
5	SO4	E	7	-	-	X	-
6	1PE	B	62	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50444 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	0	0	0
			3980	2556	639	765	20			
1	B	518	Total	C	N	O	S	0	0	0
			3929	2527	635	747	20			
1	C	518	Total	C	N	O	S	0	0	0
			3953	2544	637	752	20			
1	D	513	Total	C	N	O	S	0	0	0
			3928	2531	633	744	20			
1	E	510	Total	C	N	O	S	0	0	0
			3897	2509	626	743	19			
1	F	510	Total	C	N	O	S	0	0	0
			3873	2492	624	738	19			
1	G	516	Total	C	N	O	S	0	0	0
			3989	2560	650	760	19			
1	H	509	Total	C	N	O	S	0	0	0
			3938	2531	640	748	19			
1	I	518	Total	C	N	O	S	0	0	0
			4006	2569	651	766	20			
1	J	513	Total	C	N	O	S	0	0	0
			3954	2539	639	756	20			
1	K	509	Total	C	N	O	S	0	0	0
			3930	2525	637	749	19			
1	L	513	Total	C	N	O	S	0	0	0
			3932	2526	634	753	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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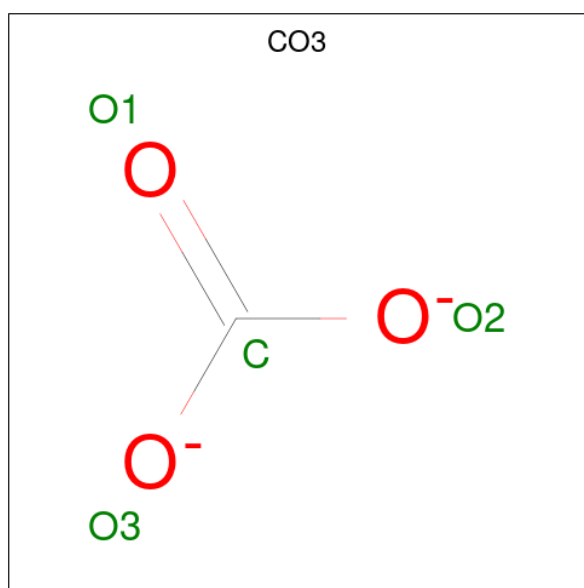
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression 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 (three-letter code: CO3) (formula: CO<sub>3</sub>).



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 (three-letter code: ZN) (formula: Zn).

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

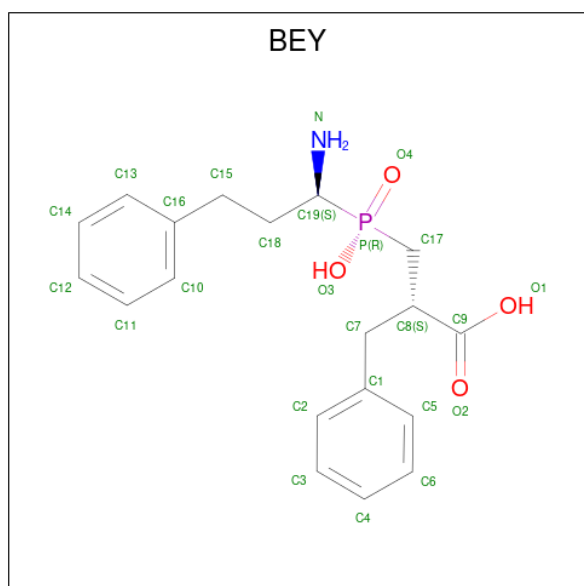
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	Zn	0	0
			2	2		
3	K	2	Total	Zn	0	0
			2	2		
3	L	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (2S)-3-[(R)-[(1S)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]-2-benzylpropionic acid (three-letter code: BEY) (formula: C<sub>19</sub>H<sub>24</sub>NO<sub>4</sub>P).



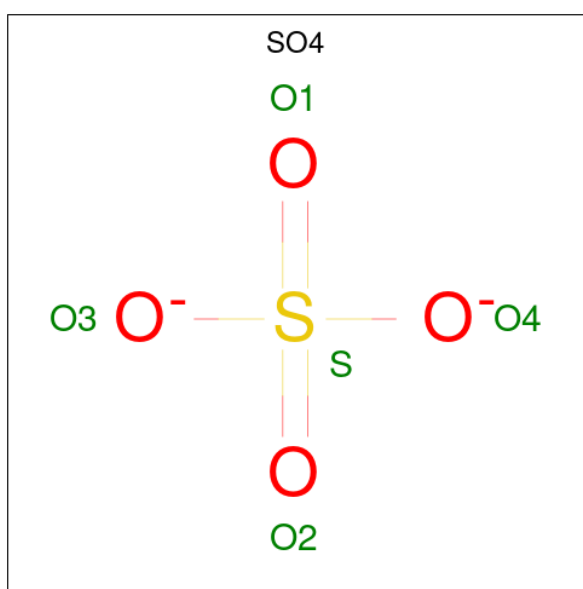
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			25	19	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	J	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	L	1	Total	C	N	O	P	0	0
			25	19	1	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



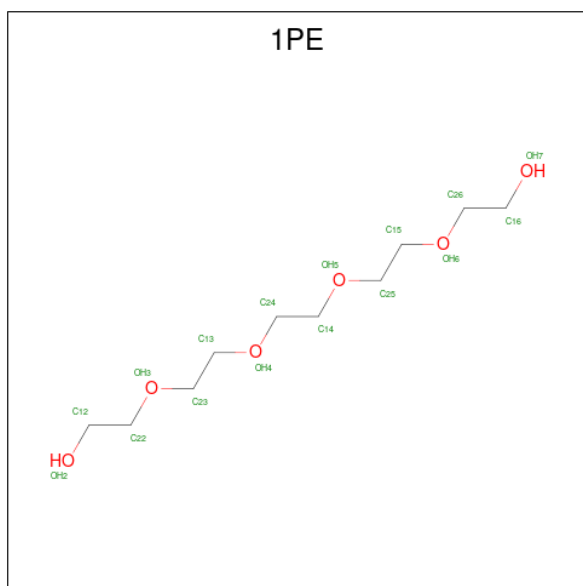
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	A	1	Total	C	O	0	0
			12	8	4		
6	B	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		
6	C	1	Total	C	O	0	0
			13	9	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			11	8	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			7	5	2		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			7	4	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			15	10	5		
6	H	1	Total	C	O	0	0
			10	7	3		
6	H	1	Total	C	O	0	0
			10	7	3		

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	217	Total	O	0	0
			217	217		
7	B	158	Total	O	0	0
			158	158		
7	C	188	Total	O	0	0
			188	188		
7	D	182	Total	O	0	0
			182	182		
7	E	203	Total	O	0	0
			203	203		
7	F	165	Total	O	0	0
			165	165		

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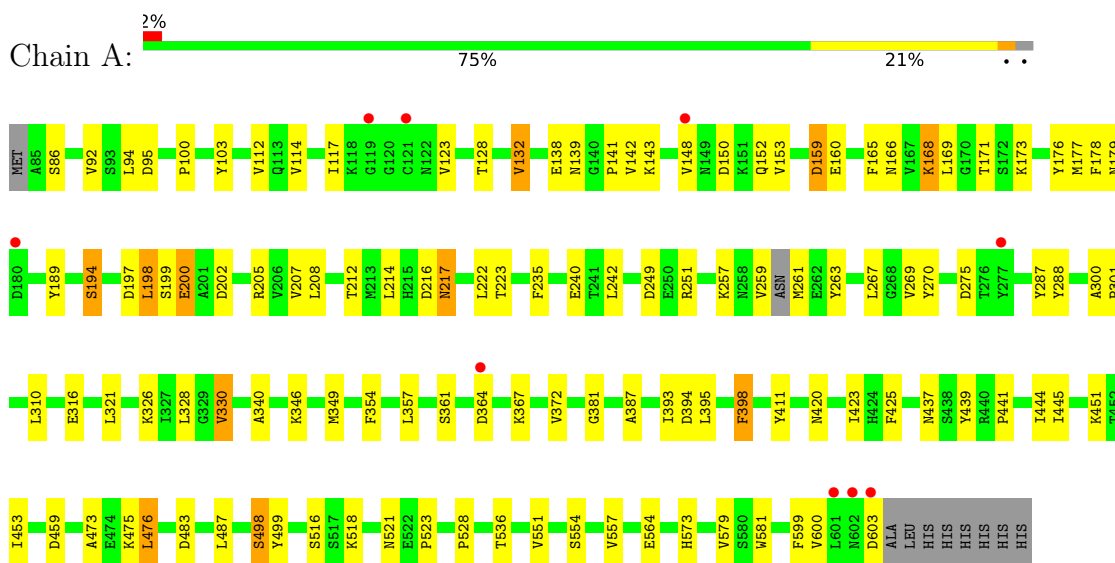
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	204	Total 204	O 204	0	0
7	H	203	Total 203	O 203	0	0
7	I	207	Total 207	O 207	0	0
7	J	207	Total 207	O 207	0	0
7	K	222	Total 222	O 222	0	0
7	L	158	Total 158	O 158	0	0

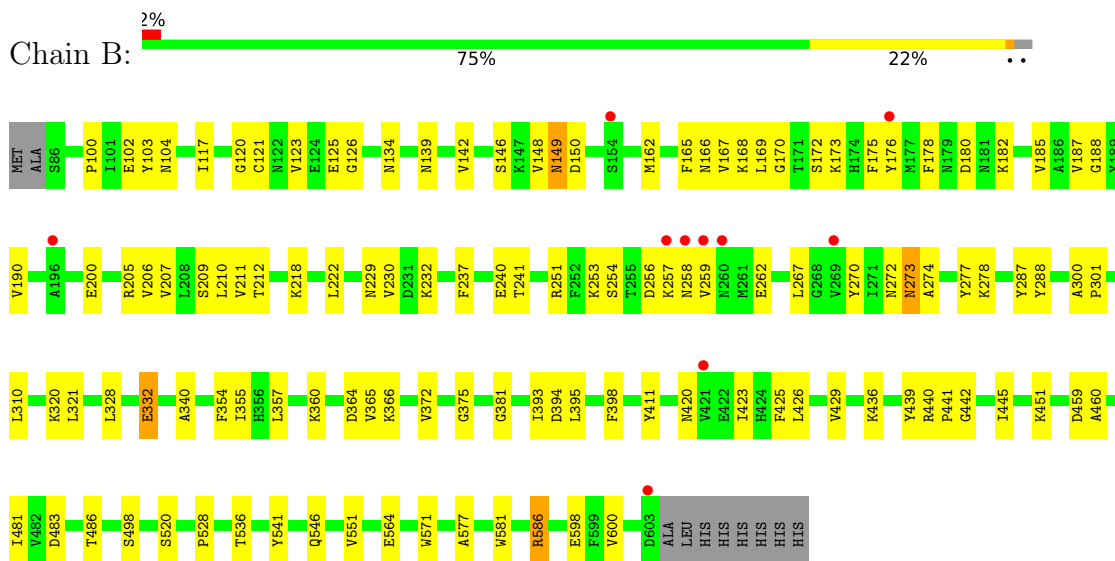
### 3 Residue-property plots [i](#)

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: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

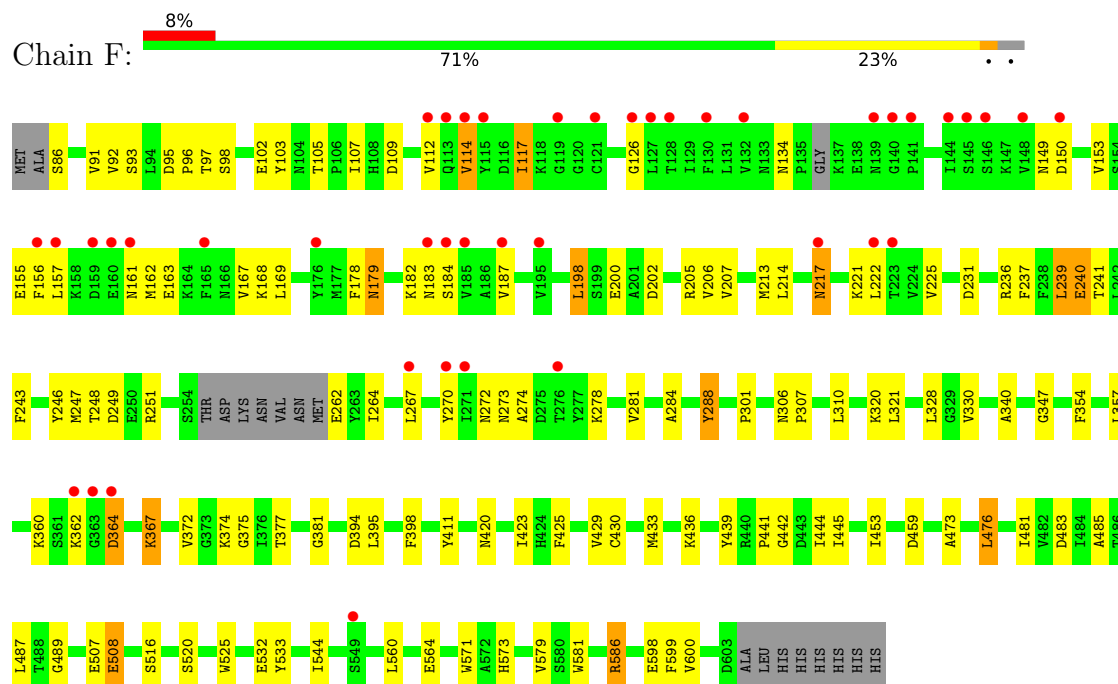


- Molecule 1: M17 leucyl aminopeptidase

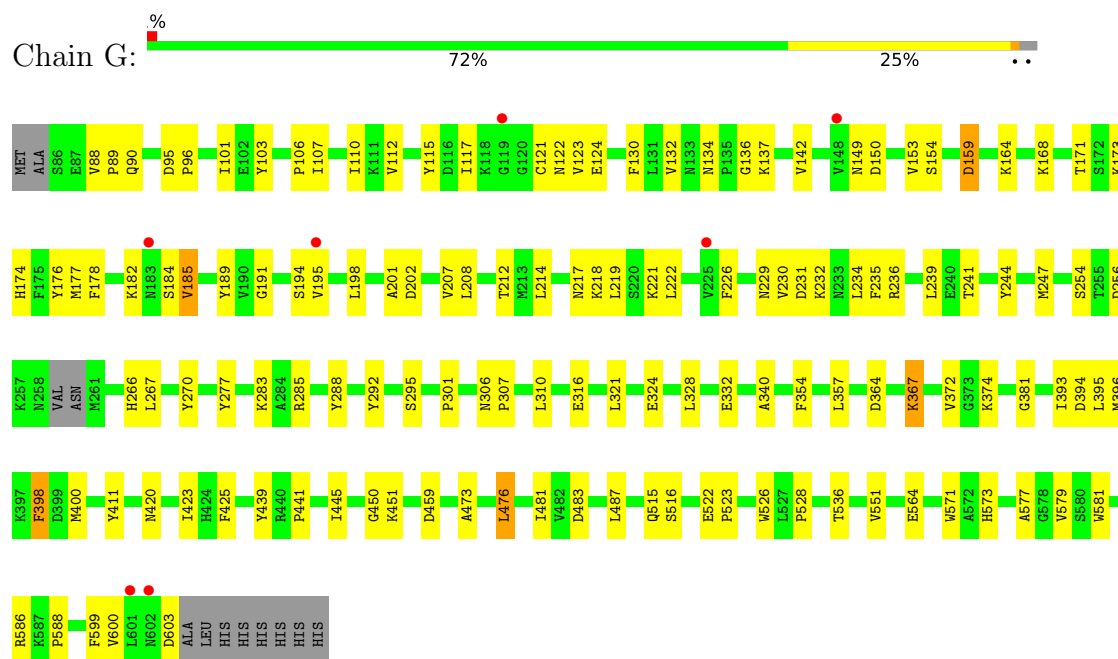




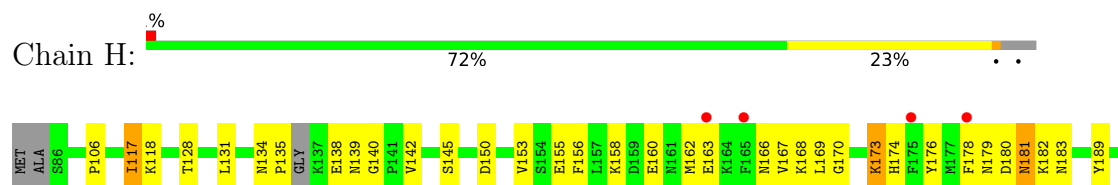
• Molecule 1: M17 leucyl aminopeptidase

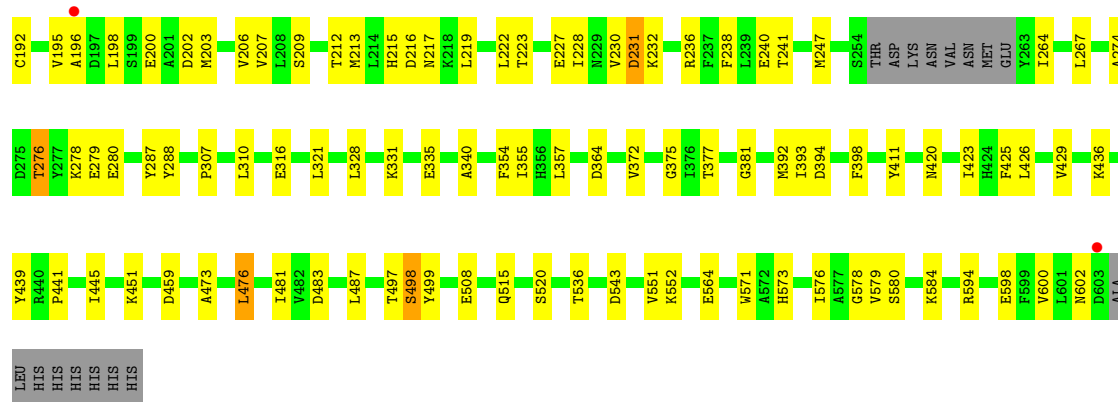


• Molecule 1: M17 leucyl aminopeptidase

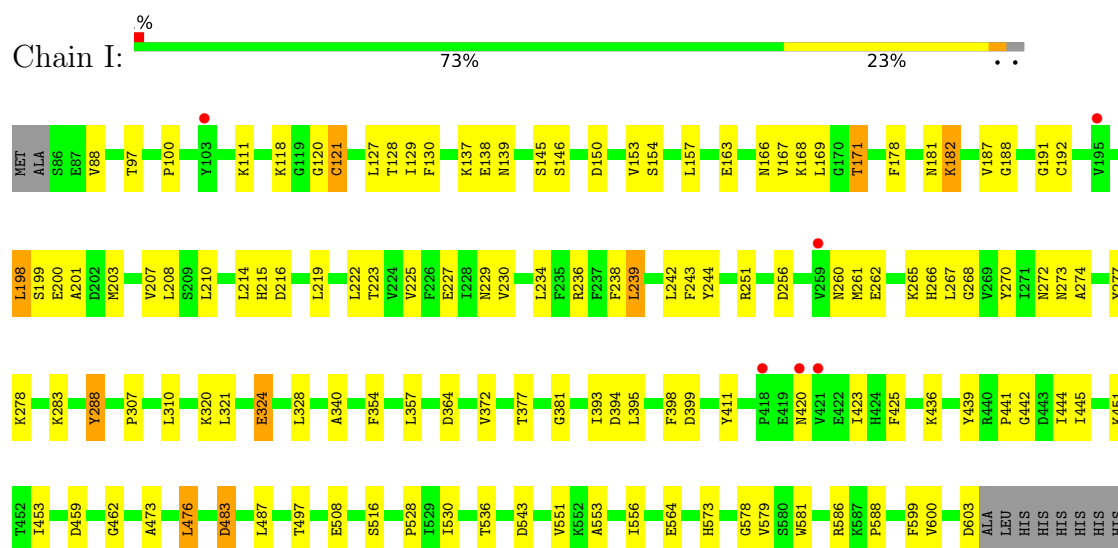


• Molecule 1: M17 leucyl aminopeptidase

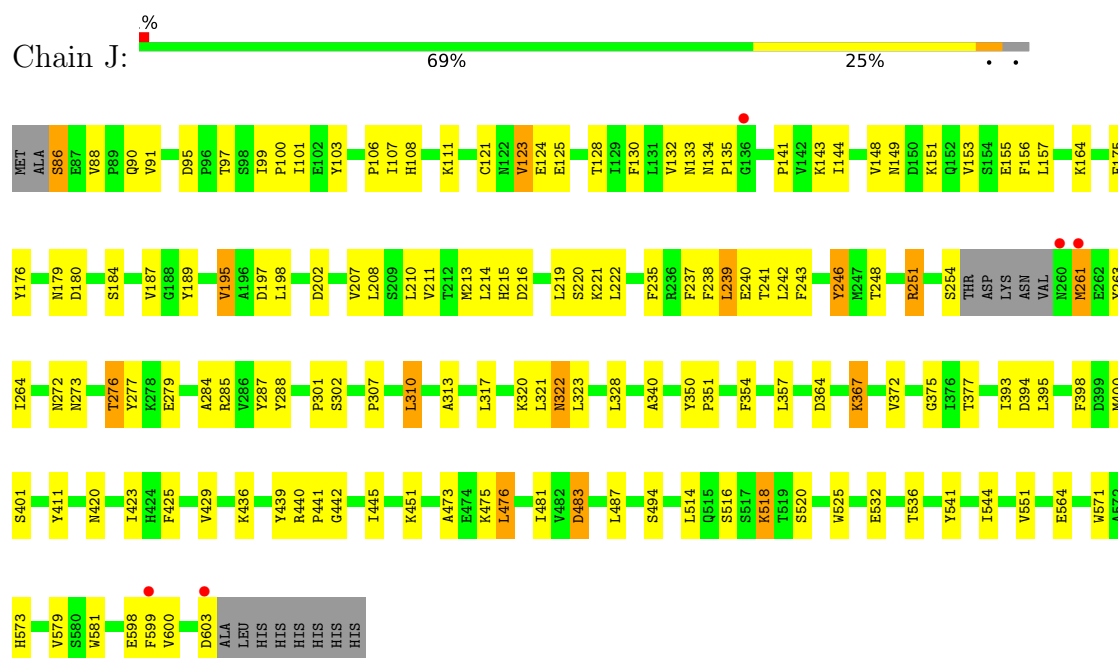




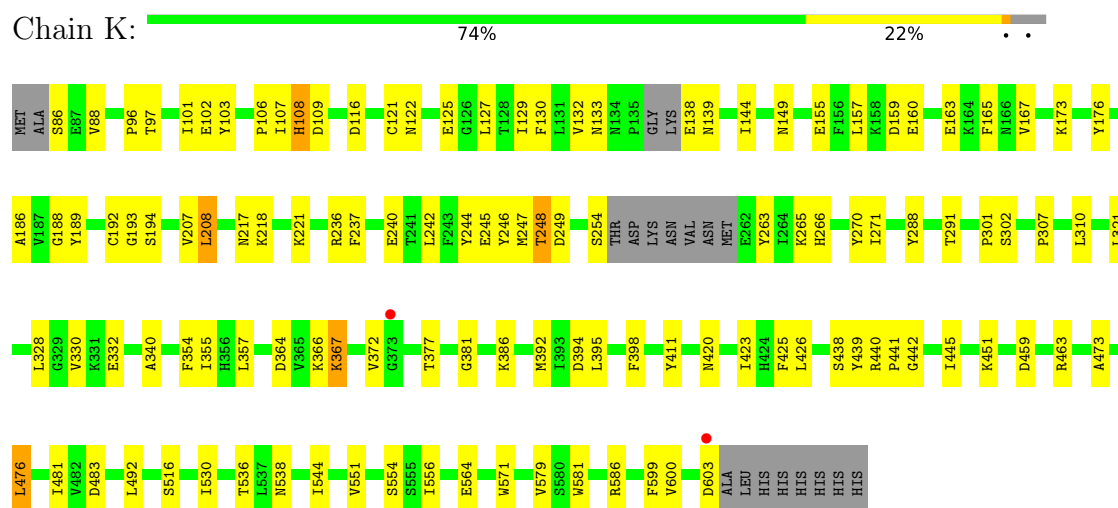
• Molecule 1: M17 leucyl aminopeptidase



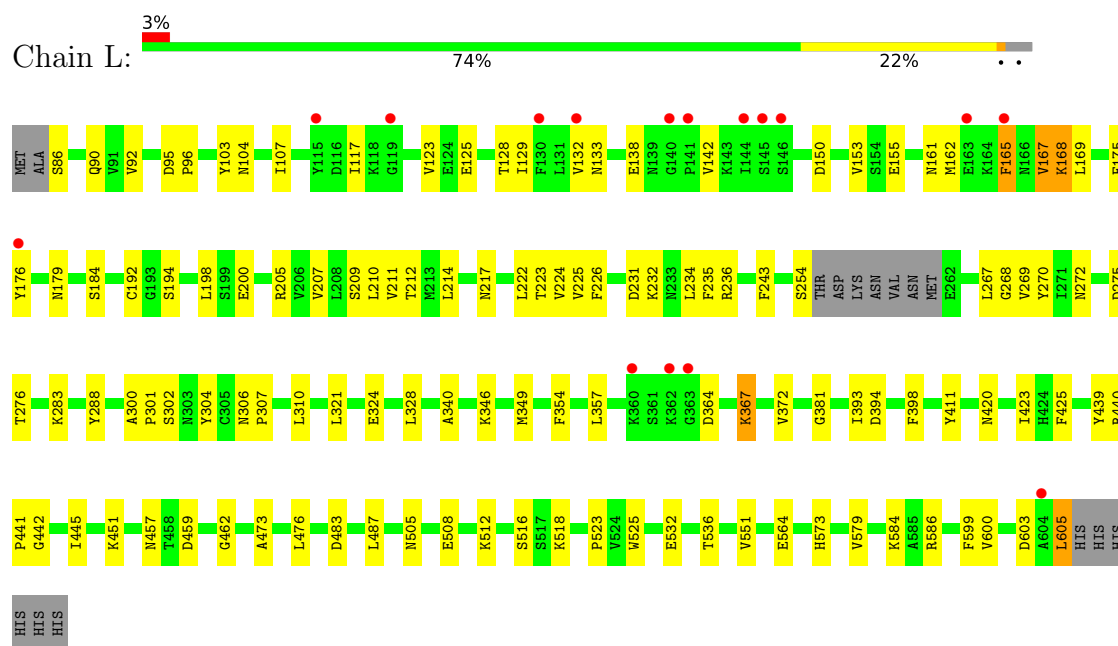
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.08Å 174.16Å 227.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.70 – 2.56 77.70 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.8 (77.70-2.56) 98.8 (77.70-2.56)	Depositor EDS
$R_{merge}$	0.55	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.220 , 0.278 0.224 , 0.281	Depositor DCC
$R_{free}$ test set	10910 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	50444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 47.88 % 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 9.3151e-05. 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: BEY, CO3, SO4, 1PE, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.67	0/4057	0.71	1/5500 (0.0%)
1	B	0.63	0/4007	0.69	2/5442 (0.0%)
1	C	0.67	1/4031 (0.0%)	0.71	0/5469
1	D	0.69	0/4005	0.74	6/5429 (0.1%)
1	E	0.71	1/3974 (0.0%)	0.76	6/5393 (0.1%)
1	F	0.64	1/3949 (0.0%)	0.76	3/5364 (0.1%)
1	G	0.69	0/4066	0.71	1/5505 (0.0%)
1	H	0.66	0/4014	0.68	0/5434
1	I	0.68	0/4084	0.79	3/5531 (0.1%)
1	J	0.70	0/4031	0.72	0/5461
1	K	0.72	0/4006	0.75	1/5427 (0.0%)
1	L	0.66	0/4009	0.69	1/5440 (0.0%)
All	All	0.68	3/48233 (0.0%)	0.72	24/65395 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	305	CYS	CB-SG	-5.60	1.72	1.81
1	C	305	CYS	CB-SG	-5.25	1.73	1.81
1	F	430	CYS	CB-SG	-5.20	1.73	1.81

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	586	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	I	586	ARG	NE-CZ-NH1	-17.07	111.76	120.30
1	F	586	ARG	NE-CZ-NH2	16.73	128.66	120.30
1	F	586	ARG	NE-CZ-NH1	-16.10	112.25	120.30
1	F	586	ARG	CD-NE-CZ	8.03	134.84	123.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3980	0	3912	93	0
1	B	3929	0	3828	87	1
1	C	3953	0	3882	89	0
1	D	3928	0	3876	102	0
1	E	3897	0	3822	92	0
1	F	3873	0	3772	98	0
1	G	3989	0	3976	95	0
1	H	3938	0	3931	84	0
1	I	4006	0	3986	93	0
1	J	3954	0	3923	120	0
1	K	3930	0	3901	84	0
1	L	3932	0	3862	86	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	2	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	1	0
2	I	4	0	0	1	0
2	J	4	0	0	1	0
2	K	4	0	0	2	0
2	L	4	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	25	0	21	4	0
4	B	25	0	22	2	0
4	C	25	0	21	5	0
4	D	25	0	22	6	0
4	E	25	0	22	2	0
4	F	25	0	21	2	0
4	G	25	0	21	2	0
4	H	25	0	22	7	0
4	I	25	0	22	2	0
4	J	25	0	22	3	0
4	K	25	0	22	4	0
4	L	25	0	22	2	0
5	A	15	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	0	0
5	E	10	0	0	3	0
5	F	5	0	0	1	0
5	G	10	0	0	0	0
5	I	5	0	0	1	0
5	J	10	0	0	2	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	A	21	0	22	2	0
6	B	30	0	30	3	0
6	C	22	0	24	1	0
6	D	38	0	38	5	0
6	E	32	0	36	3	0
6	F	30	0	39	1	0
6	G	43	0	47	4	0
6	H	20	0	20	1	0
6	I	33	0	37	5	0
6	J	31	0	36	9	0
6	K	41	0	44	8	0
6	L	33	0	40	5	0
7	A	217	0	0	12	0
7	B	158	0	0	7	0
7	C	188	0	0	6	0
7	D	182	0	0	5	1
7	E	203	0	0	15	0
7	F	165	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	204	0	0	11	0
7	H	203	0	0	6	0
7	I	207	0	0	6	0
7	J	207	0	0	18	0
7	K	222	0	0	7	0
7	L	158	0	0	11	0
All	All	50444	0	47344	1043	1

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 11.

The worst 5 of 1043 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:H:436:LYS:HE2	7:I:3958:HOH:O	1.43	1.15
1:B:257:LYS:HA	1:B:258:ASN:HB3	1.34	1.09
1:J:518:LYS:HE2	7:J:2650:HOH:O	1.52	1.08
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.39	1.03
1:G:136:GLY:HA3	1:G:137:LYS:CB	1.86	1.02

All (1) 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)
1:B:366:LYS:NZ	7:D:3762:HOH:O[4_555]	1.84	0.36

## 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	514/528 (97%)	493 (96%)	19 (4%)	2 (0%)	34 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	516/528 (98%)	488 (95%)	25 (5%)	3 (1%)	25	33
1	C	516/528 (98%)	495 (96%)	18 (4%)	3 (1%)	25	33
1	D	509/528 (96%)	492 (97%)	16 (3%)	1 (0%)	47	58
1	E	506/528 (96%)	487 (96%)	17 (3%)	2 (0%)	34	45
1	F	504/528 (96%)	484 (96%)	14 (3%)	6 (1%)	13	17
1	G	512/528 (97%)	483 (94%)	27 (5%)	2 (0%)	34	45
1	H	503/528 (95%)	477 (95%)	21 (4%)	5 (1%)	15	21
1	I	516/528 (98%)	493 (96%)	22 (4%)	1 (0%)	47	58
1	J	509/528 (96%)	483 (95%)	24 (5%)	2 (0%)	34	45
1	K	503/528 (95%)	479 (95%)	22 (4%)	2 (0%)	34	45
1	L	509/528 (96%)	484 (95%)	24 (5%)	1 (0%)	47	58
All	All	6117/6336 (96%)	5838 (95%)	249 (4%)	30 (0%)	29	39

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	149	ASN
1	E	230	VAL
1	H	139	ASN
1	B	273	ASN

### 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	426/455 (94%)	407 (96%)	19 (4%)	27	37
1	B	412/455 (90%)	403 (98%)	9 (2%)	52	66
1	C	419/455 (92%)	406 (97%)	13 (3%)	40	52
1	D	417/455 (92%)	395 (95%)	22 (5%)	22	30
1	E	414/455 (91%)	396 (96%)	18 (4%)	29	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	409/455 (90%)	385 (94%)	24 (6%)	19	25
1	G	435/455 (96%)	418 (96%)	17 (4%)	32	43
1	H	430/455 (94%)	412 (96%)	18 (4%)	30	40
1	I	437/455 (96%)	414 (95%)	23 (5%)	22	30
1	J	430/455 (94%)	404 (94%)	26 (6%)	19	24
1	K	427/455 (94%)	412 (96%)	15 (4%)	36	48
1	L	421/455 (92%)	403 (96%)	18 (4%)	29	39
All	All	5077/5460 (93%)	4855 (96%)	222 (4%)	28	38

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	367	LYS
1	L	605	LEU
1	I	163	GLU
1	L	579	VAL
1	K	398	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	511	ASN
1	I	602	ASN
1	I	166	ASN
1	K	181	ASN
1	E	161	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 24 are monoatomic - leaving 76 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	$\# Z  > 2$
5	SO4	A	24	-	4,4,4	0.17	0	6,6,6	0.33	0
2	CO3	K	1002	-	0,3,3	-	-	0,3,3	-	-
6	1PE	I	66	-	6,6,15	0.61	0	5,5,14	0.55	0
5	SO4	E	7	-	4,4,4	0.17	0	6,6,6	0.40	0
2	CO3	L	1002	-	0,3,3	-	-	0,3,3	-	-
6	1PE	K	5	-	11,11,15	0.51	0	10,10,14	0.41	0
5	SO4	L	25	-	4,4,4	0.15	0	6,6,6	0.35	0
6	1PE	D	67	-	6,6,15	0.73	0	5,5,14	0.36	0
6	1PE	I	21	-	14,14,15	0.72	0	13,13,14	0.51	0
4	BEY	C	1003	3	19,26,26	1.17	1 (5%)	21,35,35	1.42	3 (14%)
5	SO4	F	21	-	4,4,4	0.18	0	6,6,6	0.25	0
2	CO3	J	1002	-	0,3,3	-	-	0,3,3	-	-
6	1PE	F	31	-	9,9,15	0.50	0	8,8,14	0.51	0
6	1PE	H	65	-	9,9,15	0.59	0	8,8,14	0.23	0
4	BEY	B	1003	3	19,26,26	0.85	0	21,35,35	0.99	1 (4%)
2	CO3	A	1002	-	0,3,3	-	-	0,3,3	-	-
6	1PE	G	48	-	5,5,15	0.64	0	4,4,14	0.80	0
6	1PE	L	612	-	11,11,15	0.65	0	10,10,14	0.35	0
2	CO3	G	1002	-	0,3,3	-	-	0,3,3	-	-
6	1PE	K	50	-	5,5,15	0.69	0	4,4,14	0.53	0
6	1PE	F	32	-	9,9,15	0.66	0	8,8,14	0.44	0
6	1PE	D	44	-	10,10,15	0.70	0	9,9,14	0.45	0
6	1PE	G	12	-	8,8,15	0.49	0	7,7,14	0.21	0
5	SO4	G	26	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	J	18	-	4,4,4	0.28	0	6,6,6	0.31	0
6	1PE	J	3	-	9,9,15	0.59	0	8,8,14	0.54	0
4	BEY	H	1003	3	19,26,26	0.78	0	21,35,35	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BEY	L	1003	3	19,26,26	0.84	1 (5%)	21,35,35	0.97	1 (4%)
6	1PE	L	56	-	10,10,15	0.77	0	9,9,14	0.49	0
6	1PE	L	1	-	9,9,15	0.51	0	8,8,14	0.38	0
6	1PE	I	22	-	10,10,15	0.57	0	9,9,14	0.53	0
4	BEY	F	1003	3	19,26,26	1.09	1 (5%)	21,35,35	0.88	0
4	BEY	J	1003	3	19,26,26	0.83	0	21,35,35	0.74	1 (4%)
2	CO3	E	1002	-	0,3,3	-	-	0,3,3	-	-
5	SO4	A	1	-	4,4,4	0.16	0	6,6,6	0.31	0
2	CO3	I	1002	-	0,3,3	-	-	0,3,3	-	-
5	SO4	A	2	-	4,4,4	0.19	0	6,6,6	0.59	0
6	1PE	G	30	-	6,6,15	0.55	0	5,5,14	0.44	0
6	1PE	H	64	-	9,9,15	0.62	0	8,8,14	0.25	0
6	1PE	K	42	-	10,10,15	0.59	0	9,9,14	0.34	0
6	1PE	K	4	-	11,11,15	0.73	0	10,10,14	0.64	0
6	1PE	E	612	-	11,11,15	0.60	0	10,10,14	0.42	0
6	1PE	J	45	-	9,9,15	0.67	0	8,8,14	0.53	0
4	BEY	G	1003	3	19,26,26	0.92	0	21,35,35	1.05	0
5	SO4	I	17	-	4,4,4	0.09	0	6,6,6	0.15	0
6	1PE	J	2	-	10,10,15	0.60	0	9,9,14	0.37	0
2	CO3	F	1002	-	0,3,3	-	-	0,3,3	-	-
2	CO3	D	1002	-	0,3,3	-	-	0,3,3	-	-
4	BEY	K	1003	3	19,26,26	0.61	0	21,35,35	1.84	4 (19%)
6	1PE	A	19	-	8,8,15	0.61	0	7,7,14	0.20	0
6	1PE	A	20	-	11,11,15	0.63	0	10,10,14	0.35	0
6	1PE	B	62	-	9,9,15	0.68	0	8,8,14	0.44	0
4	BEY	I	1003	3	19,26,26	0.79	1 (5%)	21,35,35	1.66	2 (9%)
6	1PE	G	58	-	14,14,15	0.73	0	13,13,14	0.54	0
6	1PE	E	8	-	11,11,15	0.53	0	10,10,14	0.44	0
6	1PE	E	43	-	7,7,15	0.46	0	6,6,14	0.49	0
5	SO4	D	5	-	4,4,4	0.14	0	6,6,6	0.16	0
6	1PE	B	61	-	9,9,15	0.71	0	8,8,14	0.93	0
5	SO4	E	22	-	4,4,4	0.22	0	6,6,6	0.30	0
4	BEY	A	1003	3	19,26,26	0.72	0	21,35,35	1.22	3 (14%)
6	1PE	D	63	-	9,9,15	0.70	0	8,8,14	0.43	0
5	SO4	G	23	-	4,4,4	0.09	0	6,6,6	0.20	0
6	1PE	F	33	-	9,9,15	0.61	0	8,8,14	0.29	0
5	SO4	K	19	-	4,4,4	0.16	0	6,6,6	0.20	0
6	1PE	D	9	-	9,9,15	0.60	0	8,8,14	0.58	0
2	CO3	B	1002	-	0,3,3	-	-	0,3,3	-	-
2	CO3	C	1002	-	0,3,3	-	-	0,3,3	-	-
2	CO3	H	1002	-	0,3,3	-	-	0,3,3	-	-
5	SO4	J	20	-	4,4,4	0.12	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	1PE	B	60	-	9,9,15	0.54	0	8,8,14	0.29	0
6	1PE	C	18	-	8,8,15	0.59	0	7,7,14	0.38	0
5	SO4	C	3	-	4,4,4	0.17	0	6,6,6	0.39	0
6	1PE	G	47	-	5,5,15	0.40	0	4,4,14	0.25	0
4	BEY	D	1003	3	19,26,26	0.94	1 (5%)	21,35,35	1.10	2 (9%)
4	BEY	E	1003	3	19,26,26	0.70	0	21,35,35	0.93	0
6	1PE	C	17	-	12,12,15	0.91	0	11,11,14	1.05	1 (9%)

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
6	1PE	I	66	-	-	2/4/4/13	-
6	1PE	K	5	-	-	3/9/9/13	-
6	1PE	D	67	-	-	3/4/4/13	-
6	1PE	I	21	-	-	8/12/12/13	-
4	BEY	C	1003	3	-	10/14/24/24	0/2/2/2
6	1PE	H	65	-	-	2/7/7/13	-
6	1PE	F	31	-	-	3/7/7/13	-
4	BEY	B	1003	3	-	9/14/24/24	0/2/2/2
6	1PE	L	612	-	-	7/9/9/13	-
6	1PE	G	48	-	-	2/3/3/13	-
6	1PE	K	50	-	-	3/3/3/13	-
6	1PE	F	32	-	-	3/7/7/13	-
6	1PE	D	44	-	-	4/8/8/13	-
6	1PE	G	12	-	-	4/6/6/13	-
6	1PE	J	3	-	-	3/7/7/13	-
4	BEY	H	1003	3	-	9/14/24/24	0/2/2/2
4	BEY	L	1003	3	-	8/14/24/24	0/2/2/2
6	1PE	L	56	-	-	6/8/8/13	-
6	1PE	L	1	-	-	4/7/7/13	-
4	BEY	D	1003	3	-	8/14/24/24	0/2/2/2
6	1PE	I	22	-	-	4/8/8/13	-
4	BEY	F	1003	3	-	9/14/24/24	0/2/2/2
4	BEY	J	1003	3	-	6/14/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	H	64	-	-	5/7/7/13	-
6	1PE	G	30	-	-	2/4/4/13	-
6	1PE	K	42	-	-	5/8/8/13	-
6	1PE	K	4	-	-	1/9/9/13	-
6	1PE	E	612	-	-	2/9/9/13	-
6	1PE	J	45	-	-	4/7/7/13	-
4	BEY	G	1003	3	-	7/14/24/24	0/2/2/2
6	1PE	J	2	-	-	4/8/8/13	-
6	1PE	B	62	-	-	4/7/7/13	-
4	BEY	K	1003	3	-	10/14/24/24	0/2/2/2
6	1PE	A	19	-	-	2/6/6/13	-
6	1PE	G	58	-	-	5/12/12/13	-
4	BEY	I	1003	3	-	8/14/24/24	0/2/2/2
6	1PE	E	8	-	-	4/9/9/13	-
6	1PE	E	43	-	-	3/5/5/13	-
6	1PE	B	61	-	-	6/7/7/13	-
6	1PE	D	63	-	-	1/7/7/13	-
6	1PE	F	33	-	-	3/7/7/13	-
4	BEY	A	1003	3	-	11/14/24/24	0/2/2/2
6	1PE	D	9	-	-	3/7/7/13	-
6	1PE	B	60	-	-	4/7/7/13	-
6	1PE	C	18	-	-	3/6/6/13	-
6	1PE	G	47	-	-	1/3/3/13	-
6	1PE	A	20	-	-	3/9/9/13	-
4	BEY	E	1003	3	-	8/14/24/24	0/2/2/2
6	1PE	C	17	-	-	3/10/10/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	BEY	P-C17	3.87	1.83	1.79
4	D	1003	BEY	P-C17	2.81	1.82	1.79
4	F	1003	BEY	P-C17	2.65	1.82	1.79
4	L	1003	BEY	P-C17	2.40	1.82	1.79
4	I	1003	BEY	P-C17	2.19	1.81	1.79

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1003	BEY	C1-C7-C8	6.10	121.69	113.81
4	K	1003	BEY	C1-C7-C8	5.07	120.36	113.81
4	C	1003	BEY	C7-C8-C9	-4.08	102.27	111.09
4	K	1003	BEY	C7-C8-C9	4.02	119.79	111.09
4	K	1003	BEY	O3-P-C19	-3.44	99.15	106.87

There are no chirality outliers.

5 of 232 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	BEY	C18-C19-P-O4
4	A	1003	BEY	C8-C17-P-O3
4	A	1003	BEY	C8-C17-P-O4
4	A	1003	BEY	C16-C15-C18-C19
4	A	1003	BEY	C1-C7-C8-C9

There are no ring outliers.

49 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1002	CO3	2	0
5	E	7	SO4	2	0
2	L	1002	CO3	1	0
6	K	5	1PE	3	0
6	I	21	1PE	4	0
4	C	1003	BEY	5	0
5	F	21	SO4	1	0
2	J	1002	CO3	1	0
6	F	31	1PE	1	0
6	H	65	1PE	1	0
4	B	1003	BEY	2	0
6	L	612	1PE	3	0
6	K	50	1PE	1	0
6	D	44	1PE	4	0
5	J	18	SO4	1	0
6	J	3	1PE	5	0
4	H	1003	BEY	7	0
4	L	1003	BEY	2	0
6	L	1	1PE	2	0
6	I	22	1PE	1	0
4	F	1003	BEY	2	0
4	J	1003	BEY	3	0

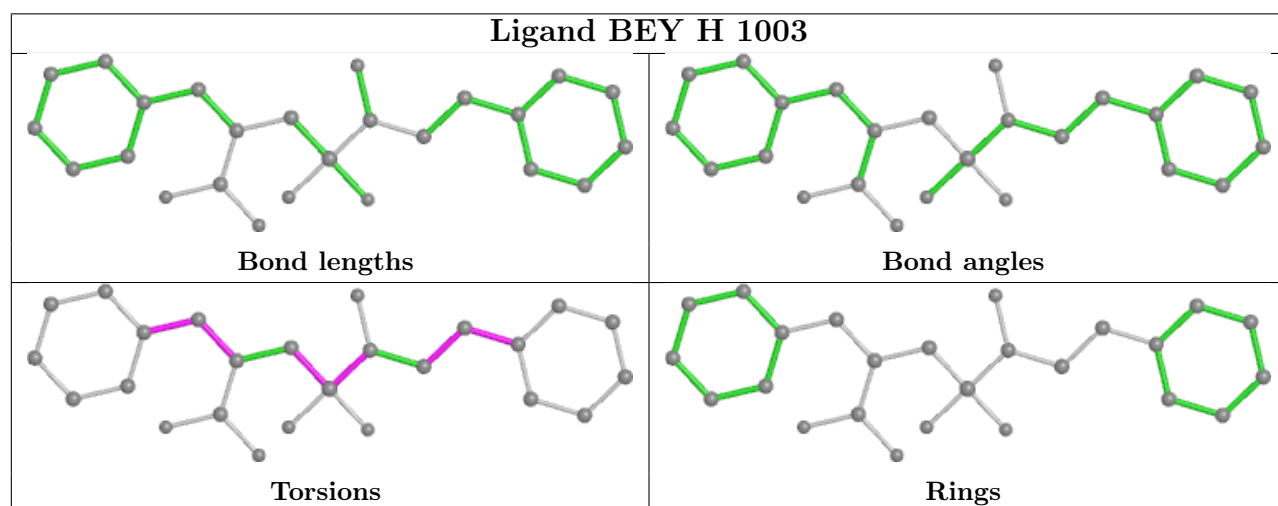
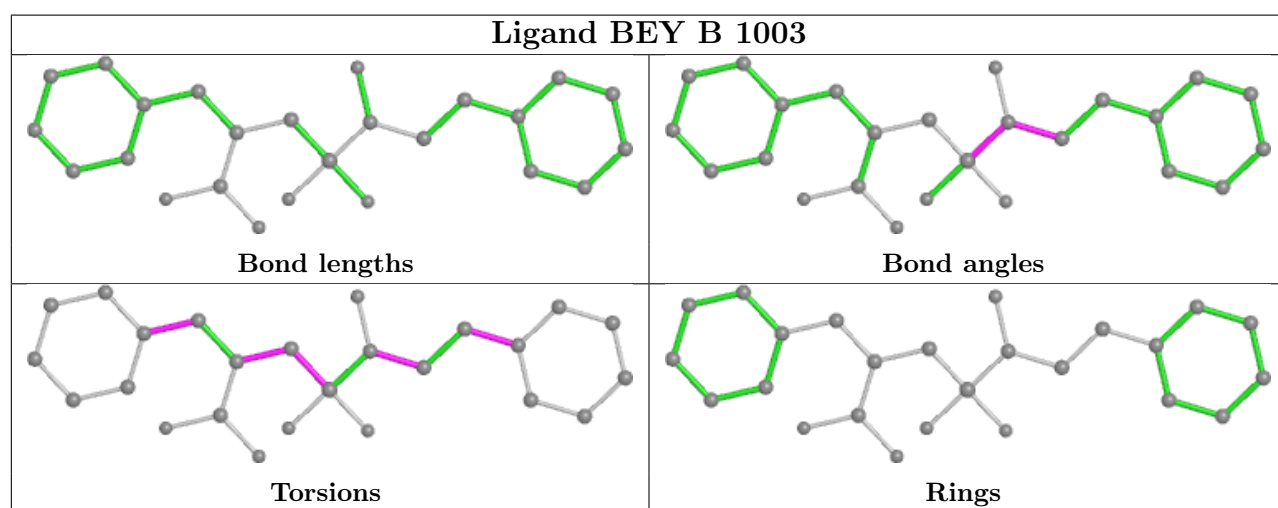
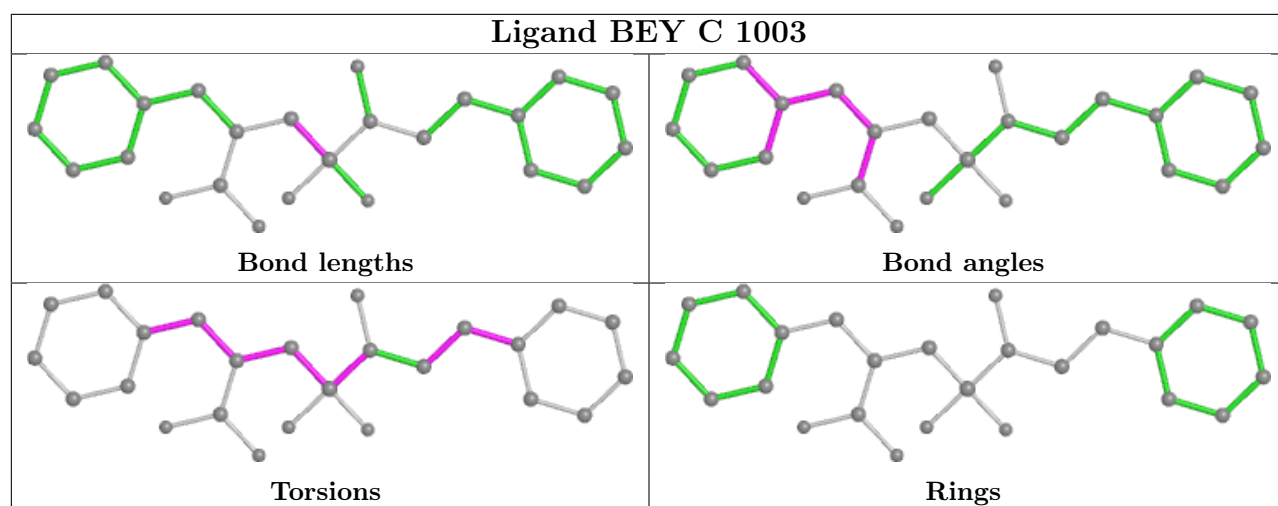
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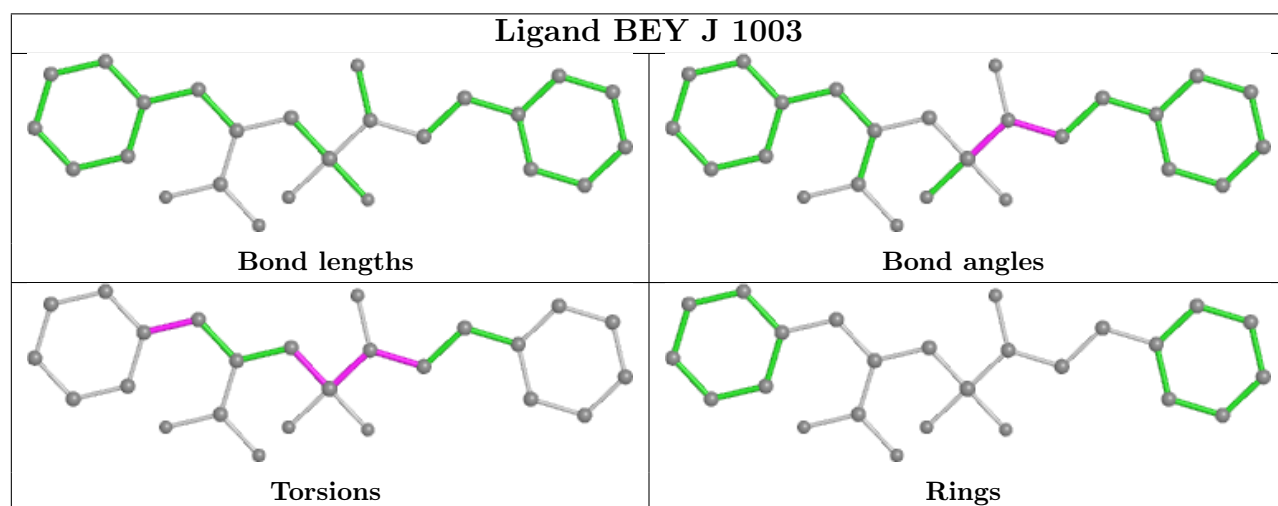
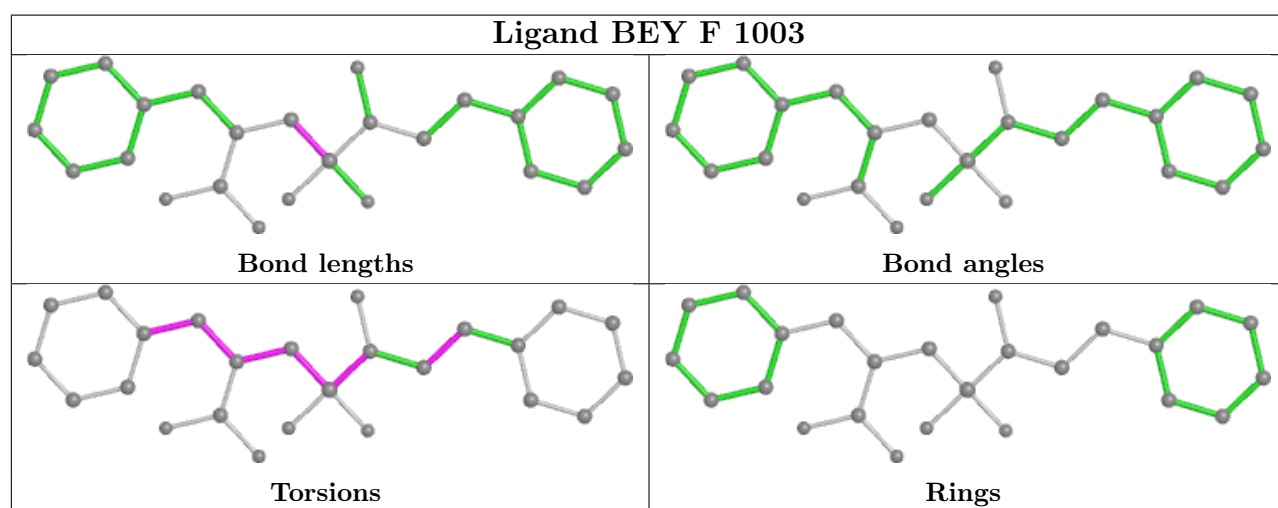
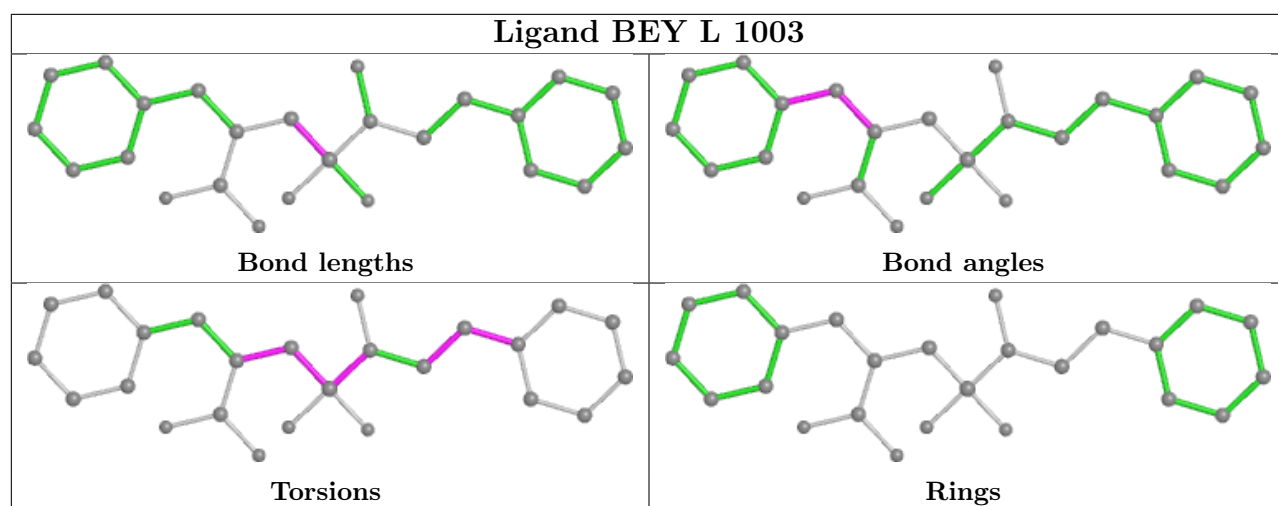
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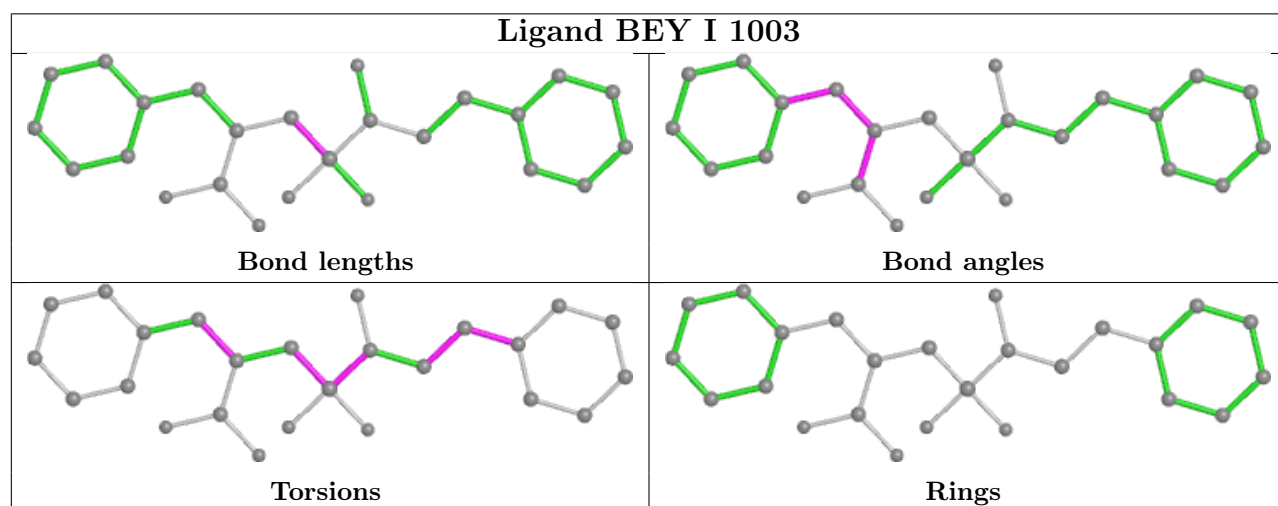
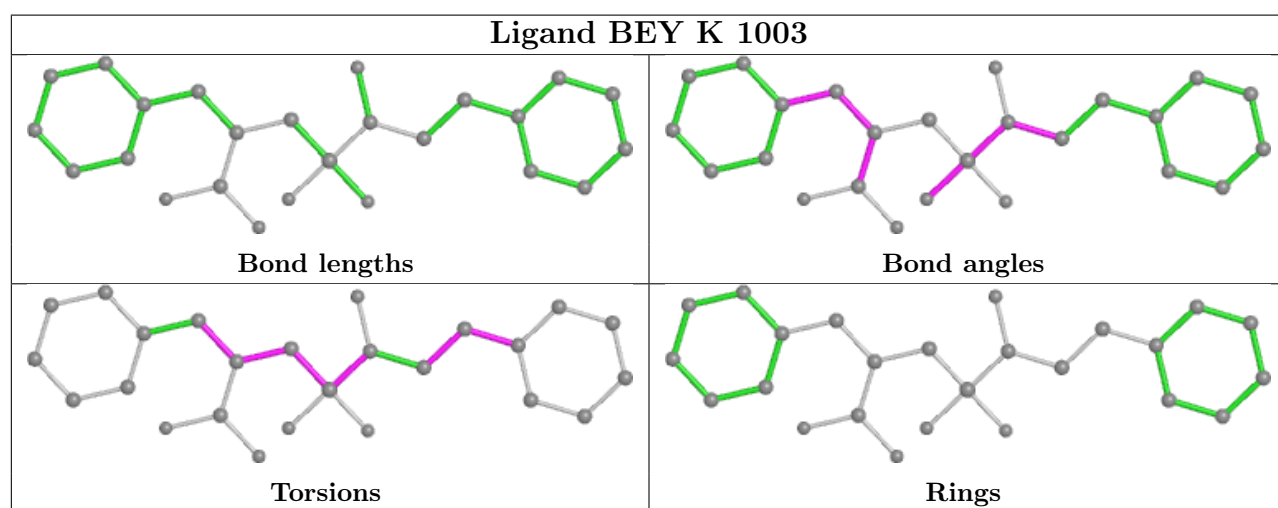
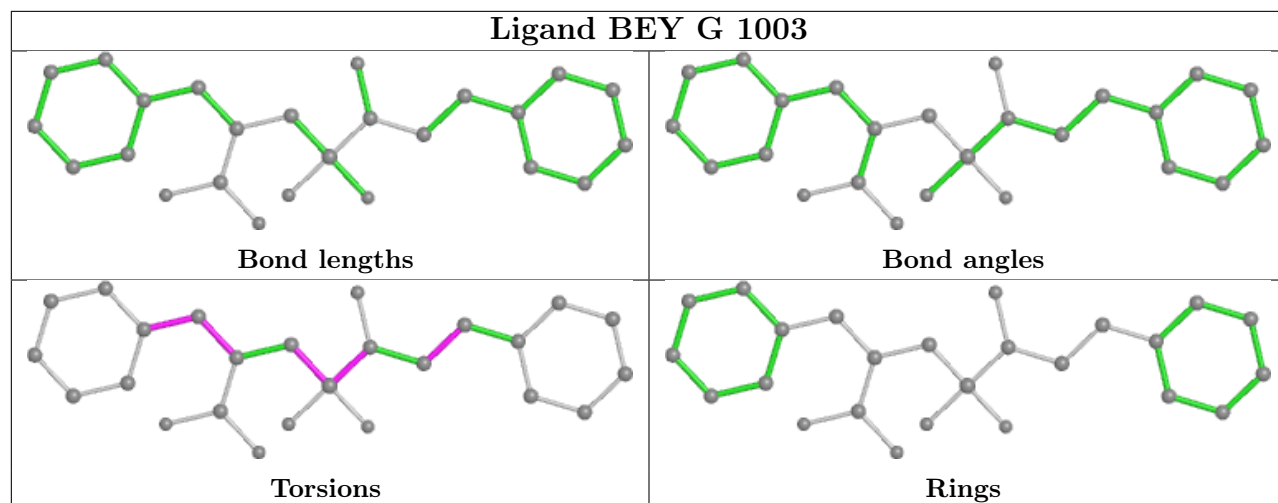
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1002	CO3	1	0
6	G	30	1PE	1	0
6	K	42	1PE	3	0
6	K	4	1PE	1	0
6	E	612	1PE	1	0
6	J	45	1PE	2	0
4	G	1003	BEY	2	0
5	I	17	SO4	1	0
6	J	2	1PE	2	0
2	D	1002	CO3	2	0
4	K	1003	BEY	4	0
6	A	20	1PE	2	0
4	I	1003	BEY	2	0
6	G	58	1PE	2	0
6	E	43	1PE	2	0
6	B	61	1PE	2	0
5	E	22	SO4	1	0
4	A	1003	BEY	4	0
6	D	63	1PE	1	0
2	H	1002	CO3	1	0
5	J	20	SO4	1	0
6	B	60	1PE	1	0
5	C	3	SO4	1	0
6	G	47	1PE	1	0
4	D	1003	BEY	6	0
4	E	1003	BEY	2	0
6	C	17	1PE	1	0

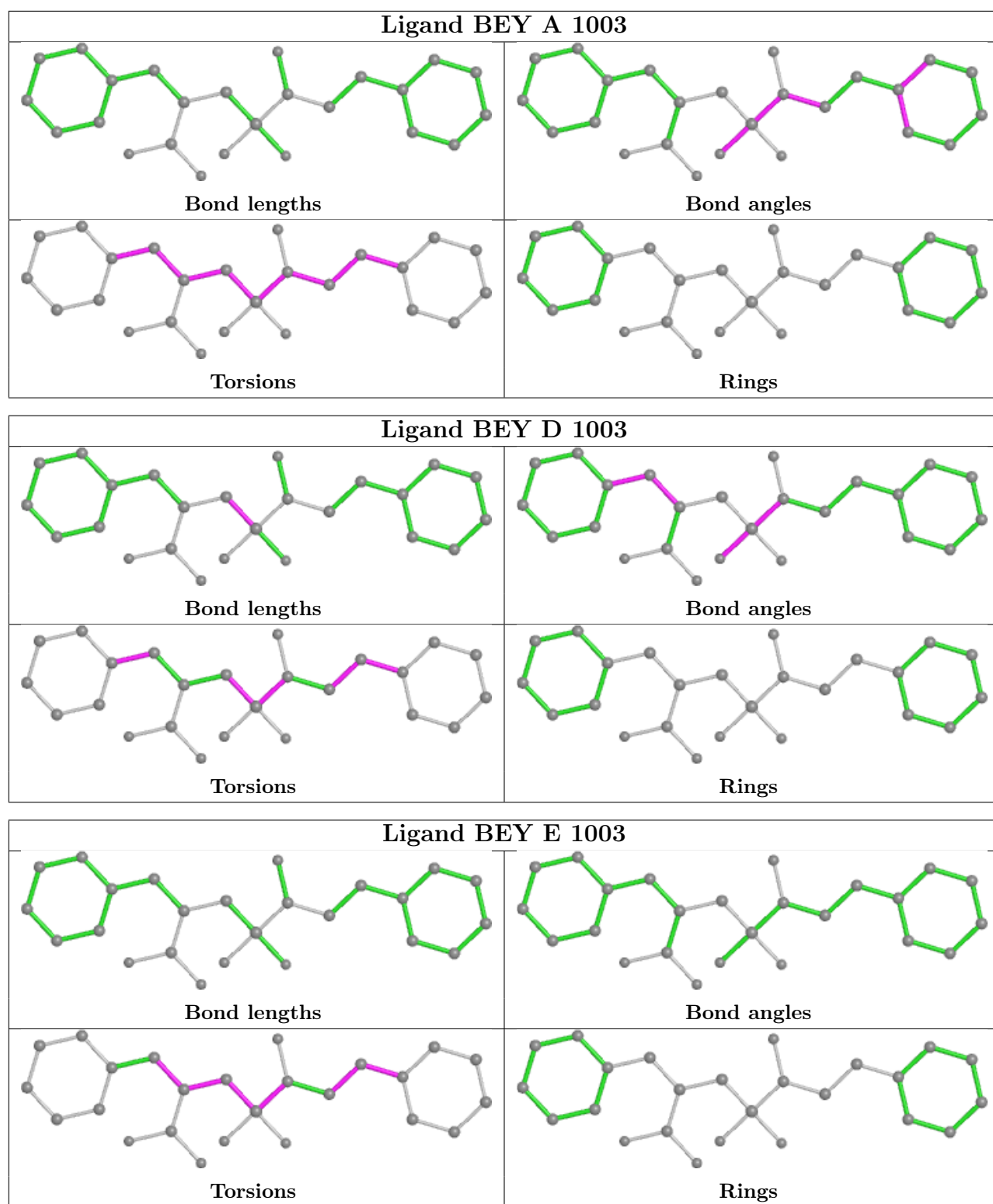
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











## 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(Å <sup>2</sup> )	Q<0.9
1	A	518/528 (98%)	0.12	9 (1%) 70 77	13, 25, 45, 61	1 (0%)
1	B	518/528 (98%)	0.15	10 (1%) 66 74	13, 29, 64, 77	0
1	C	518/528 (98%)	0.11	2 (0%) 92 96	11, 26, 49, 59	0
1	D	513/528 (97%)	-0.05	3 (0%) 89 93	15, 25, 44, 66	0
1	E	510/528 (96%)	-0.02	5 (0%) 82 87	11, 24, 40, 59	0
1	F	510/528 (96%)	0.45	42 (8%) 11 16	18, 30, 60, 72	0
1	G	516/528 (97%)	0.17	7 (1%) 75 81	13, 25, 44, 62	0
1	H	509/528 (96%)	0.09	6 (1%) 79 84	14, 28, 60, 72	0
1	I	518/528 (98%)	0.14	6 (1%) 79 84	15, 26, 52, 64	0
1	J	513/528 (97%)	0.01	5 (0%) 82 87	12, 25, 46, 69	0
1	K	509/528 (96%)	-0.04	2 (0%) 92 96	13, 24, 42, 58	0
1	L	513/528 (97%)	0.25	16 (3%) 49 58	16, 28, 55, 63	0
All	All	6165/6336 (97%)	0.12	113 (1%) 68 75	11, 26, 53, 77	1 (0%)

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	363	GLY	5.7
1	F	362	LYS	5.6
1	B	259	VAL	5.2
1	F	140	GLY	5.1
1	F	156	PHE	4.7

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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
6	1PE	B	62	10/16	0.43	0.51	74,89,91,92	0
6	1PE	J	45	10/16	0.65	0.36	50,68,73,75	0
6	1PE	D	44	11/16	0.79	0.26	37,51,60,63	0
6	1PE	K	4	12/16	0.81	0.21	27,44,55,55	0
6	1PE	D	67	7/16	0.82	0.30	30,41,53,54	0
6	1PE	L	56	11/16	0.83	0.19	30,44,50,50	0
5	SO4	A	2	5/5	0.84	0.19	60,62,74,74	0
6	1PE	L	612	12/16	0.85	0.27	41,59,63,64	0
6	1PE	B	61	10/16	0.86	0.21	34,46,48,51	0
6	1PE	E	43	8/16	0.86	0.21	43,45,55,55	0
6	1PE	F	31	10/16	0.86	0.22	36,44,74,74	0
6	1PE	F	33	10/16	0.86	0.23	33,61,63,64	0
6	1PE	A	20	12/16	0.87	0.21	49,54,58,58	0
6	1PE	E	612	12/16	0.88	0.26	31,46,54,55	0
6	1PE	D	63	10/16	0.88	0.20	37,42,46,53	0
6	1PE	K	42	11/16	0.88	0.16	30,44,49,51	0
6	1PE	K	50	6/16	0.88	0.21	11,25,55,55	0
6	1PE	G	58	15/16	0.88	0.21	43,47,56,56	0
6	1PE	H	64	10/16	0.88	0.24	43,47,52,53	0
6	1PE	J	3	10/16	0.89	0.30	33,50,53,54	0
6	1PE	D	9	10/16	0.90	0.18	27,38,45,48	0
5	SO4	E	22	5/5	0.90	0.36	90,90,94,97	0
6	1PE	H	65	10/16	0.90	0.20	42,49,54,55	0
4	BEY	H	1003	25/25	0.90	0.18	26,38,46,50	0
6	1PE	C	17	13/16	0.90	0.20	15,36,43,43	0
6	1PE	I	66	7/16	0.91	0.17	26,35,44,46	0
6	1PE	B	60	10/16	0.91	0.25	33,48,74,75	0
6	1PE	I	21	15/16	0.91	0.20	25,34,53,54	0
6	1PE	I	22	11/16	0.91	0.21	30,47,62,67	0
4	BEY	L	1003	25/25	0.92	0.20	36,57,69,71	0
6	1PE	K	5	12/16	0.92	0.14	23,35,52,53	0
4	BEY	F	1003	25/25	0.92	0.18	23,35,51,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	1PE	F	32	10/16	0.93	0.14	33,42,45,46	0
4	BEY	D	1003	25/25	0.93	0.17	20,40,59,61	0
5	SO4	G	26	5/5	0.93	0.41	30,30,30,30	0
5	SO4	J	20	5/5	0.93	0.40	72,74,78,81	0
6	1PE	A	19	9/16	0.93	0.14	20,25,34,41	0
6	1PE	E	8	12/16	0.93	0.15	18,34,63,63	0
6	1PE	C	18	9/16	0.93	0.12	27,36,38,45	0
4	BEY	J	1003	25/25	0.93	0.17	28,42,55,57	0
4	BEY	G	1003	25/25	0.94	0.16	13,29,59,61	0
5	SO4	A	24	5/5	0.94	0.16	53,57,63,64	0
5	SO4	D	5	5/5	0.94	0.29	92,94,97,97	0
6	1PE	J	2	11/16	0.94	0.21	12,25,44,48	0
4	BEY	B	1003	25/25	0.94	0.16	26,38,48,50	0
4	BEY	I	1003	25/25	0.94	0.17	21,33,40,50	0
4	BEY	E	1003	25/25	0.94	0.17	22,42,59,61	0
6	1PE	G	12	9/16	0.94	0.13	20,25,41,44	0
6	1PE	G	30	7/16	0.94	0.17	24,39,53,57	0
5	SO4	L	25	5/5	0.94	0.14	68,71,75,76	0
4	BEY	C	1003	25/25	0.94	0.17	16,33,43,47	0
5	SO4	A	1	5/5	0.94	0.18	61,62,66,66	0
4	BEY	A	1003	25/25	0.95	0.19	17,33,63,65	0
4	BEY	K	1003	25/25	0.95	0.18	19,30,45,54	0
6	1PE	G	48	6/16	0.95	0.16	16,22,26,26	0
2	CO3	A	1002	4/4	0.95	0.17	39,42,43,46	0
6	1PE	L	1	10/16	0.95	0.13	15,23,33,35	0
2	CO3	K	1002	4/4	0.95	0.17	25,30,31,37	0
5	SO4	F	21	5/5	0.95	0.15	69,70,71,75	0
2	CO3	C	1002	4/4	0.96	0.15	13,21,22,28	0
3	ZN	K	1004	1/1	0.96	0.04	39,39,39,39	0
6	1PE	G	47	6/16	0.96	0.29	15,22,28,39	0
2	CO3	E	1002	4/4	0.96	0.16	31,33,34,34	0
2	CO3	H	1002	4/4	0.96	0.17	15,23,23,28	0
2	CO3	B	1002	4/4	0.97	0.18	11,14,16,19	0
2	CO3	L	1002	4/4	0.97	0.18	27,27,28,33	0
3	ZN	B	1004	1/1	0.97	0.05	36,36,36,36	0
5	SO4	G	23	5/5	0.97	0.20	45,45,49,50	0
3	ZN	C	1004	1/1	0.97	0.05	42,42,42,42	0
3	ZN	D	1001	1/1	0.97	0.05	41,41,41,41	0
5	SO4	K	19	5/5	0.97	0.32	71,71,76,77	0
2	CO3	G	1002	4/4	0.97	0.16	19,20,22,26	0
2	CO3	D	1002	4/4	0.97	0.14	22,24,25,27	0
3	ZN	H	1004	1/1	0.98	0.04	32,32,32,32	0

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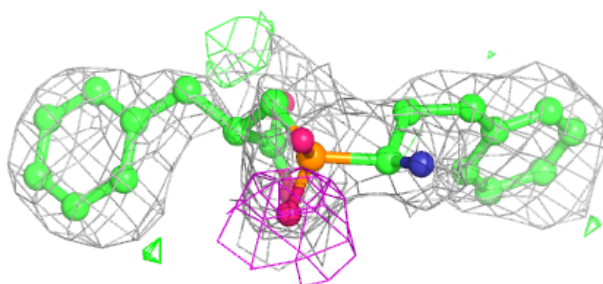
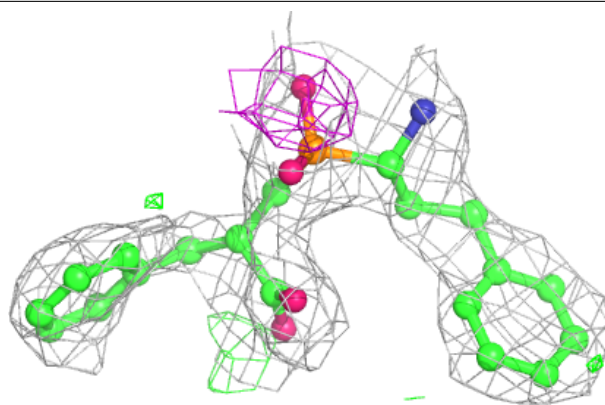
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	J	1001	1/1	0.98	0.06	39,39,39,39	0
2	CO3	J	1002	4/4	0.98	0.18	27,27,29,31	0
2	CO3	F	1002	4/4	0.98	0.18	35,38,39,44	0
2	CO3	I	1002	4/4	0.98	0.12	18,19,22,23	0
3	ZN	E	1004	1/1	0.98	0.04	45,45,45,45	0
3	ZN	G	1004	1/1	0.98	0.08	35,35,35,35	0
3	ZN	J	1004	1/1	0.99	0.05	46,46,46,46	0
3	ZN	D	1004	1/1	0.99	0.06	39,39,39,39	0
3	ZN	L	1001	1/1	0.99	0.08	29,29,29,29	0
3	ZN	L	1004	1/1	0.99	0.05	39,39,39,39	0
3	ZN	E	1001	1/1	0.99	0.07	30,30,30,30	0
5	SO4	C	3	5/5	0.99	0.14	17,18,25,26	0
3	ZN	B	1001	1/1	0.99	0.06	35,35,35,35	0
5	SO4	E	7	5/5	0.99	0.12	16,24,35,37	0
3	ZN	F	1001	1/1	0.99	0.08	29,29,29,29	0
3	ZN	F	1004	1/1	0.99	0.04	37,37,37,37	0
3	ZN	C	1001	1/1	0.99	0.07	26,26,26,26	0
3	ZN	H	1001	1/1	0.99	0.07	39,39,39,39	0
5	SO4	I	17	5/5	0.99	0.10	8,10,15,22	0
5	SO4	J	18	5/5	0.99	0.16	22,28,36,37	0
3	ZN	A	1001	1/1	0.99	0.07	30,30,30,30	0
3	ZN	I	1004	1/1	0.99	0.06	35,35,35,35	0
3	ZN	I	1001	1/1	0.99	0.08	26,26,26,26	0
3	ZN	A	1004	1/1	0.99	0.06	37,37,37,37	0
3	ZN	K	1001	1/1	1.00	0.05	23,23,23,23	0
3	ZN	G	1001	1/1	1.00	0.06	28,28,28,28	0

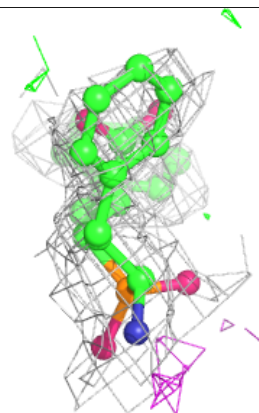
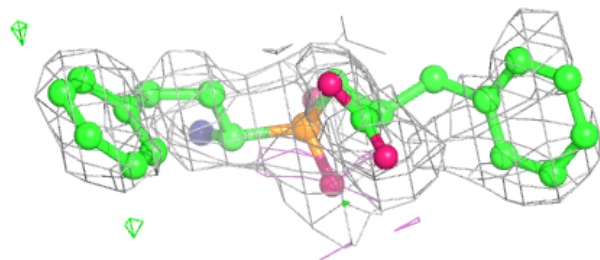
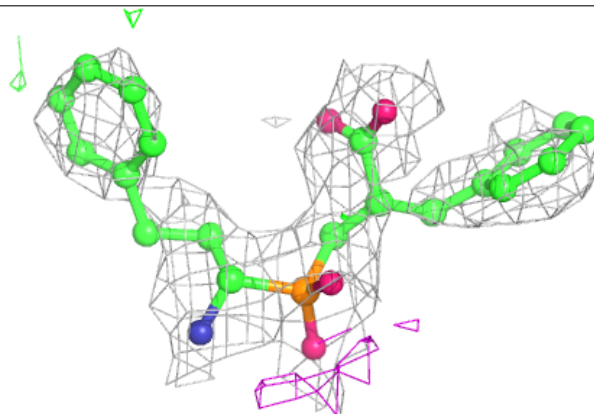
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BEY H 1003:**

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

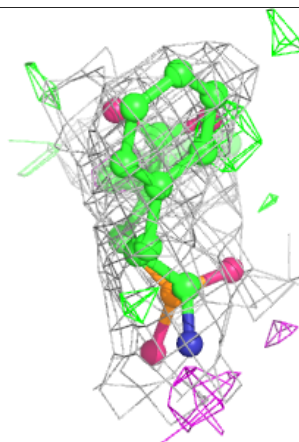
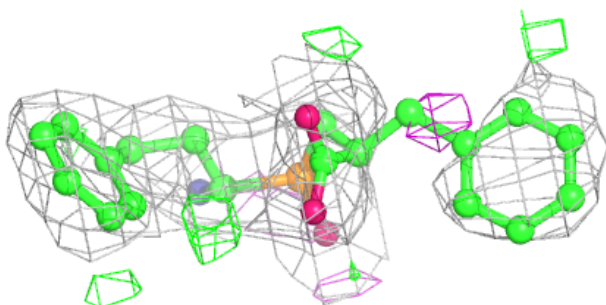
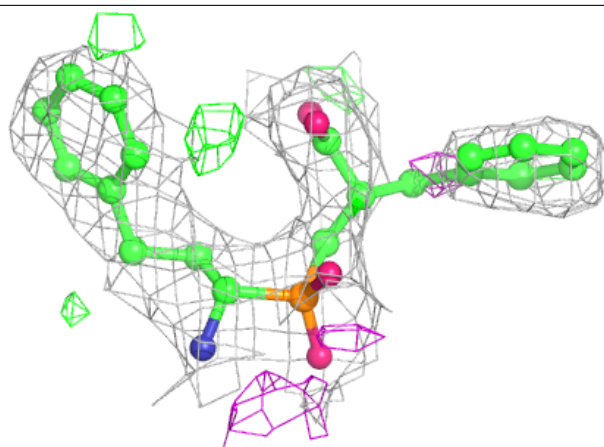
**Electron density around BEY L 1003:**

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

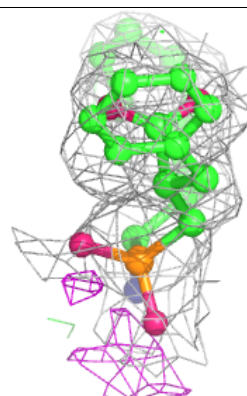
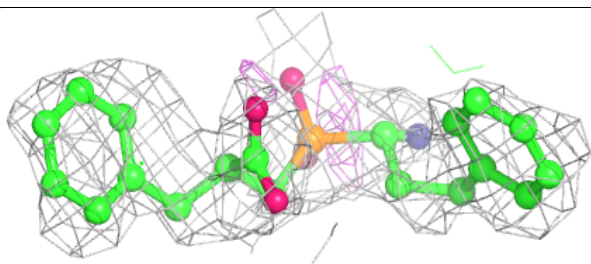
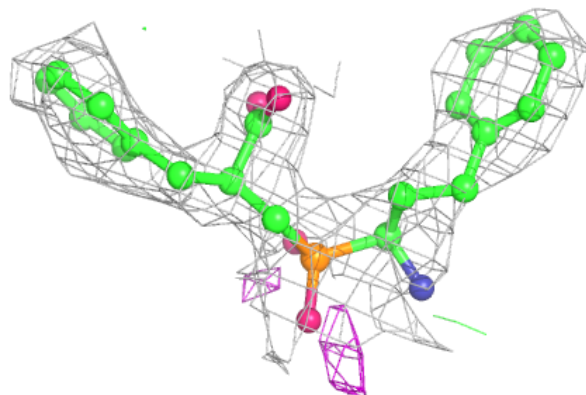


**Electron density around BEY F 1003:**

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

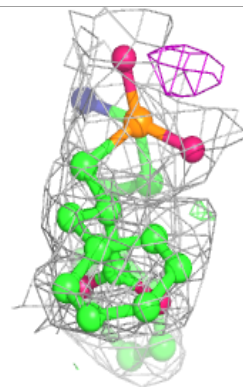
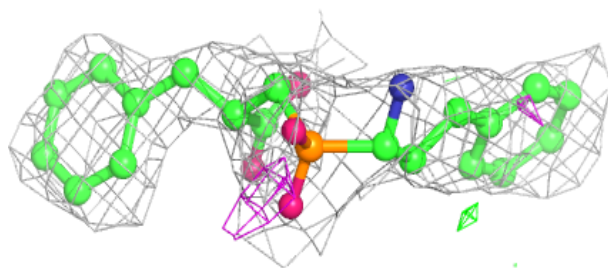
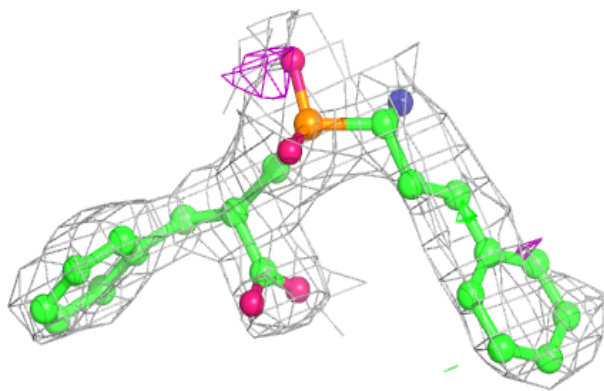
**Electron density around BEY D 1003:**

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

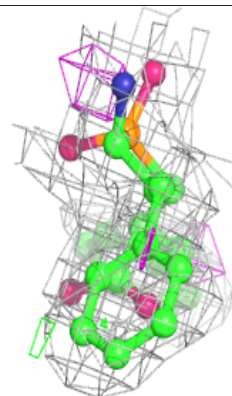
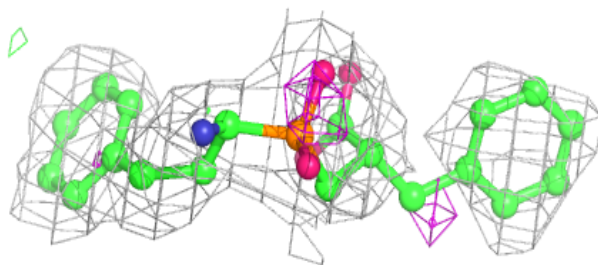
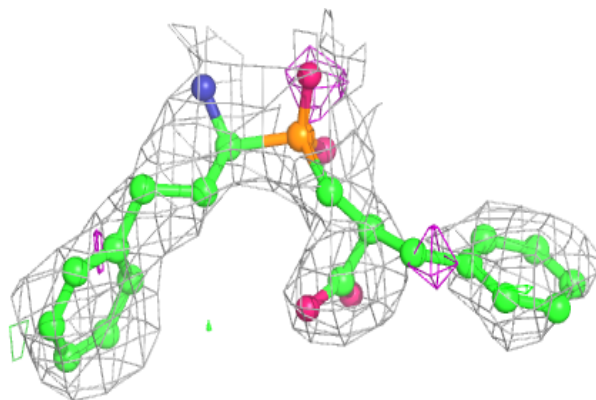


**Electron density around BEY J 1003:**

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

**Electron density around BEY G 1003:**

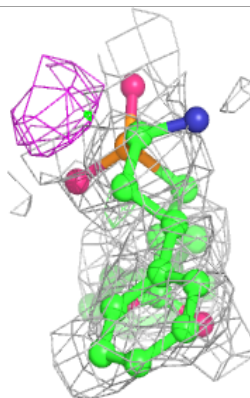
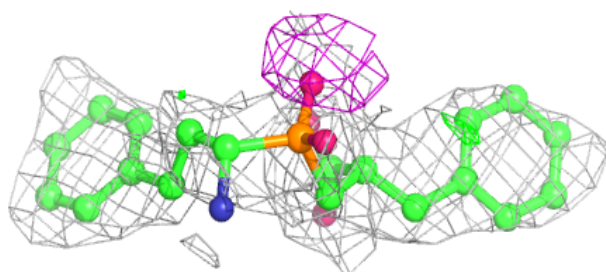
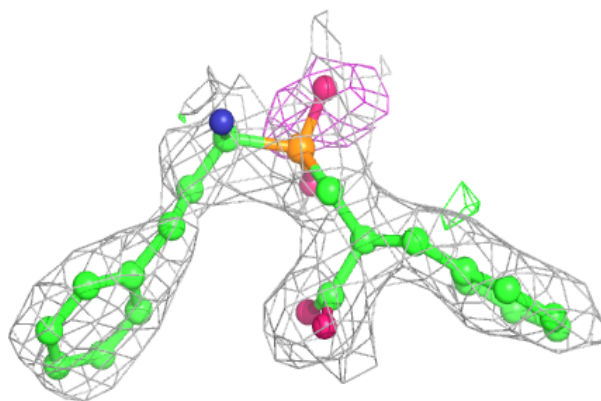
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



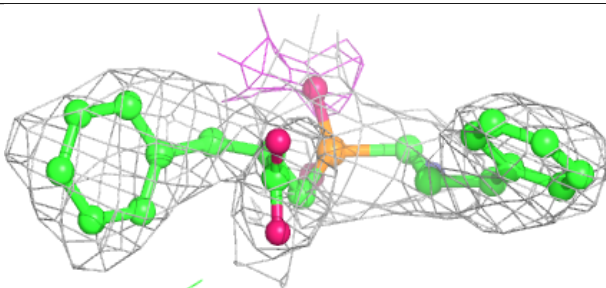
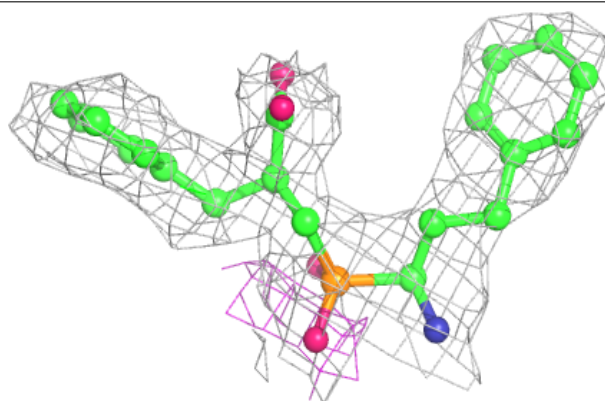


**Electron density around BEY B 1003:**

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

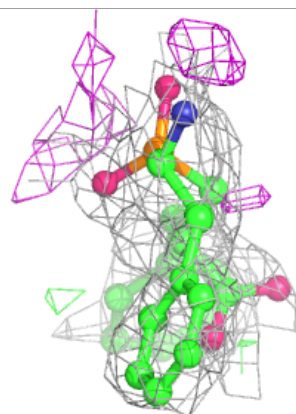
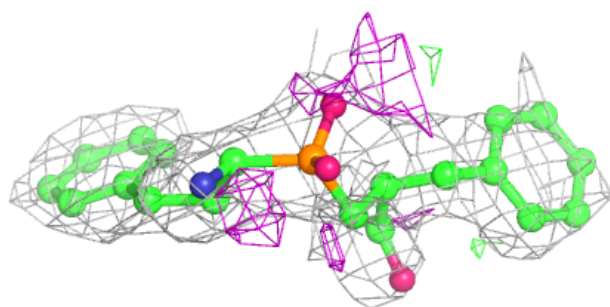
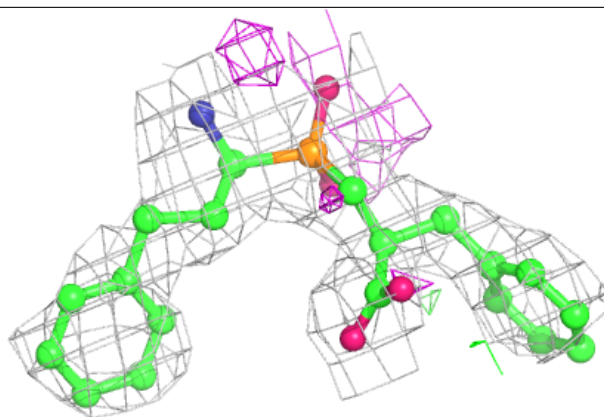
**Electron density around BEY I 1003:**

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

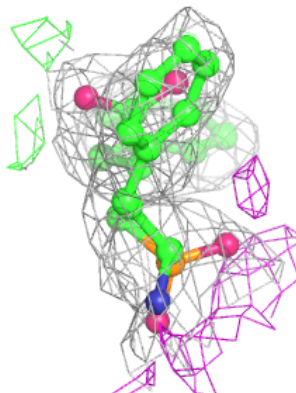
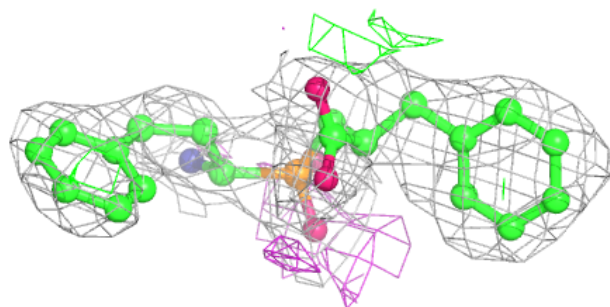
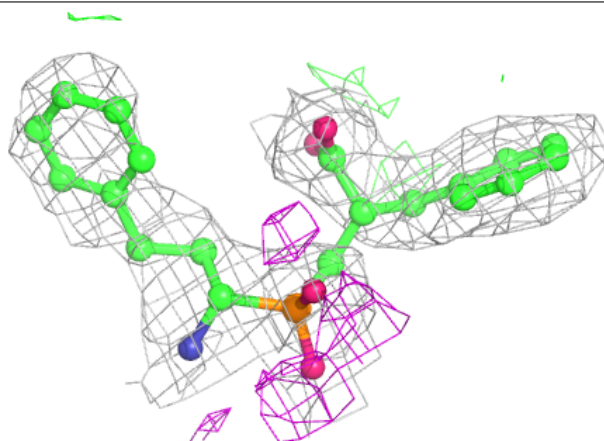


**Electron density around BEY E 1003:**

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

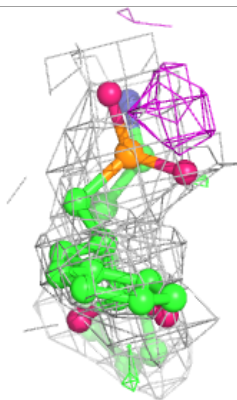
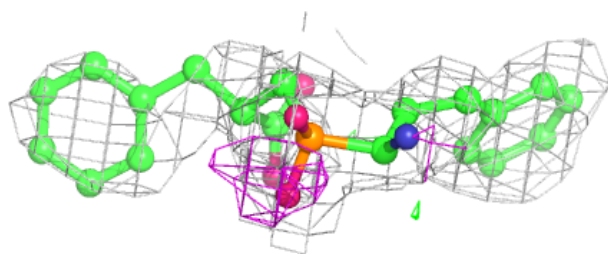
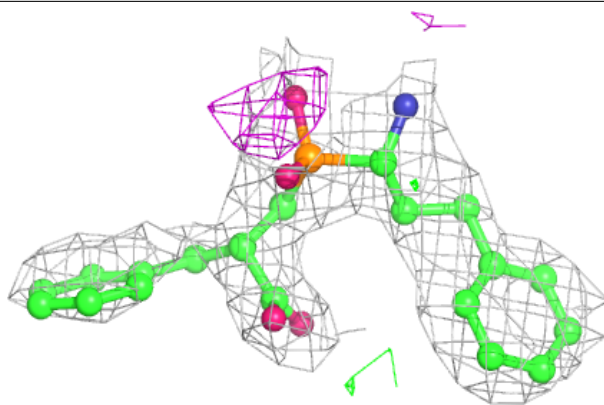
**Electron density around BEY C 1003:**

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

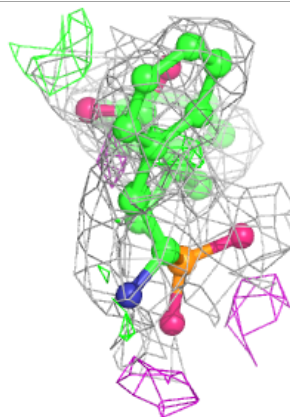
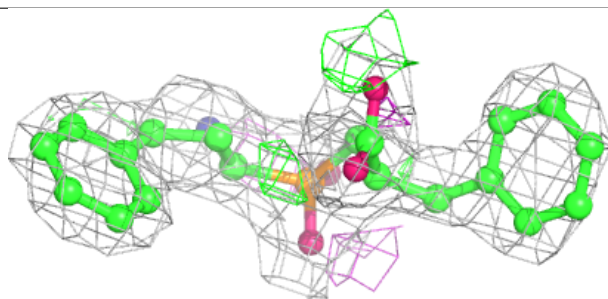
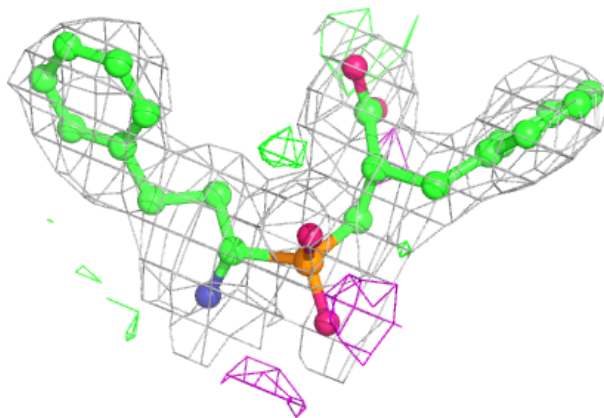


**Electron density around BEY A 1003:**

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

**Electron density around BEY K 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.