WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2023 – 05:15 AM EDT

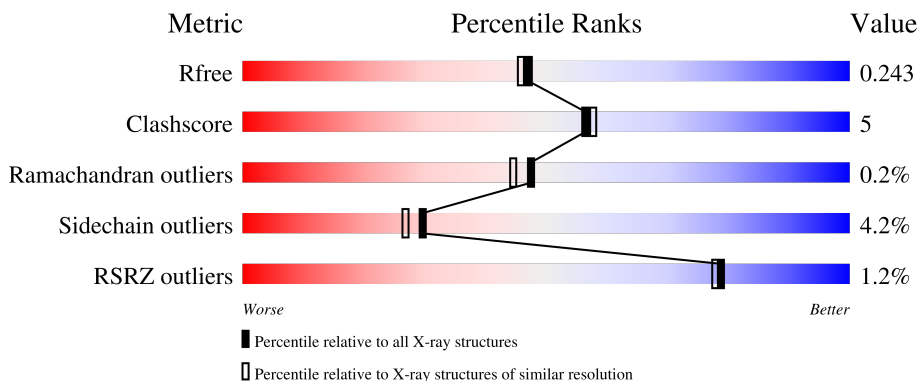|		
PDB ID	:	3KR4
Title	:	Structure of a protease 3
Authors	:	McGowan, S.; Whisstock, J.C.
Deposited on	:	2009-11-17
Resolution	:	2.00 Å(reported)

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		4.2%
RSRZ outliers		1.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	% 91% 7% ·
1	B	528	3% 86% 11% · ·
1	C	528	% 86% 11% · ·
1	D	528	% 86% 9% · ·
1	E	528	% 84% 10% · ·

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Mol	Chain	Length	Quality of chain
1	F	528	%　83%　　　13%　· ·
1	G	528	%　88%　　　9%　· ·
1	H	528	2%　85%　　　9%　· ·
1	I	528	86%　　　10%　· ·
1	J	528	%　86%　　　9%　· ·
1	K	528	%　87%　　　8%　· ·
1	L	528	%　86%　　　10%　· ·

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 (i)

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

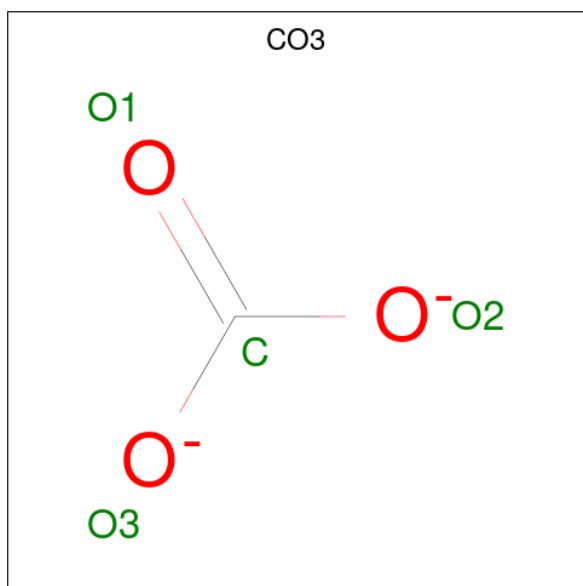*Continued on next page...*

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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_3).

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 4	C 1	O 3	0	0
2	D	1	Total 4	C 1	O 3	0	0
2	E	1	Total 4	C 1	O 3	0	0
2	F	1	Total 4	C 1	O 3	0	0
2	G	1	Total 4	C 1	O 3	0	0
2	H	1	Total 4	C 1	O 3	0	0
2	I	1	Total 4	C 1	O 3	0	0
2	J	1	Total 4	C 1	O 3	0	0
2	K	1	Total 4	C 1	O 3	0	0
2	L	1	Total 4	C 1	O 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 4 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: $C_{16}H_{24}N_2O_4$).
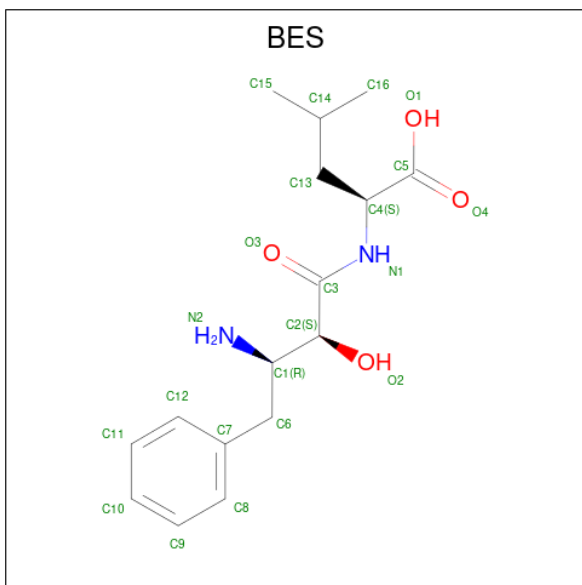
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 22	C 16	N 2	O 4	0	0
4	B	1	Total 22	C 16	N 2	O 4	0	0
4	C	1	Total 22	C 16	N 2	O 4	0	0
4	D	1	Total 22	C 16	N 2	O 4	0	0
4	E	1	Total 22	C 16	N 2	O 4	0	0
4	F	1	Total 22	C 16	N 2	O 4	0	0
4	G	1	Total 22	C 16	N 2	O 4	0	0
4	H	1	Total 22	C 16	N 2	O 4	0	0

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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 (three-letter code: 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 (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
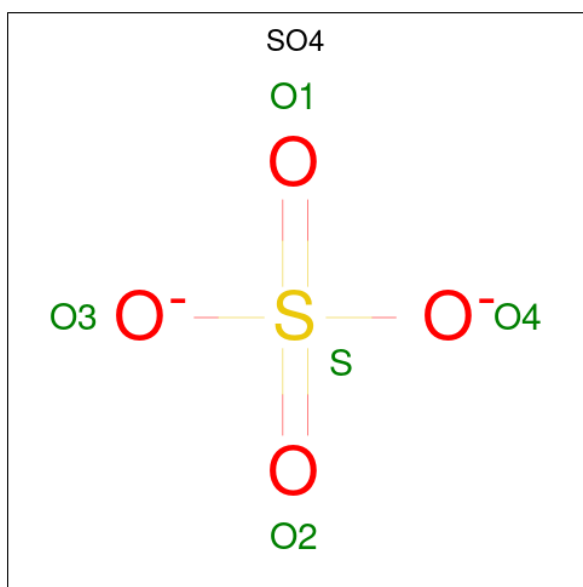
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	E	1	Total 5	O 4	S 1	0	0
6	F	1	Total 5	O 4	S 1	0	0
6	G	1	Total 5	O 4	S 1	0	0
6	G	1	Total 5	O 4	S 1	0	0
6	J	1	Total 5	O 4	S 1	0	0
6	J	1	Total 5	O 4	S 1	0	0
6	K	1	Total 5	O 4	S 1	0	0
6	L	1	Total 5	O 4	S 1	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
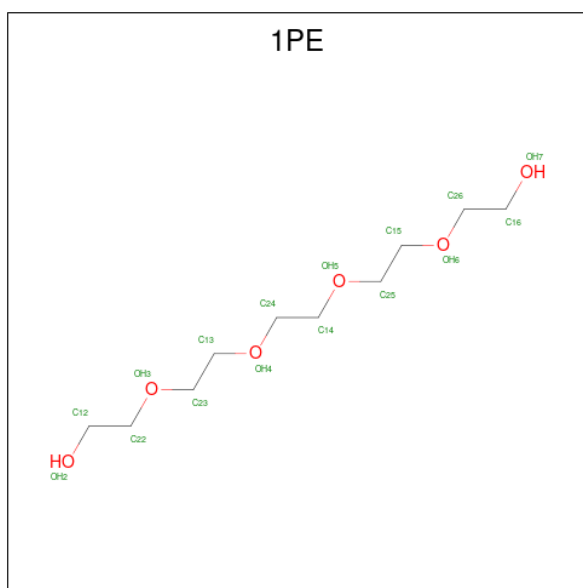
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 9	C 6	O 3	0	0
7	A	1	Total 12	C 8	O 4	0	0
7	B	1	Total 10	C 7	O 3	0	0
7	B	1	Total 10	C 7	O 3	0	0
7	B	1	Total 10	C 7	O 3	0	0
7	C	1	Total 13	C 9	O 4	0	0
7	C	1	Total 9	C 6	O 3	0	0
7	D	1	Total 10	C 7	O 3	0	0
7	D	1	Total 11	C 8	O 3	0	0
7	D	1	Total 10	C 7	O 3	0	0
7	D	1	Total 7	C 5	O 2	0	0
7	E	1	Total 12	C 8	O 4	0	0
7	E	1	Total 12	C 8	O 4	0	0

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

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

- Molecule 8 is water.

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

3 Residue-property plots ⓘ

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.
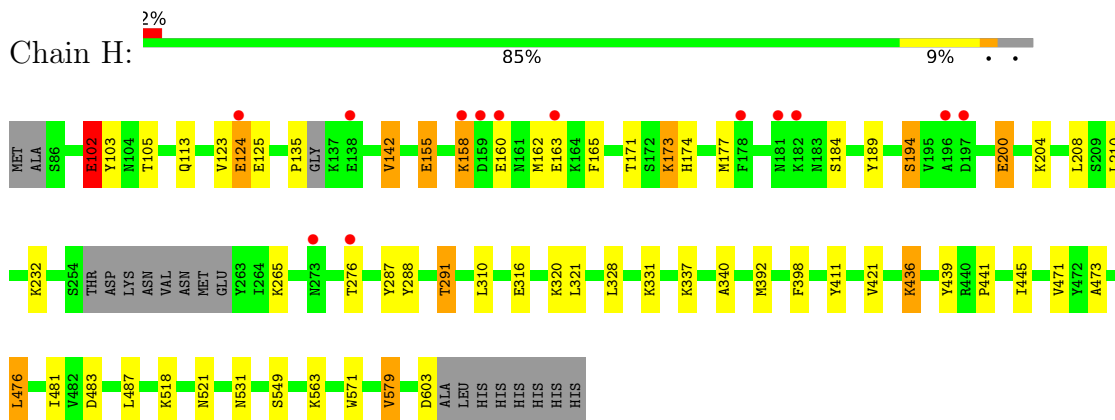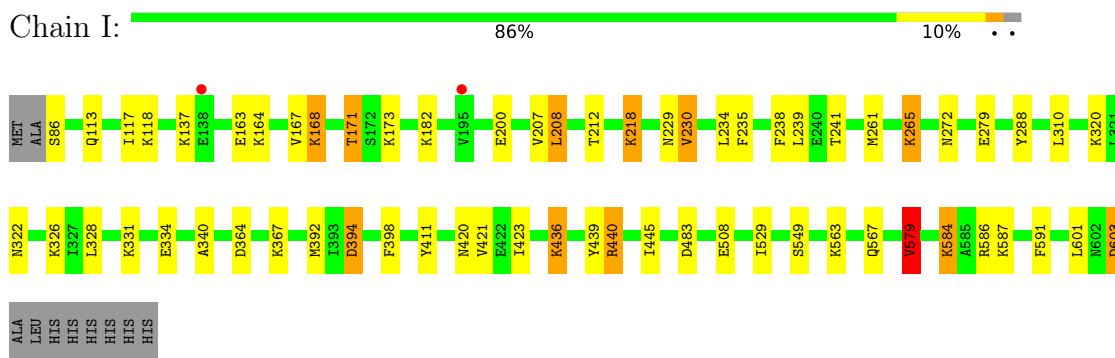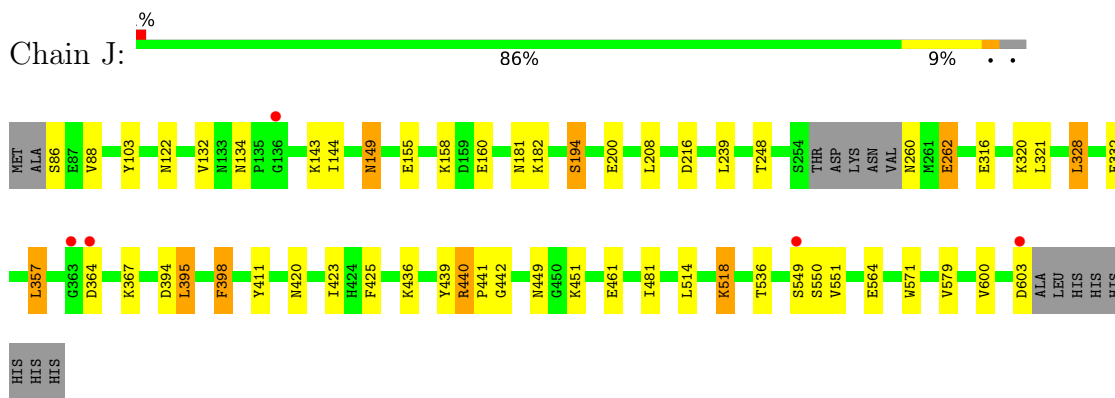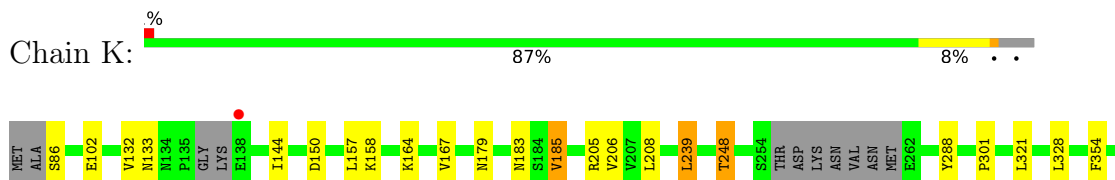
- Molecule 1: M17 leucyl aminopeptidase
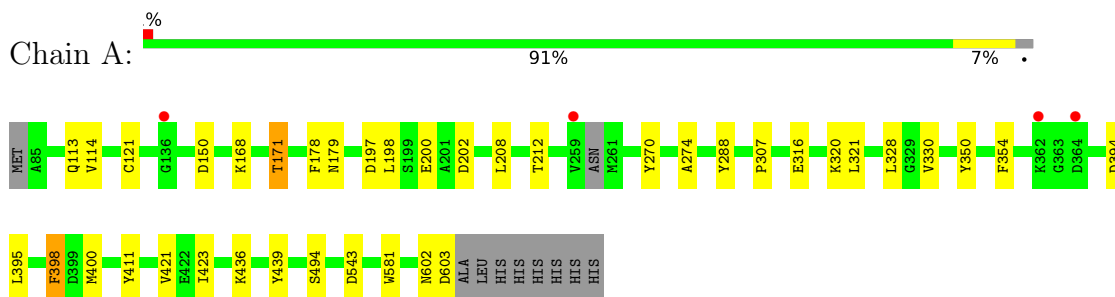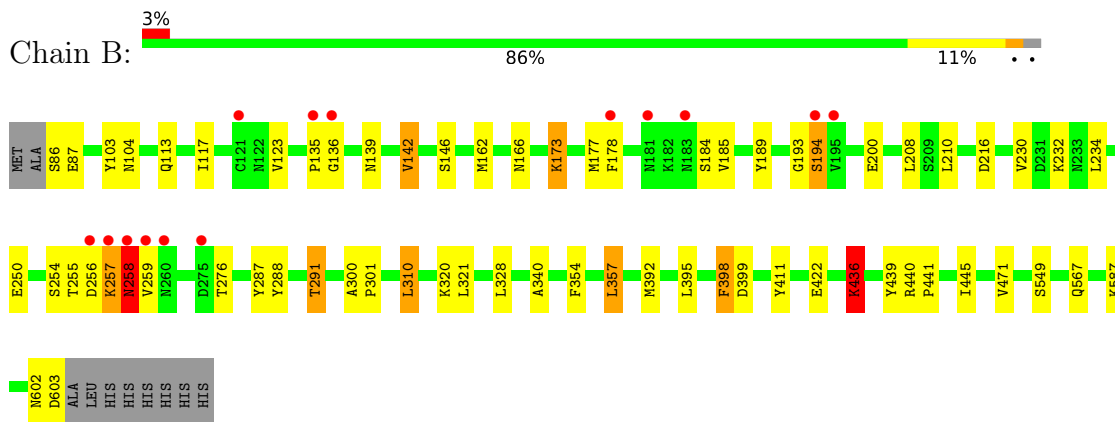
- Molecule 1: M17 leucyl aminopeptidase

- Molecule 1: M17 leucyl aminopeptidase

- Molecule 1: M17 leucyl aminopeptidase

Chain D:

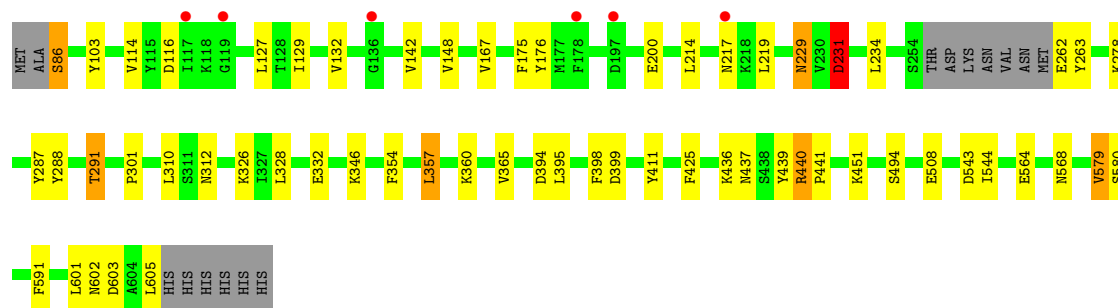• Molecule 1: M17 leucyl aminopeptidase

Chain E:

• Molecule 1: M17 leucyl aminopeptidase

Chain F:

• Molecule 1: M17 leucyl aminopeptidase

Chain G:

HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain H:

• Molecule 1: M17 leucyl aminopeptidase

Chain I:

• Molecule 1: M17 leucyl aminopeptidase

Chain J:

• Molecule 1: M17 leucyl aminopeptidase

Chain K:

G363 D364 M392 I393 D394 L395 F398 D399 Y411 N420 I423 K436 Y439 R440 P441 G442 L487 T536 I544 S549 S550 V551 E564 V579 S580 W581 K589 T597 V600 L601 N602 D603 ALA LEU HIS HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain L:

%

86%　　　　　　　10%

MET ALA S86 Y103 V114 Y115 D116 I117 K118 G119 L127 T128 I129 V132 G136 V142 V148 V167 F175 Y176 M177 F178 D197 E200 L214 N217 K218 L219 N229 V230 D231 L234 S254 THR ASP LYS ASN VAL ASN MET E262 Y263 K278

Y287 Y288 T291 P301 L310 S311 N312 K326 I327 L328 E332 K346 F354 L357 K360 V365 D394 L395 F398 D399 Y411 F425 K436 N437 S438 Y439 R440 P441 K451 S494 E508 D543 I544 E564 N568 V579 S580

F591 L601 N602 D603 A604 L605 HIS HIS HIS HIS HIS
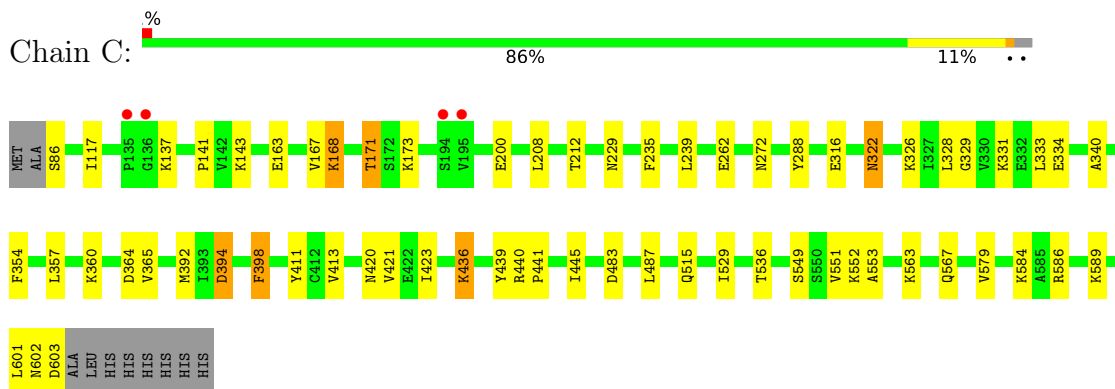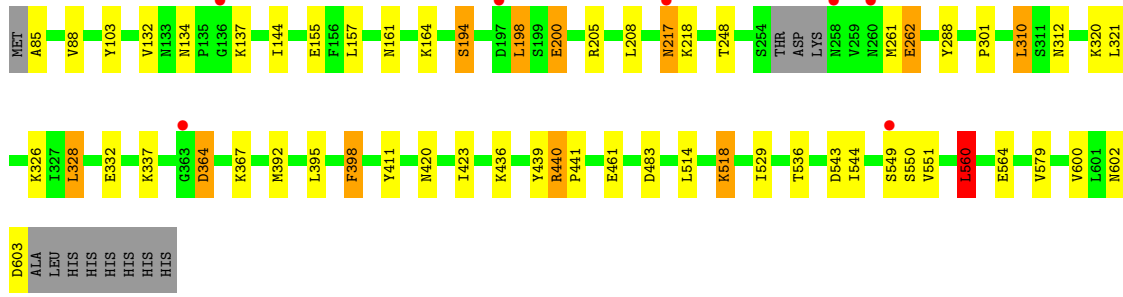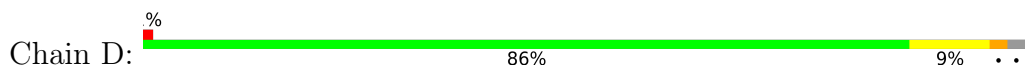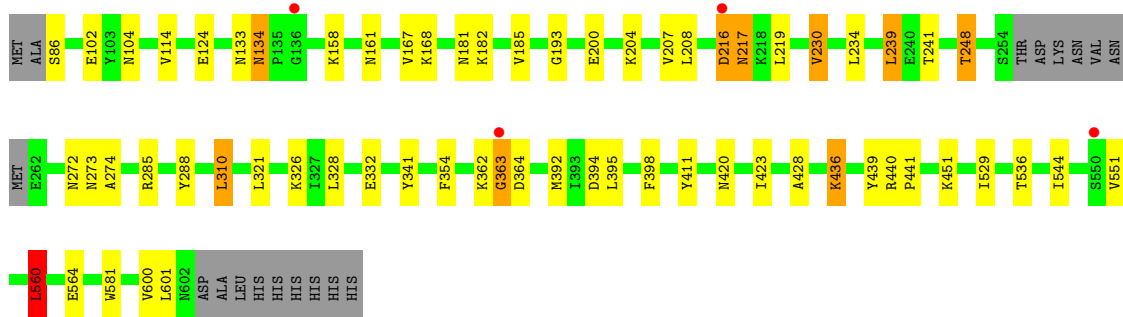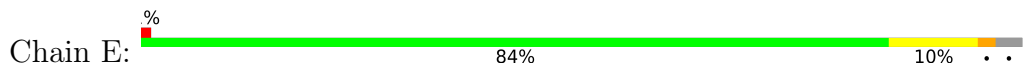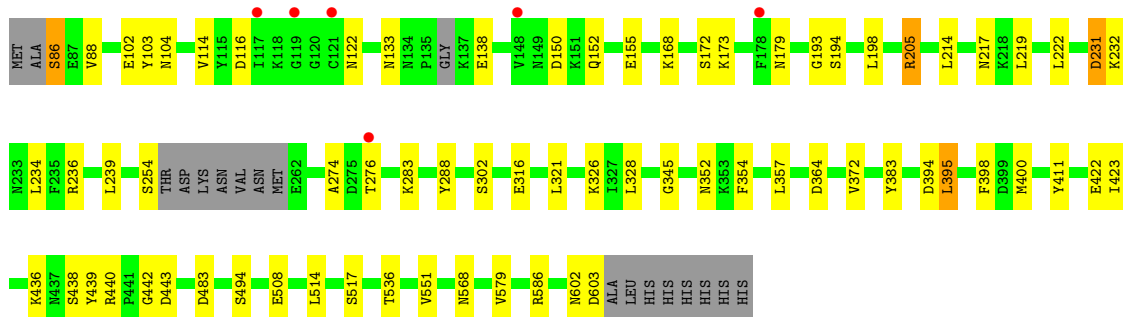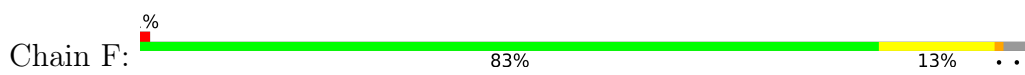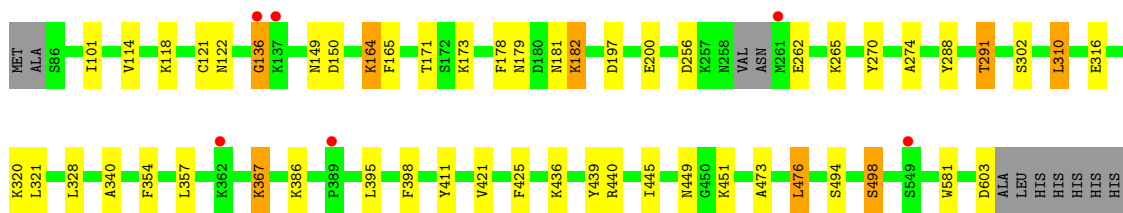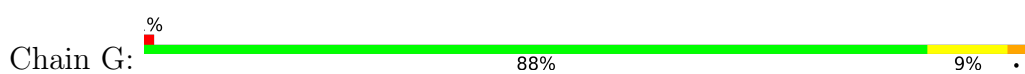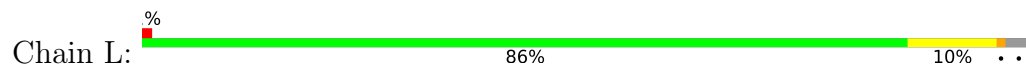
4 Data and refinement statistics ⓘ

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 43.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.15-2.00) 98.3 (43.13-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.192 , 0.242 0.196 , 0.243	Depositor DCC
R_{free} test set	23578 reflections (5.03%)	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 , 53.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, BES, ZN, MG, SO4, 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	0.85	0/4063	0.76	0/5508
1	B	0.81	2/4014 (0.0%)	0.79	8/5450 (0.1%)
1	C	0.84	0/4036	0.80	4/5477 (0.1%)
1	D	0.84	0/4023	0.81	8/5454 (0.1%)
1	E	0.86	0/3973	0.83	9/5392 (0.2%)
1	F	0.83	0/3949	0.81	5/5364 (0.1%)
1	G	0.86	2/4073 (0.0%)	0.77	6/5513 (0.1%)
1	H	0.80	2/4022 (0.0%)	0.78	3/5445 (0.1%)
1	I	0.84	0/4089	0.83	6/5539 (0.1%)
1	J	0.86	0/4043	0.81	4/5476 (0.1%)
1	K	0.87	2/4014 (0.0%)	0.83	7/5438 (0.1%)
1	L	0.85	0/4024	0.81	4/5460 (0.1%)
All	All	0.84	8/48323 (0.0%)	0.80	64/65516 (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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	262	GLU	CB-CG	-5.83	1.41	1.52
1	K	206	VAL	CB-CG2	-5.61	1.41	1.52
1	B	422	GLU	CD-OE1	-5.53	1.19	1.25
1	K	206	VAL	CB-CG1	-5.39	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	421	VAL	CB-CG2	-5.33	1.41	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	440	ARG	NE-CZ-NH2	-15.18	112.71	120.30
1	I	440	ARG	NE-CZ-NH2	-13.93	113.34	120.30
1	B	440	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	L	440	ARG	NE-CZ-NH2	-12.05	114.28	120.30
1	F	440	ARG	NE-CZ-NH2	-11.99	114.31	120.30

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   ⓘ

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	25	0
1	B	3936	0	3843	51	0
1	C	3955	0	3881	36	0
1	D	3946	0	3888	45	0
1	E	3896	0	3819	50	0
1	F	3873	0	3771	46	0
1	G	3996	0	3988	36	0
1	H	3943	0	3937	37	0
1	I	4008	0	3985	38	0
1	J	3963	0	3940	49	0
1	K	3935	0	3907	39	0
1	L	3944	0	3874	44	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
4	D	22	0	22	3	0
4	E	22	0	22	3	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	3	0
4	J	22	0	22	2	0
4	K	22	0	22	4	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
7	C	22	0	24	5	0
7	D	38	0	38	6	0
7	E	32	0	36	4	0
7	F	30	0	39	3	0
7	G	43	0	47	7	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	9	0
8	C	427	0	0	9	0
8	D	411	0	0	12	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	482	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.

The worst 5 of 482 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

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%)	25	19
1	C	517/528 (98%)	509 (98%)	8 (2%)	0	100	100
1	D	512/528 (97%)	492 (96%)	18 (4%)	2 (0%)	34	30
1	E	506/528 (96%)	493 (97%)	10 (2%)	3 (1%)	25	19
1	F	504/528 (96%)	487 (97%)	17 (3%)	0	100	100
1	G	512/528 (97%)	500 (98%)	11 (2%)	1 (0%)	47	44
1	H	504/528 (96%)	493 (98%)	10 (2%)	1 (0%)	47	44
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%)	47	44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	124	GLU

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Mol	Chain	Res	Type
1	B	136	GLY
1	B	258	ASN
1	B	259	VAL
1	E	362	LYS

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%)	50	53
1	B	414/455 (91%)	395 (95%)	19 (5%)	27	23
1	C	419/455 (92%)	401 (96%)	18 (4%)	29	26
1	D	418/455 (92%)	397 (95%)	21 (5%)	24	20
1	E	413/455 (91%)	398 (96%)	15 (4%)	35	34
1	F	409/455 (90%)	391 (96%)	18 (4%)	28	25
1	G	437/455 (96%)	422 (97%)	15 (3%)	37	36
1	H	431/455 (95%)	409 (95%)	22 (5%)	24	19
1	I	437/455 (96%)	411 (94%)	26 (6%)	19	15
1	J	432/455 (95%)	415 (96%)	17 (4%)	32	30
1	K	428/455 (94%)	415 (97%)	13 (3%)	41	41
1	L	424/455 (93%)	404 (95%)	20 (5%)	26	22
All	All	5089/5460 (93%)	4875 (96%)	214 (4%)	30	27

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	603	ASP
1	I	173	LYS
1	L	229	ASN
1	H	155	GLU
1	H	398	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	113	GLN
1	L	181	ASN
1	L	217	ASN
1	L	215	HIS
1	G	149	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 monosaccharides 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	$\#|Z| > 2$
7	1PE	B	60	-	9,9,15	0.44	0	8,8,14	0.56	0
6	SO4	G	23	-	4,4,4	0.20	0	6,6,6	0.31	0
4	BES	J	1003	5,3	22,22,22	0.92	1 (4%)	27,29,29	1.63	5 (18%)
7	1PE	G	48	-	5,5,15	0.64	0	4,4,14	0.80	0
7	1PE	J	45	-	9,9,15	0.52	0	8,8,14	0.36	0
7	1PE	L	1	-	9,9,15	0.31	0	8,8,14	0.53	0
7	1PE	C	18	-	8,8,15	0.54	0	7,7,14	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert>2$	Counts	RMSZ	$\#\lvert Z\rvert>2$
7	1PE	F	33	-	9,9,15	0.54	0	8,8,14	0.32	0
2	CO3	C	1002	-	2,3,3	0.62	0	2,3,3	1.17	0
6	SO4	A	24	-	4,4,4	0.17	0	6,6,6	0.15	0
7	1PE	E	43	-	7,7,15	0.53	0	6,6,14	0.29	0
7	1PE	I	66	-	6,6,15	0.60	0	5,5,14	0.33	0
7	1PE	K	5	-	11,11,15	0.44	0	10,10,14	0.64	0
4	BES	L	1003	5,3	22,22,22	0.75	0	27,29,29	1.49	6 (22%)
7	1PE	I	21	-	14,14,15	0.66	0	13,13,14	0.76	0
2	CO3	E	1002	-	2,3,3	0.39	0	2,3,3	0.92	0
7	1PE	J	3	-	9,9,15	0.54	0	8,8,14	0.50	0
2	CO3	G	1002	-	2,3,3	0.61	0	2,3,3	0.77	0
7	1PE	L	56	-	10,10,15	0.56	0	9,9,14	0.28	0
4	BES	F	1003	5,3	22,22,22	0.76	0	27,29,29	1.57	5 (18%)
7	1PE	H	64	-	9,9,15	0.52	0	8,8,14	0.56	0
2	CO3	K	1002	-	2,3,3	0.51	0	2,3,3	0.90	0
7	1PE	G	47	-	5,5,15	0.51	0	4,4,14	0.51	0
6	SO4	G	17	-	4,4,4	0.08	0	6,6,6	0.37	0
7	1PE	D	9	-	9,9,15	0.47	0	8,8,14	0.29	0
7	1PE	D	63	-	9,9,15	0.74	0	8,8,14	0.80	0
7	1PE	I	22	-	10,10,15	0.49	0	9,9,14	0.34	0
4	BES	D	1003	5,3	22,22,22	0.79	0	27,29,29	1.12	3 (11%)
7	1PE	G	58	-	14,14,15	0.71	0	13,13,14	0.54	0
6	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.34	0
7	1PE	A	19	-	8,8,15	0.51	0	7,7,14	0.25	0
7	1PE	B	61	-	9,9,15	0.64	0	8,8,14	0.83	0
6	SO4	K	19	-	4,4,4	0.24	0	6,6,6	0.22	0
4	BES	C	1003	5,3	22,22,22	0.88	0	27,29,29	1.41	2 (7%)
7	1PE	B	62	-	9,9,15	0.61	0	8,8,14	0.41	0
4	BES	E	1003	5,3	22,22,22	0.85	1 (4%)	27,29,29	1.37	2 (7%)
7	1PE	C	17	-	12,12,15	0.56	0	11,11,14	0.49	0
7	1PE	G	30	-	6,6,15	0.48	0	5,5,14	0.32	0
7	1PE	H	65	-	9,9,15	0.64	0	8,8,14	0.73	0
4	BES	K	1003	5,3	22,22,22	0.89	0	27,29,29	1.56	4 (14%)
7	1PE	K	4	-	11,11,15	0.57	0	10,10,14	0.38	0
4	BES	G	1003	5,3	22,22,22	0.94	2 (9%)	27,29,29	1.61	2 (7%)
2	CO3	J	1002	-	2,3,3	0.51	0	2,3,3	1.61	0
4	BES	A	1003	5,3	22,22,22	0.83	0	27,29,29	1.55	4 (14%)
2	CO3	H	1002	-	2,3,3	0.26	0	2,3,3	1.22	0
4	BES	H	1003	5,3	22,22,22	0.75	0	27,29,29	1.41	4 (14%)
2	CO3	A	1002	-	2,3,3	0.13	0	2,3,3	1.36	0
2	CO3	I	1002	-	2,3,3	0.67	0	2,3,3	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	BES	I	1003	5,3	22,22,22	0.92	0	27,29,29	1.65	6 (22%)
7	1PE	E	7	-	11,11,15	0.54	0	10,10,14	0.44	0
6	SO4	D	7	-	4,4,4	0.34	0	6,6,6	0.54	0
6	SO4	F	21	-	4,4,4	0.17	0	6,6,6	0.24	0
7	1PE	F	32	-	9,9,15	0.57	0	8,8,14	0.39	0
4	BES	B	1003	5,3	22,22,22	0.71	0	27,29,29	1.66	9 (33%)
7	1PE	K	42	-	10,10,15	0.58	0	9,9,14	0.41	0
6	SO4	E	22	-	4,4,4	0.18	0	6,6,6	0.25	0
6	SO4	J	20	-	4,4,4	0.11	0	6,6,6	0.22	0
7	1PE	A	20	-	11,11,15	0.61	0	10,10,14	0.53	0
7	1PE	G	12	-	8,8,15	0.57	0	7,7,14	0.37	0
7	1PE	K	50	-	5,5,15	0.60	0	4,4,14	0.31	0
2	CO3	F	1002	-	2,3,3	0.74	0	2,3,3	1.58	0
2	CO3	L	1002	-	2,3,3	0.36	0	2,3,3	1.30	0
6	SO4	D	5	-	4,4,4	0.18	0	6,6,6	0.25	0
7	1PE	L	612	-	11,11,15	0.45	0	10,10,14	0.51	0
7	1PE	D	44	-	10,10,15	0.72	0	9,9,14	0.66	0
7	1PE	F	31	-	9,9,15	0.36	0	8,8,14	0.62	0
6	SO4	L	25	-	4,4,4	0.24	0	6,6,6	0.34	0
7	1PE	J	2	-	10,10,15	0.41	0	9,9,14	0.58	0
6	SO4	J	18	-	4,4,4	0.35	0	6,6,6	0.62	0
7	1PE	D	67	-	6,6,15	0.50	0	5,5,14	0.28	0
6	SO4	B	3	-	4,4,4	0.32	0	6,6,6	0.43	0
2	CO3	B	1002	-	2,3,3	0.53	0	2,3,3	2.21	2 (100%)
2	CO3	D	1002	-	2,3,3	0.72	0	2,3,3	1.64	1 (50%)
6	SO4	A	2	-	4,4,4	0.20	0	6,6,6	0.28	0
7	1PE	E	8	-	11,11,15	0.39	0	10,10,14	0.53	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	B	60	-	-	3/7/7/13	-
7	1PE	L	1	-	-	5/7/7/13	-
4	BES	J	1003	5,3	-	5/24/24/24	0/1/1/1
7	1PE	G	48	-	-	2/3/3/13	-
7	1PE	J	45	-	-	4/7/7/13	-
7	1PE	C	18	-	-	4/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	F	33	-	-	4/7/7/13	-
7	1PE	K	5	-	-	2/9/9/13	-
7	1PE	E	43	-	-	2/5/5/13	-
4	BES	L	1003	5,3	-	5/24/24/24	0/1/1/1
7	1PE	I	21	-	-	4/12/12/13	-
7	1PE	J	3	-	-	4/7/7/13	-
7	1PE	L	56	-	-	1/8/8/13	-
4	BES	F	1003	5,3	-	10/24/24/24	0/1/1/1
7	1PE	H	64	-	-	2/7/7/13	-
7	1PE	G	47	-	-	3/3/3/13	-
7	1PE	D	9	-	-	6/7/7/13	-
7	1PE	D	63	-	-	3/7/7/13	-
7	1PE	I	22	-	-	5/8/8/13	-
4	BES	D	1003	5,3	-	5/24/24/24	0/1/1/1
7	1PE	G	58	-	-	5/12/12/13	-
7	1PE	A	19	-	-	2/6/6/13	-
7	1PE	B	61	-	-	7/7/7/13	-
4	BES	C	1003	5,3	-	6/24/24/24	0/1/1/1
7	1PE	B	62	-	-	1/7/7/13	-
4	BES	E	1003	5,3	-	6/24/24/24	0/1/1/1
7	1PE	C	17	-	-	2/10/10/13	-
7	1PE	G	30	-	-	3/4/4/13	-
7	1PE	H	65	-	-	3/7/7/13	-
4	BES	K	1003	5,3	-	8/24/24/24	0/1/1/1
7	1PE	K	4	-	-	1/9/9/13	-
4	BES	G	1003	5,3	-	6/24/24/24	0/1/1/1
4	BES	A	1003	5,3	-	2/24/24/24	0/1/1/1
4	BES	H	1003	5,3	-	6/24/24/24	0/1/1/1
4	BES	I	1003	5,3	-	7/24/24/24	0/1/1/1
7	1PE	E	7	-	-	3/9/9/13	-
7	1PE	K	42	-	-	4/8/8/13	-
7	1PE	F	32	-	-	3/7/7/13	-
7	1PE	K	50	-	-	3/3/3/13	-
4	BES	B	1003	5,3	-	6/24/24/24	0/1/1/1
7	1PE	G	12	-	-	6/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	A	20	-	-	4/9/9/13	-
7	1PE	L	612	-	-	6/9/9/13	-
7	1PE	D	44	-	-	2/8/8/13	-
7	1PE	F	31	-	-	0/7/7/13	-
7	1PE	J	2	-	-	6/8/8/13	-
7	1PE	D	67	-	-	3/4/4/13	-
7	1PE	I	66	-	-	2/4/4/13	-
7	1PE	E	8	-	-	0/9/9/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1003	BES	O4-C5	2.12	1.28	1.22
4	E	1003	BES	C2-C3	-2.10	1.48	1.52
4	J	1003	BES	O2-C2	2.09	1.46	1.42
4	G	1003	BES	C2-C1	2.09	1.56	1.54

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1003	BES	O2-C2-C1	5.42	121.01	109.64
4	G	1003	BES	O2-C2-C1	5.14	120.41	109.64
4	F	1003	BES	O2-C2-C1	4.66	119.42	109.64
4	G	1003	BES	O2-C2-C3	-4.62	100.69	110.63
4	K	1003	BES	O2-C2-C3	-4.43	101.08	110.63

There are no chirality outliers.

5 of 192 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

There are no ring outliers.

35 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1003	BES	2	0
7	J	45	1PE	2	0
7	L	1	1PE	3	0
7	C	18	1PE	4	0
7	E	43	1PE	4	0
7	I	21	1PE	3	0
7	J	3	1PE	6	0
7	H	64	1PE	1	0
7	D	9	1PE	1	0
7	D	63	1PE	2	0
7	I	22	1PE	5	0
4	D	1003	BES	3	0
7	G	58	1PE	6	0
7	A	19	1PE	1	0
7	B	61	1PE	8	0
4	C	1003	BES	3	0
4	E	1003	BES	3	0
7	C	17	1PE	1	0
7	H	65	1PE	3	0
4	K	1003	BES	4	0
4	A	1003	BES	1	0
4	H	1003	BES	3	0
4	I	1003	BES	3	0
6	D	7	SO4	1	0
7	F	32	1PE	3	0
4	B	1003	BES	3	0
7	K	42	1PE	1	0
6	J	20	SO4	1	0
7	A	20	1PE	1	0
7	G	12	1PE	1	0
7	L	612	1PE	8	0
7	D	44	1PE	2	0
6	L	25	SO4	2	0
7	J	2	1PE	2	0
7	D	67	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BES J 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES L 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES F 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES D 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES C 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES E 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES K 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES G 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES A 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES H 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES I 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand BES B 1003

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	518/528 (98%)	-0.40	4 (0%)	86	85	7, 14, 29, 39	1 (0%)
1	B	518/528 (98%)	-0.22	14 (2%)	54	53	7, 16, 42, 51	0
1	C	518/528 (98%)	-0.37	4 (0%)	86	85	7, 15, 31, 42	0
1	D	516/528 (97%)	-0.37	7 (1%)	75	74	8, 15, 29, 39	0
1	E	510/528 (96%)	-0.46	4 (0%)	86	85	8, 14, 25, 37	0
1	F	510/528 (96%)	-0.25	6 (1%)	79	78	8, 17, 37, 46	0
1	G	516/528 (97%)	-0.36	6 (1%)	79	78	7, 14, 28, 40	0
1	H	509/528 (96%)	-0.22	13 (2%)	56	54	7, 16, 42, 52	0
1	I	518/528 (98%)	-0.34	2 (0%)	92	92	7, 14, 31, 41	0
1	J	513/528 (97%)	-0.34	5 (0%)	82	81	8, 15, 29, 40	0
1	K	509/528 (96%)	-0.47	5 (0%)	82	81	9, 14, 25, 38	0
1	L	513/528 (97%)	-0.26	6 (1%)	79	78	8, 16, 40, 46	0
All	All	6168/6336 (97%)	-0.34	76 (1%)	79	78	7, 15, 34, 52	1 (0%)

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	GLY	7.4
1	J	136	GLY	7.0
1	D	136	GLY	7.0
1	B	259	VAL	5.0
1	E	136	GLY	4.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	1PE	B	62	10/16	-0.02	0.71	91,95,97,98	0
7	1PE	K	50	6/16	0.66	0.21	37,40,45,46	0
7	1PE	D	63	10/16	0.79	0.18	22,30,33,36	0
7	1PE	A	20	12/16	0.80	0.18	40,43,46,47	0
7	1PE	D	44	11/16	0.80	0.29	36,38,43,44	0
7	1PE	D	67	7/16	0.82	0.23	29,33,41,41	0
7	1PE	G	58	15/16	0.83	0.20	37,42,52,53	0
7	1PE	H	65	10/16	0.83	0.17	32,40,41,41	0
7	1PE	J	45	10/16	0.83	0.27	44,48,51,51	0
7	1PE	B	61	10/16	0.83	0.19	38,40,42,43	0
7	1PE	J	3	10/16	0.85	0.15	36,37,40,41	0
7	1PE	G	30	7/16	0.86	0.17	35,38,42,43	0
7	1PE	I	21	15/16	0.87	0.20	26,33,46,47	0
7	1PE	C	17	13/16	0.87	0.20	22,36,38,38	0
5	MG	J	1004	1/1	0.87	0.58	22,22,22,22	0
7	1PE	K	4	12/16	0.87	0.14	31,32,34,35	0
7	1PE	K	42	11/16	0.87	0.18	33,42,47,47	0
7	1PE	E	7	12/16	0.87	0.15	32,34,36,36	0
7	1PE	L	56	11/16	0.87	0.18	43,45,48,50	0
4	BES	G	1003	22/22	0.88	0.17	13,28,34,39	0
7	1PE	I	66	7/16	0.88	0.15	30,32,34,34	0
4	BES	F	1003	22/22	0.88	0.20	13,27,36,40	0
7	1PE	F	32	10/16	0.88	0.16	37,39,39,39	0
4	BES	B	1003	22/22	0.89	0.18	17,30,39,45	0
6	SO4	A	2	5/5	0.89	0.15	45,46,50,51	0
6	SO4	A	24	5/5	0.89	0.14	52,55,56,57	0
4	BES	C	1003	22/22	0.89	0.15	22,27,36,36	0
7	1PE	E	43	8/16	0.89	0.18	33,35,35,39	0
4	BES	H	1003	22/22	0.89	0.18	15,25,34,37	0
7	1PE	G	12	9/16	0.89	0.16	27,28,32,32	0
4	BES	K	1003	22/22	0.89	0.16	16,26,32,39	0
7	1PE	L	612	12/16	0.89	0.18	22,36,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	MG	B	1004	1/1	0.89	0.41	16,16,16,16	0
4	BES	A	1003	22/22	0.90	0.15	20,29,35,40	0
7	1PE	J	2	11/16	0.91	0.13	23,26,37,42	0
7	1PE	D	9	10/16	0.91	0.16	21,25,35,37	0
7	1PE	G	48	6/16	0.91	0.13	25,31,33,36	0
4	BES	D	1003	22/22	0.91	0.15	13,28,32,33	0
5	MG	L	1004	1/1	0.92	0.51	33,33,33,33	0
7	1PE	F	33	10/16	0.92	0.18	21,29,31,34	0
4	BES	E	1003	22/22	0.92	0.13	19,29,35,39	0
4	BES	I	1003	22/22	0.92	0.13	11,27,30,32	0
7	1PE	A	19	9/16	0.92	0.17	20,24,28,31	0
5	MG	C	1004	1/1	0.92	0.44	27,27,27,27	0
5	MG	D	1004	1/1	0.92	0.42	28,28,28,28	0
4	BES	J	1003	22/22	0.92	0.15	11,28,37,40	0
7	1PE	I	22	11/16	0.92	0.13	18,23,36,38	0
4	BES	L	1003	22/22	0.93	0.17	12,26,33,34	0
5	MG	F	1004	1/1	0.93	0.45	37,37,37,37	0
7	1PE	C	18	9/16	0.93	0.10	20,21,26,29	0
7	1PE	G	47	6/16	0.93	0.13	30,31,32,35	0
7	1PE	B	60	10/16	0.93	0.14	23,28,33,35	0
5	MG	A	1004	1/1	0.93	0.55	24,24,24,24	0
7	1PE	K	5	12/16	0.94	0.12	25,27,38,38	0
2	CO3	A	1002	4/4	0.94	0.14	13,14,14,17	0
5	MG	I	1004	1/1	0.94	0.50	15,15,15,15	0
6	SO4	D	5	5/5	0.94	0.20	53,53,56,56	0
6	SO4	J	20	5/5	0.94	0.25	60,62,62,62	0
7	1PE	E	8	12/16	0.95	0.13	20,23,35,35	0
7	1PE	H	64	10/16	0.95	0.11	19,26,34,35	0
5	MG	K	1004	1/1	0.95	0.35	23,23,23,23	0
7	1PE	L	1	10/16	0.95	0.11	25,27,32,38	0
5	MG	H	1004	1/1	0.95	0.51	40,40,40,40	0
6	SO4	K	19	5/5	0.95	0.20	52,53,54,54	0
6	SO4	G	23	5/5	0.96	0.22	46,49,50,50	0
7	1PE	F	31	10/16	0.96	0.09	26,27,29,29	0
6	SO4	L	25	5/5	0.96	0.24	56,59,59,60	0
5	MG	G	1004	1/1	0.96	0.40	23,23,23,23	0
6	SO4	F	21	5/5	0.97	0.20	56,59,59,59	0
2	CO3	D	1002	4/4	0.97	0.11	11,12,12,16	0
5	MG	E	1004	1/1	0.97	0.33	26,26,26,26	0
2	CO3	F	1002	4/4	0.97	0.09	12,12,13,15	0
2	CO3	J	1002	4/4	0.97	0.11	12,14,15,16	0
6	SO4	E	22	5/5	0.97	0.27	44,45,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO3	C	1002	4/4	0.98	0.10	12,13,13,16	0
2	CO3	G	1002	4/4	0.98	0.08	11,12,12,15	0
2	CO3	H	1002	4/4	0.98	0.09	10,10,11,14	0
2	CO3	I	1002	4/4	0.98	0.10	14,15,15,18	0
2	CO3	B	1002	4/4	0.98	0.11	11,12,12,16	0
2	CO3	K	1002	4/4	0.98	0.10	13,14,14,18	0
2	CO3	L	1002	4/4	0.98	0.10	14,15,15,16	0
6	SO4	A	1	5/5	0.98	0.17	50,51,53,53	0
2	CO3	E	1002	4/4	0.98	0.13	16,17,18,19	0
3	ZN	E	1001	1/1	0.99	0.04	38,38,38,38	0
3	ZN	F	1001	1/1	0.99	0.08	40,40,40,40	0
3	ZN	G	1001	1/1	0.99	0.09	38,38,38,38	0
3	ZN	H	1001	1/1	0.99	0.08	34,34,34,34	0
3	ZN	I	1001	1/1	0.99	0.08	36,36,36,36	0
6	SO4	B	3	5/5	0.99	0.06	8,9,10,10	0
3	ZN	J	1001	1/1	0.99	0.04	38,38,38,38	0
3	ZN	K	1001	1/1	0.99	0.07	37,37,37,37	0
3	ZN	L	1001	1/1	0.99	0.08	37,37,37,37	0
6	SO4	G	17	5/5	0.99	0.07	10,11,13,14	0
3	ZN	A	1001	1/1	0.99	0.08	39,39,39,39	0
6	SO4	J	18	5/5	0.99	0.09	11,11,12,14	0
3	ZN	C	1001	1/1	0.99	0.10	39,39,39,39	0
3	ZN	D	1001	1/1	1.00	0.04	34,34,34,34	0
3	ZN	B	1001	1/1	1.00	0.07	37,37,37,37	0
6	SO4	D	7	5/5	1.00	0.09	8,11,11,12	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 G 1003:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
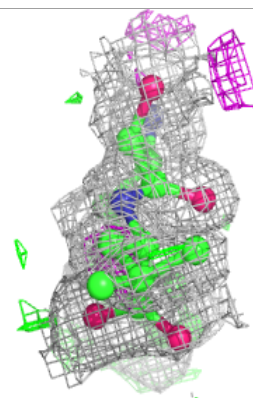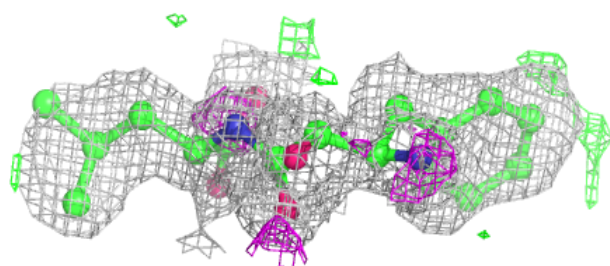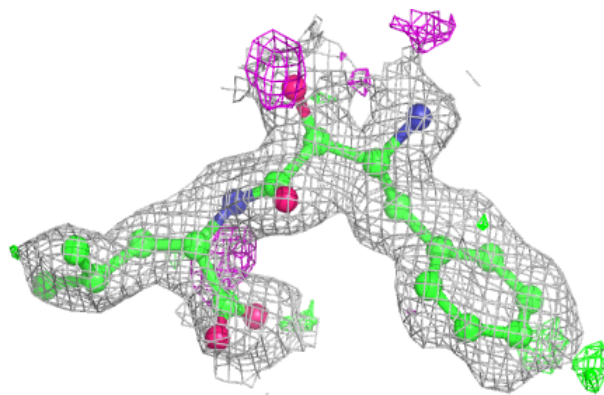
Electron density around BES F 1003:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
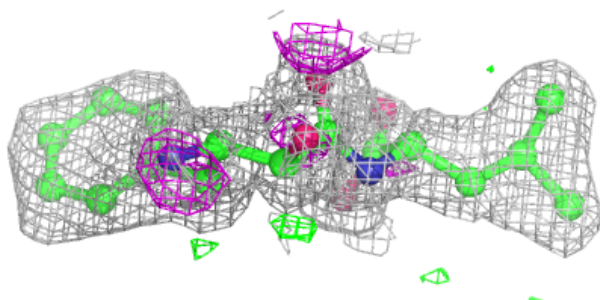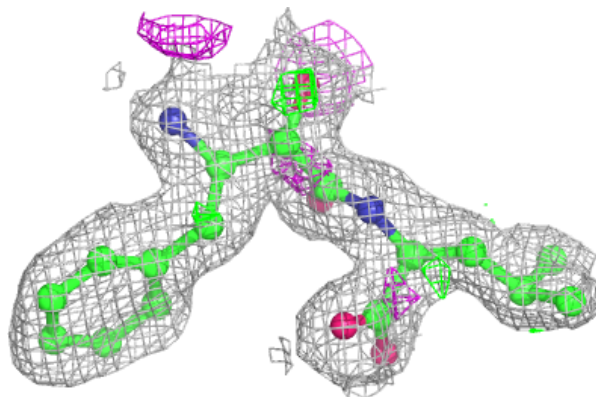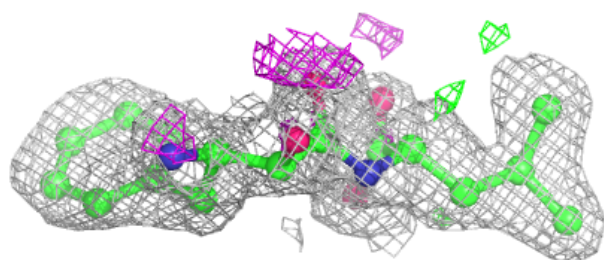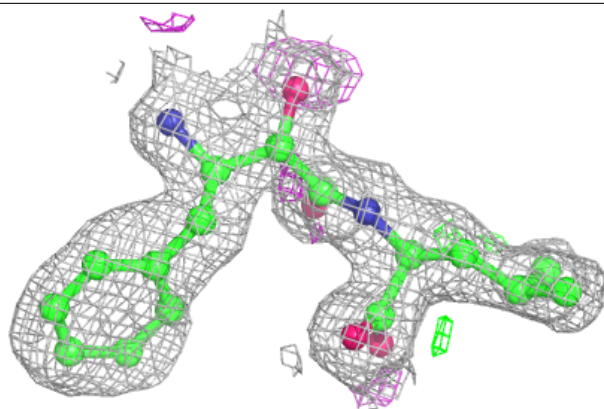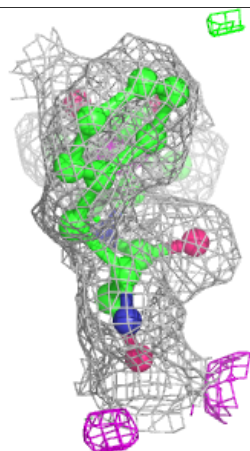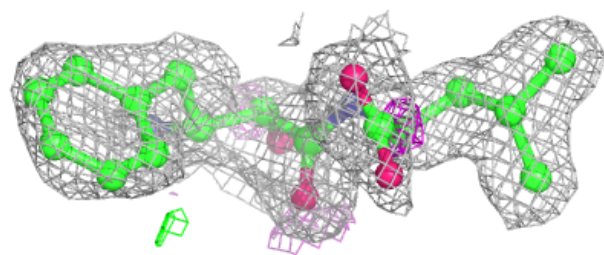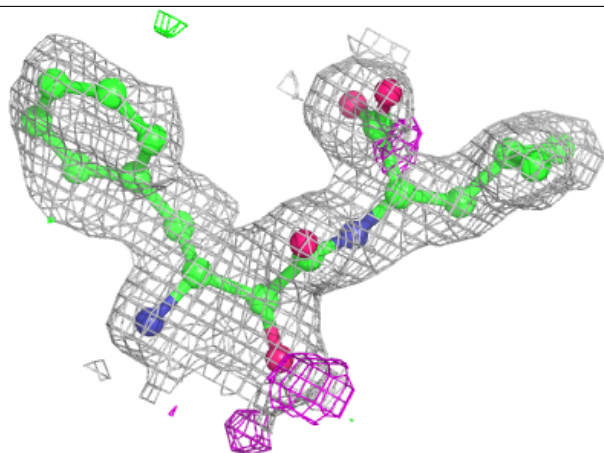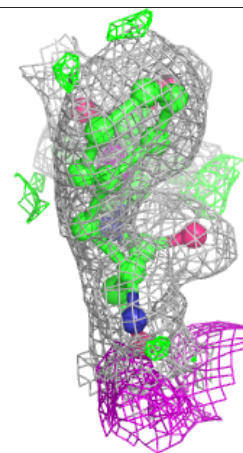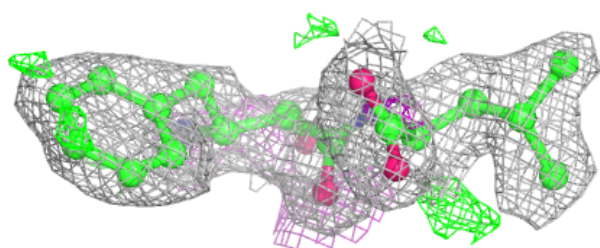$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
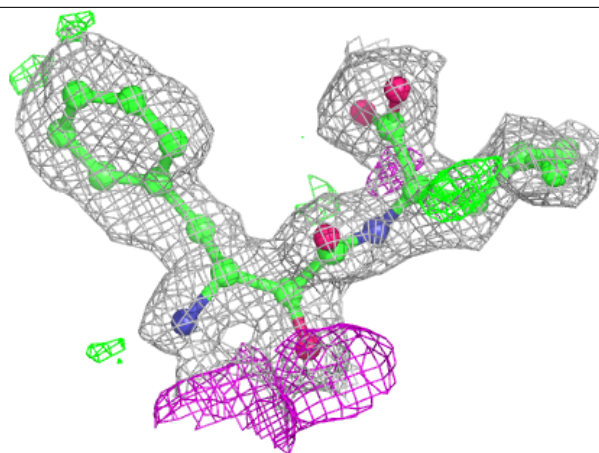and green (positive)
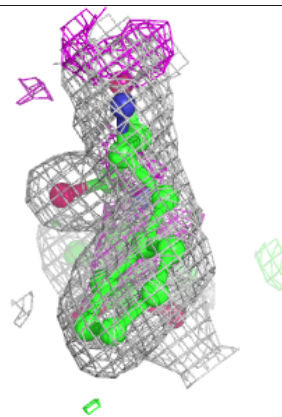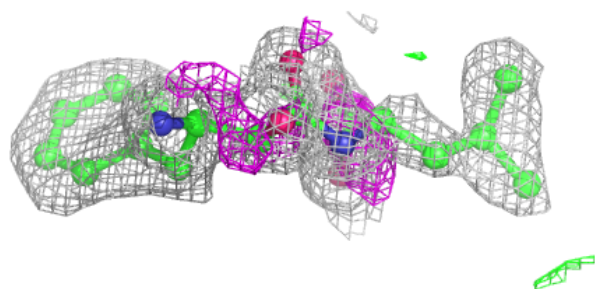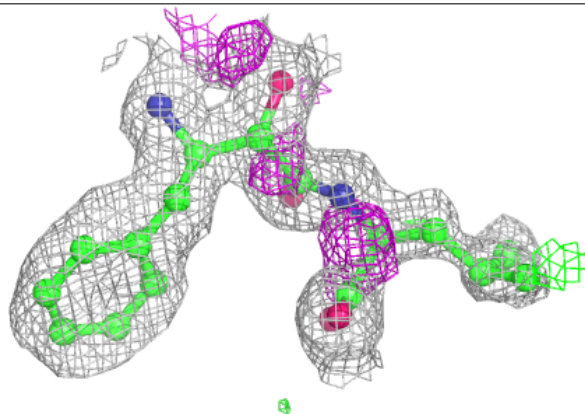
Electron density around BES B 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
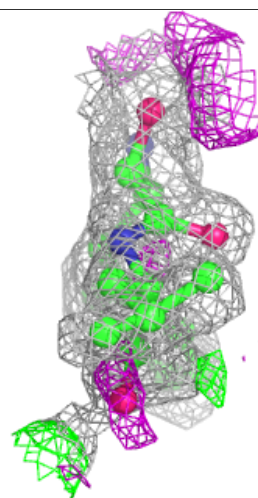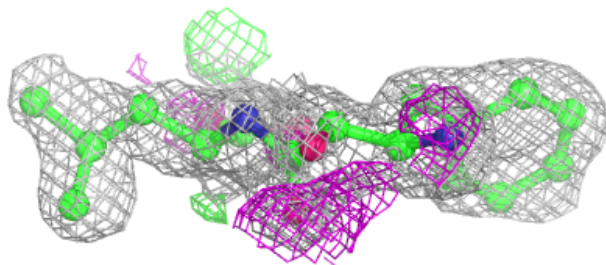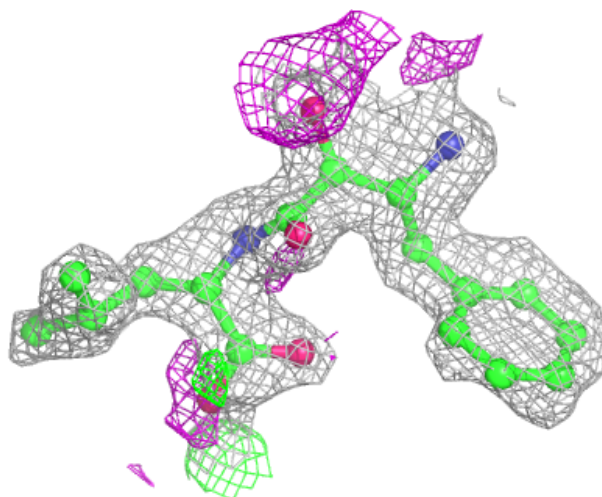
Electron density around BES C 1003:

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

Electron density around BES 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)
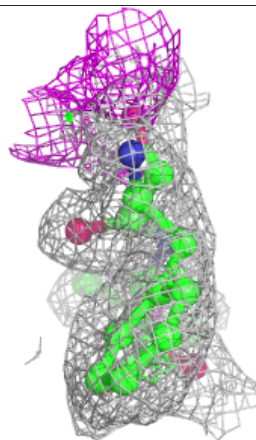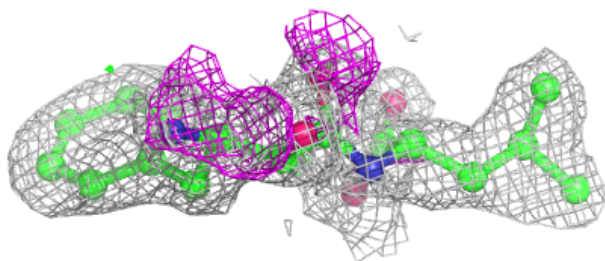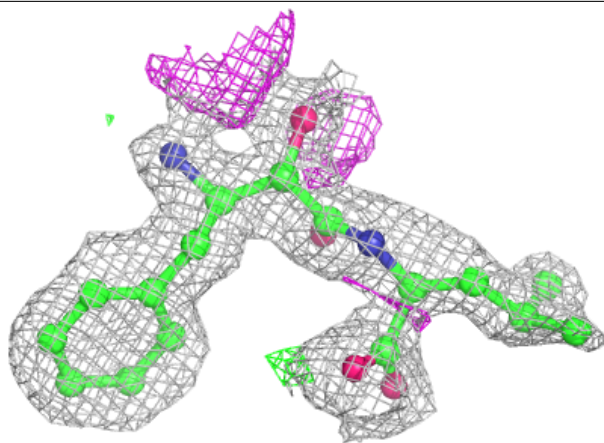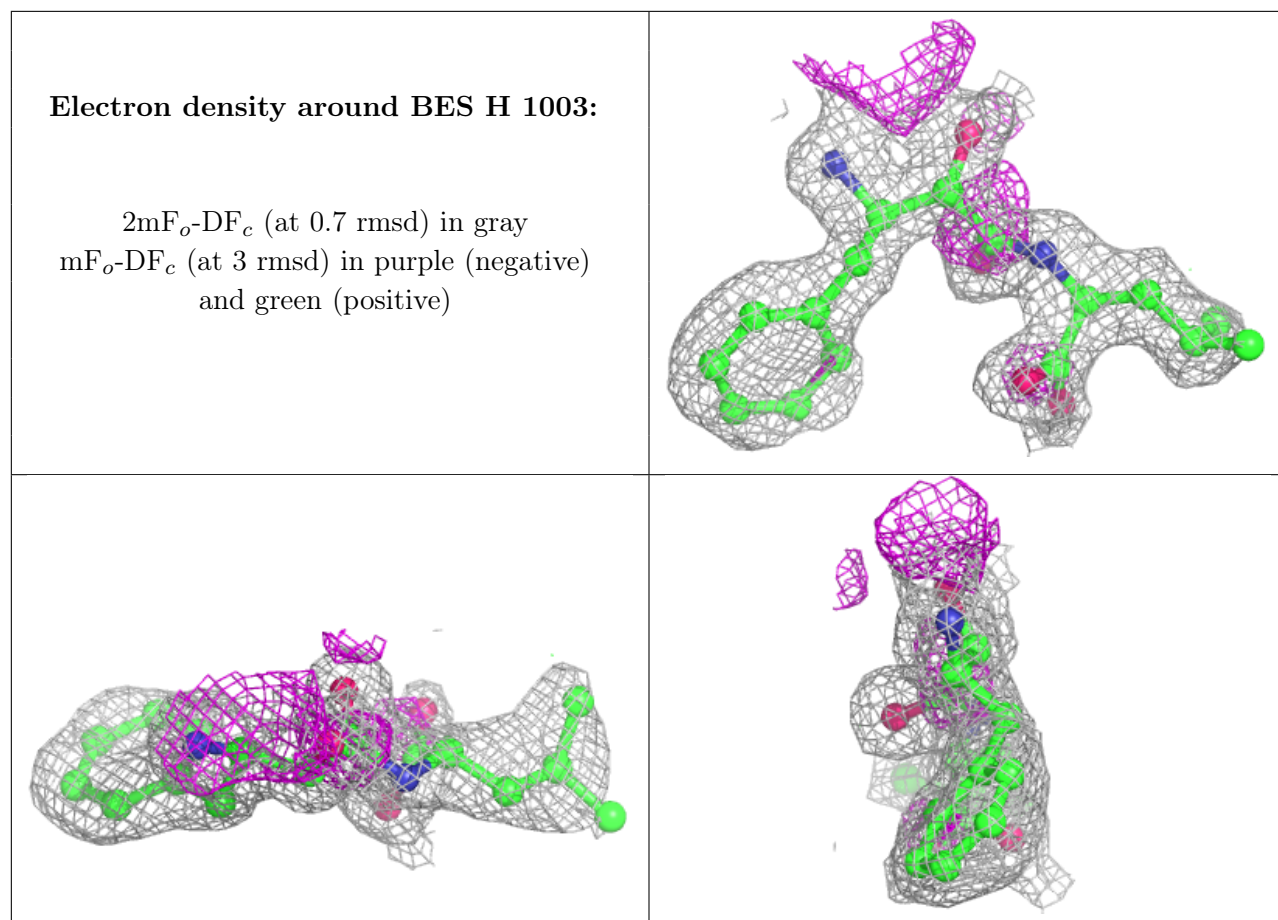
Electron density around BES K 1003:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
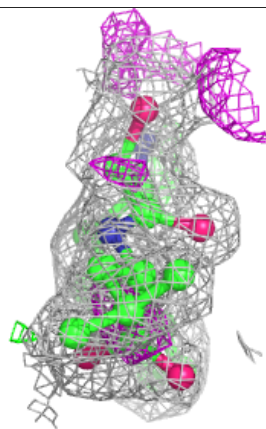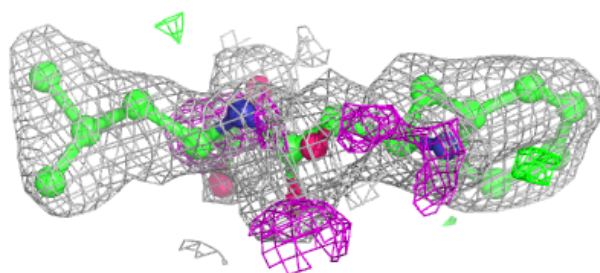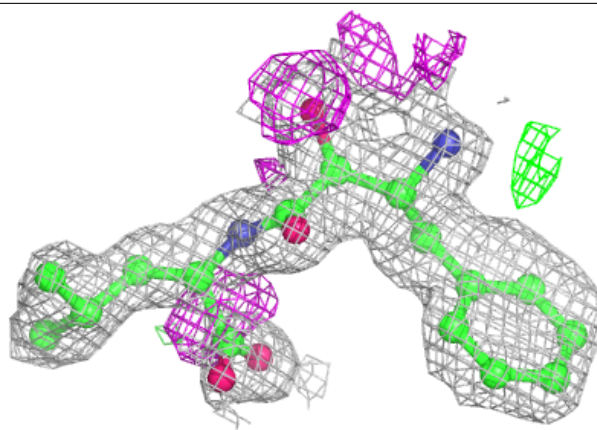
Electron density around BES A 1003:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 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)

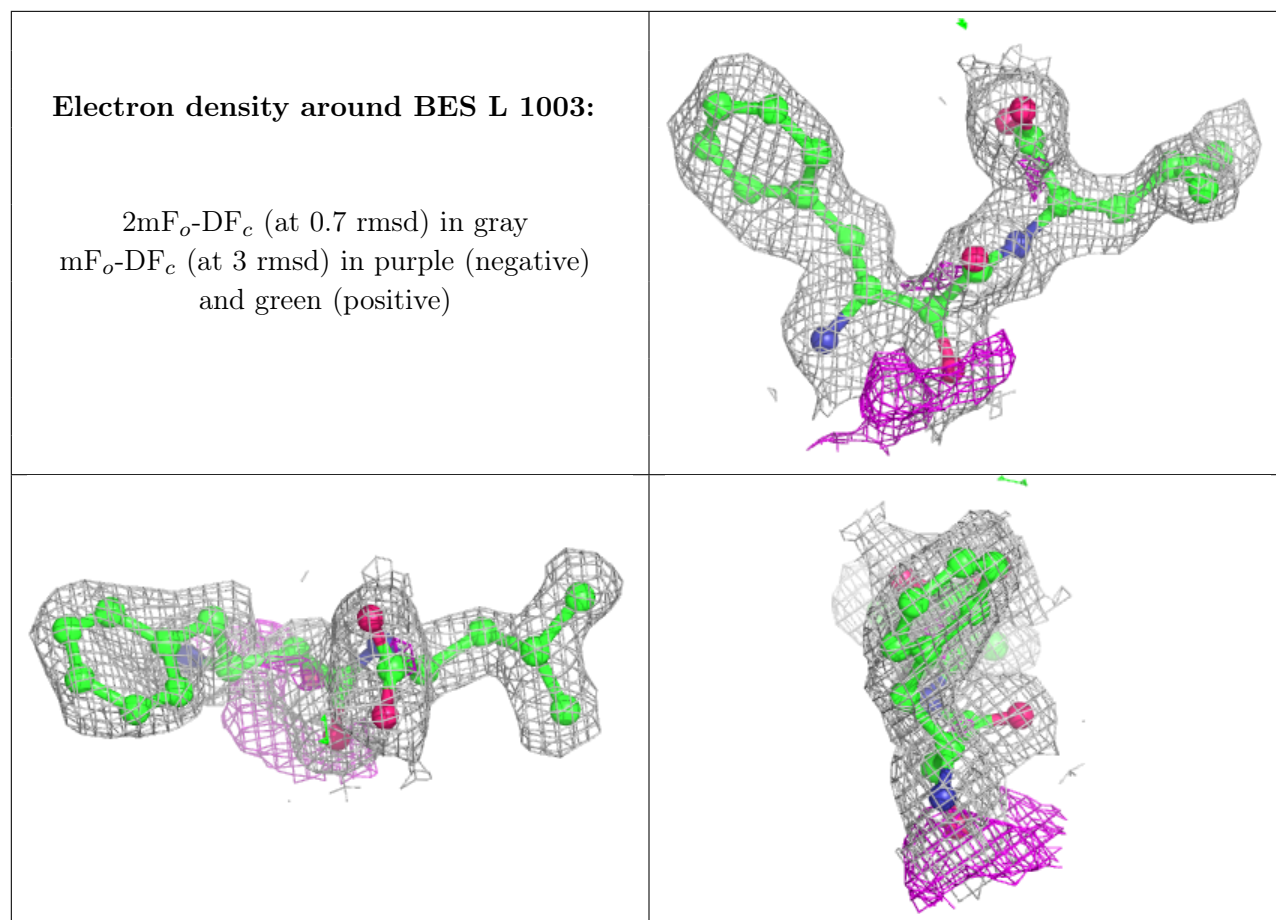**Electron density around BES I 1003:**

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

Electron density around BES J 1003:

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

Electron density around BES L 1003:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
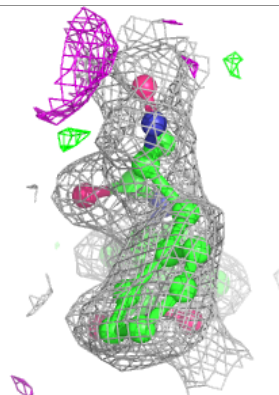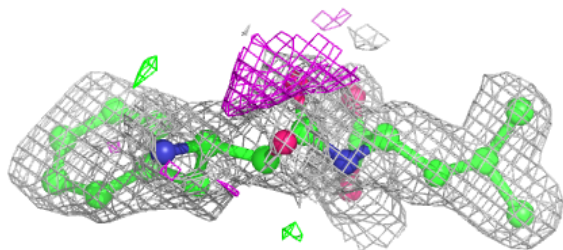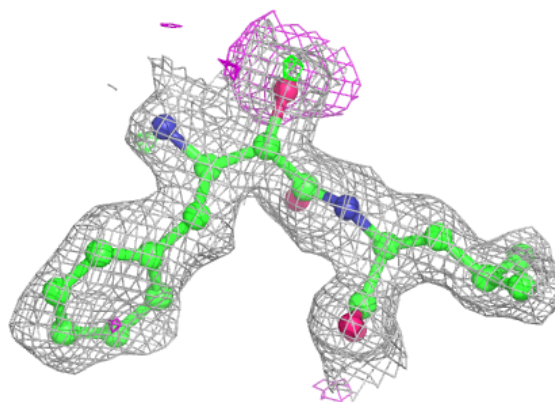
6.5   Other polymers (i)

There are no such residues in this entry.