



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:32 PM UTC

PDB ID : 3KQX / pdb_00003kqx
Title : Structure of a protease 1
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.01 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

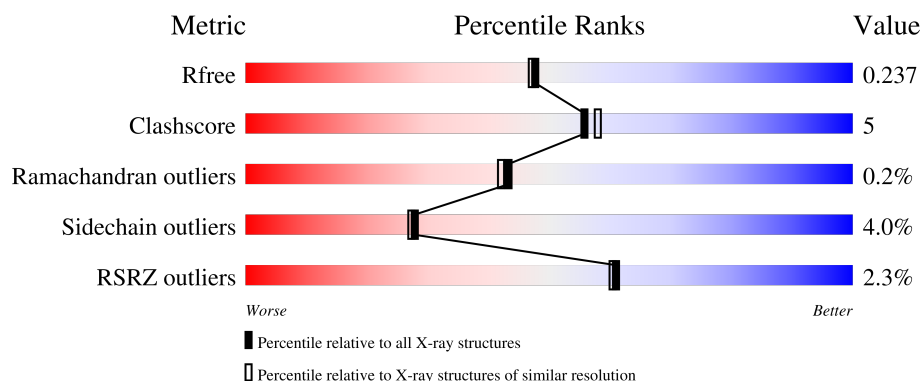
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	 88% 9% ..
1	B	528	 6% 86% 10% ..
1	C	528	 0% 88% 10% ..
1	D	528	 0% 84% 12% ..
1	E	528	 84% 12% ..

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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
5	1PE	I	27	-	-	X	-
5	1PE	I	61	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50931 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	514	Total	C	N	O	S	3	1	0
			3944	2536	632	757	19			
1	B	510	Total	C	N	O	S	0	0	0
			3867	2489	624	735	19			
1	C	518	Total	C	N	O	S	0	1	0
			3954	2544	638	753	19			
1	D	514	Total	C	N	O	S	0	0	0
			3931	2532	633	746	20			
1	E	509	Total	C	N	O	S	0	0	0
			3888	2506	622	741	19			
1	F	510	Total	C	N	O	S	0	0	0
			3776	2428	611	718	19			
1	G	514	Total	C	N	O	S	0	0	0
			3945	2536	632	758	19			
1	H	510	Total	C	N	O	S	0	0	0
			3873	2491	625	738	19			
1	I	515	Total	C	N	O	S	0	0	0
			3924	2527	632	746	19			
1	J	514	Total	C	N	O	S	0	0	0
			3931	2532	633	746	20			
1	K	509	Total	C	N	O	S	0	0	0
			3888	2506	623	740	19			
1	L	508	Total	C	N	O	S	0	0	0
			3809	2450	613	727	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 ZINC ION (CCD ID: ZN) (formula: Zn).

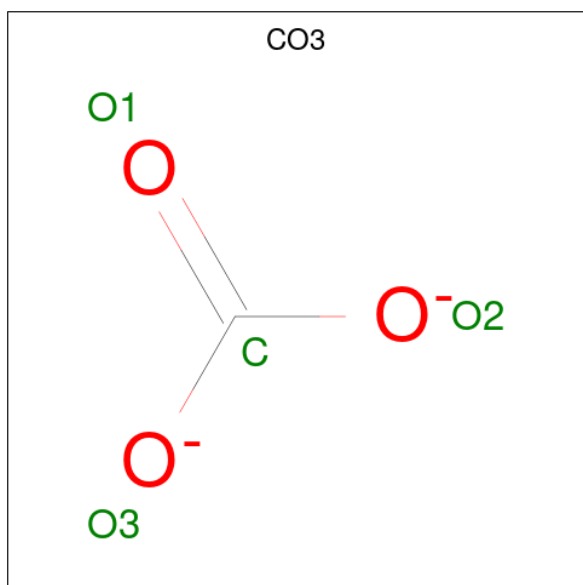
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0

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

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



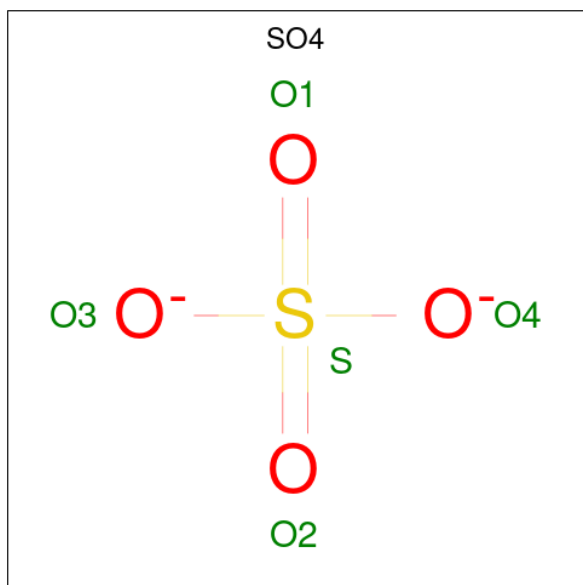
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	C	O	0	0
			4	1	3		
3	K	1	Total	C	O	0	0
			4	1	3		
3	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



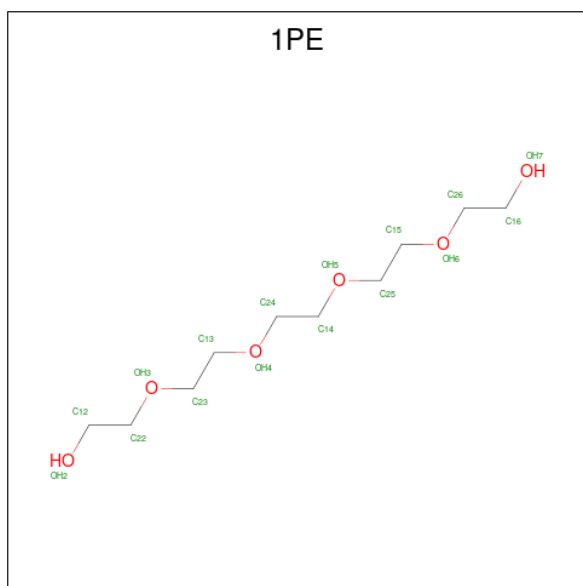
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

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

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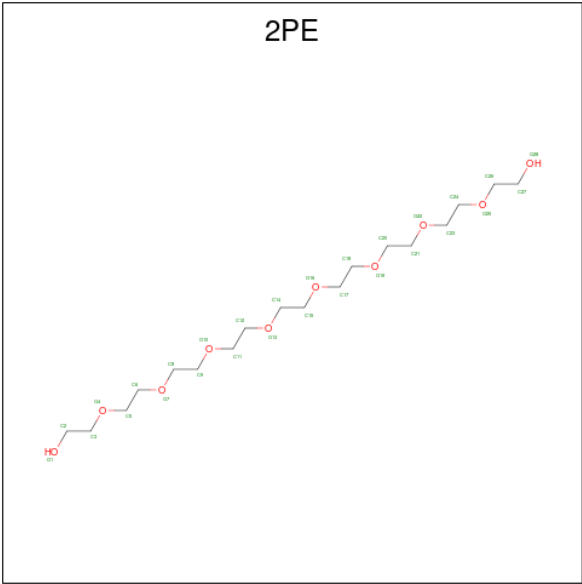
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			9	6	3		
5	G	1	Total	C	O	0	0
			10	6	4		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			6	4	2		
5	G	1	Total	C	O	0	0
			6	4	2		
5	G	1	Total	C	O	0	0
			15	10	5		
5	H	1	Total	C	O	0	0
			6	4	2		
5	H	1	Total	C	O	0	0
			11	7	4		
5	I	1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

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

- Molecule 6 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			24	16	8		
6	B	1	Total	C	O	0	0
			26	17	9		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			6	4	2		
6	H	1	Total	C	O	0	0
			25	16	9		

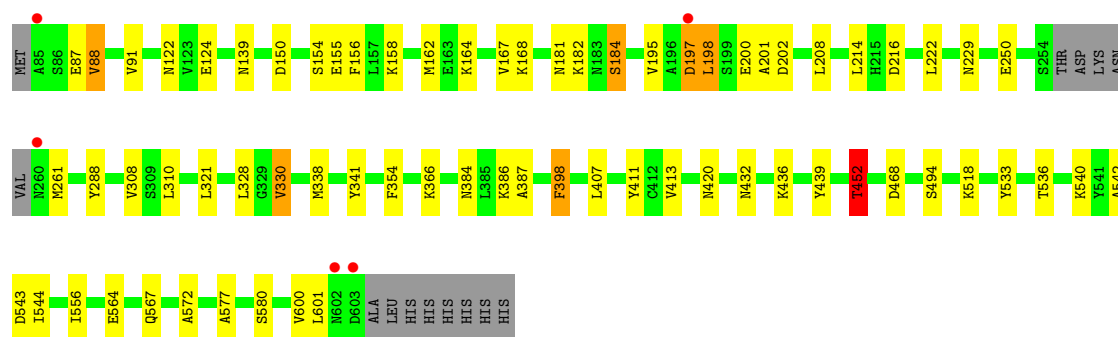
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	308	Total	O		0	0
			308	308			
7	B	238	Total	O		0	0
			238	238			
7	C	330	Total	O		0	0
			330	330			
7	D	310	Total	O		0	0
			310	310			
7	E	326	Total	O		0	0
			326	326			
7	F	225	Total	O		0	0
			225	225			
7	G	301	Total	O		0	0
			301	301			
7	H	220	Total	O		0	0
			220	220			
7	I	264	Total	O		0	0
			264	264			
7	J	322	Total	O		0	0
			322	322			
7	K	327	Total	O		0	0
			327	327			
7	L	272	Total	O		0	0
			272	272			

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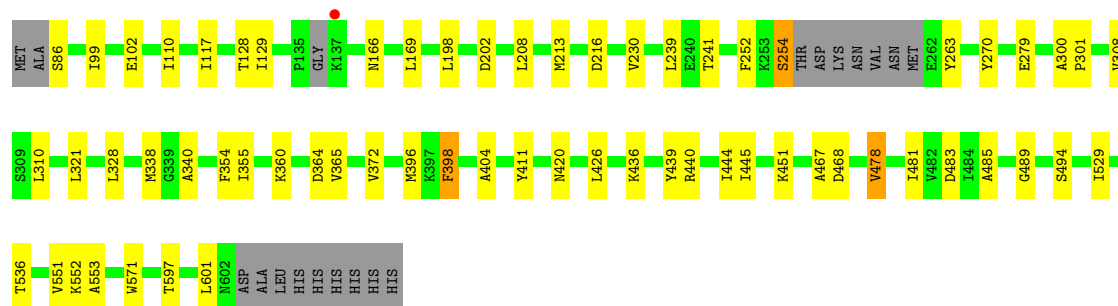
- Molecule 1: M17 leucyl aminopeptidase





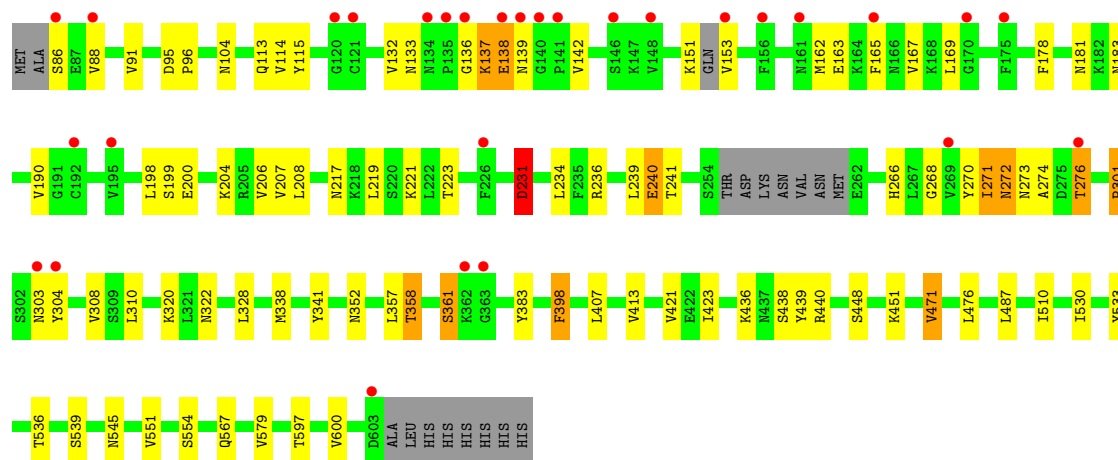
• Molecule 1: M17 leucyl aminopeptidase

Chain E: 84% 12% . .



• Molecule 1: M17 leucyl aminopeptidase

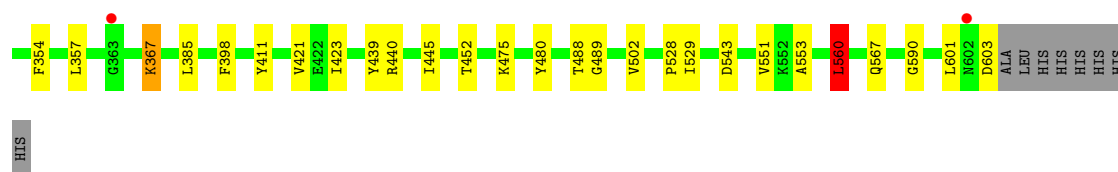
Chain F: 5% 79% 15% . .



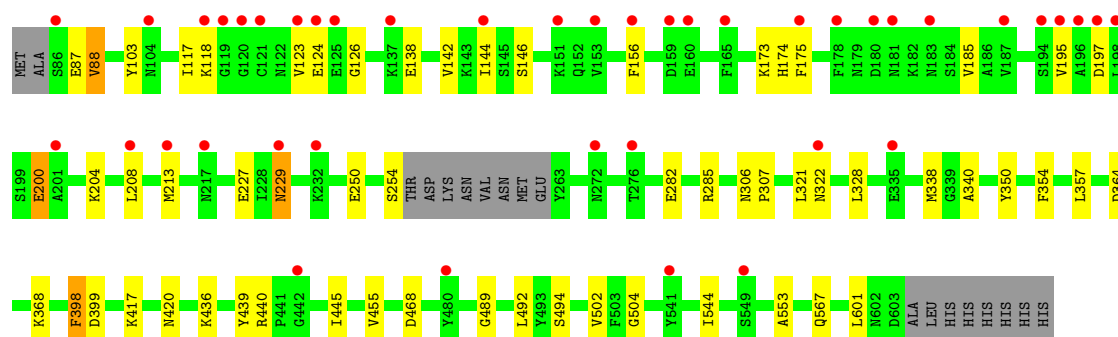
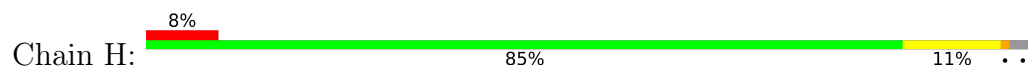
• Molecule 1: M17 leucyl aminopeptidase

Chain G: 87% 10% .

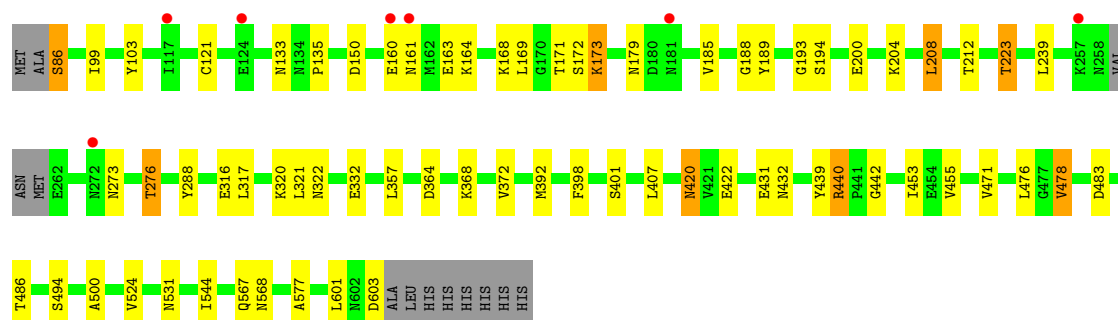
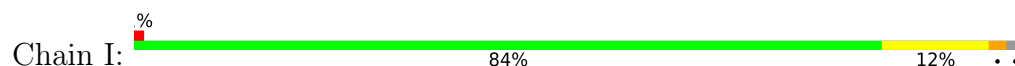




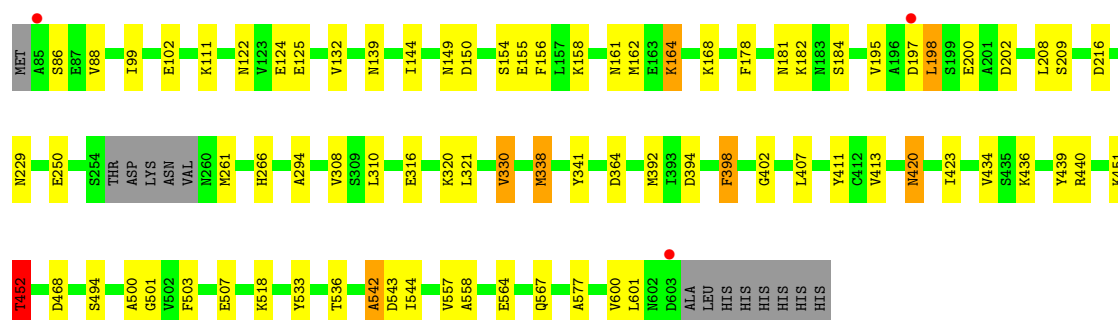
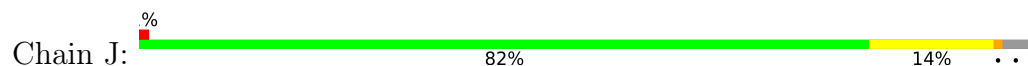
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

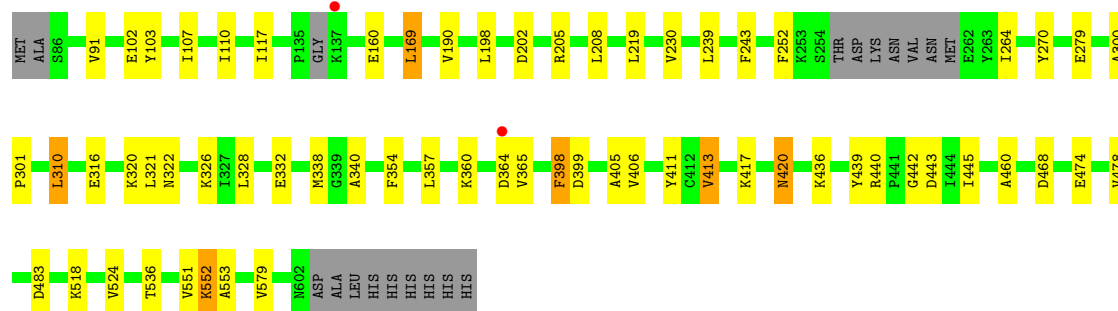


- Molecule 1: M17 leucyl aminopeptidase



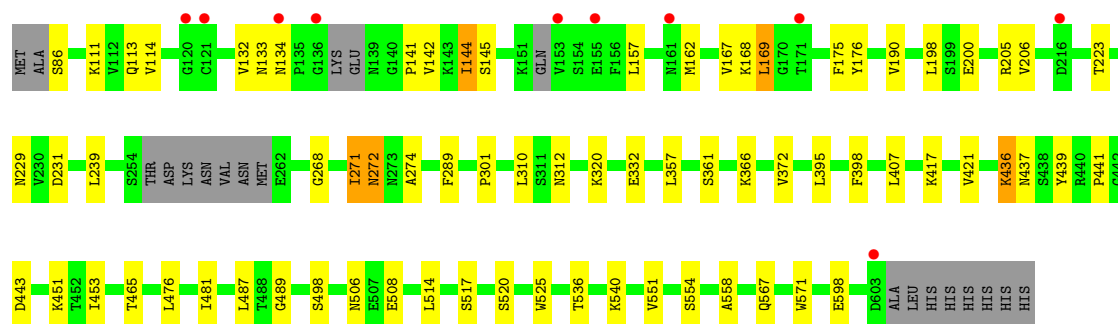
- Molecule 1: M17 leucyl aminopeptidase

Chain K:  84% 11% . .



• Molecule 1: M17 leucyl aminopeptidase

Chain L:  2% 82% 13% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.40Å 176.81Å 224.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.08 – 2.01 56.08 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.08-2.01) 100.0 (56.08-2.01)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.232 0.188 , 0.237	Depositor DCC
R_{free} test set	22860 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50931	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 50.61 % 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 6.3078e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, 2PE, SO4, ZN, CO3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.36	8/4023 (0.2%)	1.11	6/5456 (0.1%)
1	B	1.23	4/3944 (0.1%)	1.11	13/5357 (0.2%)
1	C	1.36	10/4035 (0.2%)	1.12	12/5476 (0.2%)
1	D	1.41	9/4008 (0.2%)	1.11	10/5435 (0.2%)
1	E	1.43	9/3964 (0.2%)	1.16	7/5378 (0.1%)
1	F	1.19	4/3850 (0.1%)	1.13	6/5243 (0.1%)
1	G	1.36	8/4022 (0.2%)	1.09	3/5455 (0.1%)
1	H	1.20	7/3950 (0.2%)	1.10	12/5365 (0.2%)
1	I	1.38	15/4001 (0.4%)	1.12	9/5429 (0.2%)
1	J	1.38	12/4008 (0.3%)	1.13	10/5435 (0.2%)
1	K	1.41	14/3964 (0.4%)	1.12	4/5378 (0.1%)
1	L	1.38	7/3883 (0.2%)	1.18	8/5279 (0.2%)
All	All	1.34	107/47652 (0.2%)	1.12	100/64686 (0.2%)

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

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	161	ASN	C-N	11.26	1.50	1.33
1	D	88	VAL	C-N	10.63	1.47	1.33
1	L	443	ASP	N-CA	8.80	1.57	1.46
1	L	289	PHE	C-N	8.71	1.44	1.33
1	J	558	ALA	CA-CB	8.39	1.66	1.53

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	SER	O-C-N	-11.26	104.98	123.00
1	E	440	ARG	NE-CZ-NH1	-9.11	112.39	121.50
1	E	440	ARG	NE-CZ-NH2	9.06	127.35	119.20
1	H	321	LEU	CA-C-N	-8.67	104.98	121.54
1	H	321	LEU	C-N-CA	-8.67	104.98	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3944	0	3873	32	0
1	B	3867	0	3762	32	2
1	C	3954	0	3879	18	0
1	D	3931	0	3866	38	1
1	E	3888	0	3810	31	0
1	F	3776	0	3585	61	0
1	G	3945	0	3873	31	0
1	H	3873	0	3768	27	2
1	I	3924	0	3849	34	0
1	J	3931	0	3866	61	0
1	K	3888	0	3812	34	0
1	L	3809	0	3651	45	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
4	K	10	0	0	2	0
5	A	36	0	36	6	0
5	B	11	0	12	6	0
5	C	30	0	32	2	0
5	D	56	0	60	7	0
5	E	62	0	71	7	0
5	F	42	0	51	6	0
5	G	53	0	59	4	0
5	H	17	0	16	3	0
5	I	40	0	45	20	0
5	J	64	0	74	23	0
5	K	71	0	76	5	0
5	L	55	0	66	11	0
6	B	50	0	64	11	0
6	F	6	0	4	0	0
6	H	25	0	33	1	0
7	A	308	0	0	4	0
7	B	238	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	330	0	0	5	1
7	D	310	0	0	4	0
7	E	326	0	0	2	0
7	F	225	0	0	4	0
7	G	301	0	0	8	0
7	H	220	0	0	6	0
7	I	264	0	0	5	0
7	J	322	0	0	13	0
7	K	327	0	0	7	0
7	L	272	0	0	8	0
All	All	50931	0	46293	439	4

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 439 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:E:338:MET:HE3	1:E:468:ASP:HB3	1.27	1.17
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.23	1.14
1:L:271:ILE:O	1:L:272:ASN:HB2	1.41	1.11
5:H:54:1PE:H251	7:H:4310:HOH:O	1.52	1.09
1:F:271:ILE:O	1:F:272:ASN:HB2	1.47	1.07

All (4) 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:D:366:LYS:CE	7:B:895:HOH:O[4_455]	1.60	0.60
1:B:322:ASN:ND2	1:H:322:ASN:ND2[2_664]	1.72	0.48
1:B:322:ASN:CG	1:H:322:ASN:ND2[2_664]	2.10	0.10
1:L:332:GLU:OE1	7:C:3017:HOH:O[1_556]	2.12	0.08

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	511/528 (97%)	501 (98%)	10 (2%)	0	100	100
1	B	506/528 (96%)	493 (97%)	11 (2%)	2 (0%)	30	27
1	C	517/528 (98%)	508 (98%)	9 (2%)	0	100	100
1	D	510/528 (97%)	500 (98%)	10 (2%)	0	100	100
1	E	503/528 (95%)	492 (98%)	11 (2%)	0	100	100
1	F	504/528 (96%)	483 (96%)	16 (3%)	5 (1%)	12	8
1	G	510/528 (97%)	499 (98%)	11 (2%)	0	100	100
1	H	506/528 (96%)	491 (97%)	13 (3%)	2 (0%)	30	27
1	I	511/528 (97%)	503 (98%)	8 (2%)	0	100	100
1	J	510/528 (97%)	499 (98%)	11 (2%)	0	100	100
1	K	503/528 (95%)	490 (97%)	13 (3%)	0	100	100
1	L	500/528 (95%)	486 (97%)	13 (3%)	1 (0%)	43	42
All	All	6091/6336 (96%)	5945 (98%)	136 (2%)	10 (0%)	43	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	138	GLU
1	F	272	ASN
1	L	272	ASN
1	B	138	GLU
1	H	138	GLU

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	421/455 (92%)	414 (98%)	7 (2%)	53	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/455 (89%)	394 (97%)	11 (3%)	39	42
1	C	419/455 (92%)	398 (95%)	21 (5%)	22	20
1	D	416/455 (91%)	394 (95%)	22 (5%)	20	18
1	E	412/455 (90%)	399 (97%)	13 (3%)	34	35
1	F	380/455 (84%)	358 (94%)	22 (6%)	18	15
1	G	421/455 (92%)	411 (98%)	10 (2%)	43	47
1	H	407/455 (90%)	395 (97%)	12 (3%)	37	40
1	I	415/455 (91%)	391 (94%)	24 (6%)	18	15
1	J	416/455 (91%)	397 (95%)	19 (5%)	24	22
1	K	412/455 (90%)	397 (96%)	15 (4%)	31	31
1	L	391/455 (86%)	370 (95%)	21 (5%)	20	17
All	All	4915/5460 (90%)	4718 (96%)	197 (4%)	28	27

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	436	LYS
1	J	164	LYS
1	I	121	CYS
1	I	276	THR
1	J	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	322	ASN
1	J	266	HIS
1	H	531	ASN
1	J	139	ASN
1	J	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 12 are monoatomic - leaving 86 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	1PE	H	51	-	5,5,15	0.75	0	4,4,14	0.58	0
5	1PE	K	42	-	10,10,15	0.59	0	9,9,14	0.48	0
5	1PE	C	18	-	8,8,15	0.46	0	7,7,14	0.84	0
5	1PE	D	9	-	9,9,15	0.58	0	8,8,14	0.54	0
5	1PE	I	22	-	10,10,15	0.77	0	9,9,14	0.82	0
6	2PE	F	63	-	5,5,27	0.74	0	4,4,26	0.52	0
4	SO4	A	2	-	4,4,4	0.44	0	6,6,6	0.56	0
5	1PE	B	40	-	10,10,15	0.67	0	9,9,14	0.92	1 (11%)
4	SO4	A	1	-	4,4,4	0.40	0	6,6,6	0.43	0
3	CO3	D	1002	-	3,3,3	1.21	0	2,3,3	1.62	0
5	1PE	J	49	-	10,10,15	0.69	0	9,9,14	0.89	0
4	SO4	D	7	-	4,4,4	0.50	0	6,6,6	0.35	0
5	1PE	E	43	-	7,7,15	0.54	0	6,6,14	0.46	0
4	SO4	C	6	-	4,4,4	1.04	0	6,6,6	0.82	0
3	CO3	G	1002	-	3,3,3	0.40	0	2,3,3	2.50	2 (100%)
5	1PE	E	35	-	9,9,15	0.57	0	8,8,14	0.54	0
5	1PE	G	12	-	8,8,15	0.67	0	7,7,14	0.55	0
3	CO3	B	1002	-	3,3,3	0.48	0	2,3,3	2.59	2 (100%)
5	1PE	E	7	-	11,11,15	0.73	0	10,10,14	0.68	0
5	1PE	E	8	-	11,11,15	0.62	0	10,10,14	0.80	0
3	CO3	L	1002	-	3,3,3	1.38	0	2,3,3	1.43	0
5	1PE	D	34	-	9,9,15	0.55	0	8,8,14	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	F	31	-	9,9,15	0.51	0	8,8,14	0.52	0
5	1PE	L	1	-	9,9,15	0.46	0	8,8,14	0.75	0
5	1PE	F	32	-	9,9,15	0.61	0	8,8,14	0.49	0
5	1PE	J	15	-	11,11,15	0.70	0	10,10,14	0.68	0
5	1PE	C	41	-	7,7,15	0.59	0	6,6,14	0.45	0
4	SO4	B	3	-	4,4,4	0.40	0	6,6,6	0.43	0
5	1PE	K	36	-	10,10,15	0.79	0	9,9,14	0.52	0
5	1PE	F	33	-	9,9,15	0.61	0	8,8,14	0.65	0
5	1PE	G	30	-	6,6,15	0.33	0	5,5,14	0.51	0
4	SO4	B	12	-	4,4,4	0.41	0	6,6,6	0.29	0
5	1PE	L	59	-	11,11,15	0.66	0	10,10,14	0.76	0
5	1PE	L	56	-	10,10,15	0.66	0	9,9,14	0.51	0
4	SO4	K	18	-	4,4,4	0.49	0	6,6,6	0.53	0
5	1PE	A	24	-	8,8,15	0.62	0	7,7,14	0.90	0
4	SO4	J	20	-	4,4,4	0.32	0	6,6,6	0.29	0
3	CO3	E	1002	-	3,3,3	0.43	0	2,3,3	1.79	0
4	SO4	G	23	-	4,4,4	0.50	0	6,6,6	0.25	0
5	1PE	G	16	-	9,9,15	0.55	0	8,8,14	0.70	0
5	1PE	E	28	-	10,10,15	0.91	0	9,9,14	0.75	0
5	1PE	D	44	-	10,10,15	0.75	0	9,9,14	0.77	0
5	1PE	F	53	-	11,11,15	0.77	0	10,10,14	0.47	0
5	1PE	K	52	-	10,10,15	0.48	0	9,9,14	0.66	0
5	1PE	G	47	-	5,5,15	0.62	0	4,4,14	0.82	0
6	2PE	H	6	-	24,24,27	0.51	0	23,23,26	0.75	0
5	1PE	J	45	-	10,10,15	0.63	0	9,9,14	0.50	0
6	2PE	B	13	-	23,23,27	0.61	0	22,22,26	0.36	0
5	1PE	L	29	-	9,9,15	0.38	0	8,8,14	0.87	0
3	CO3	J	1002	-	3,3,3	2.00	1 (33%)	2,3,3	1.81	1 (50%)
5	1PE	K	5	-	11,11,15	0.55	0	10,10,14	0.68	0
5	1PE	I	21	-	14,14,15	0.58	0	13,13,14	0.57	0
5	1PE	A	20	-	11,11,15	0.92	0	10,10,14	0.90	0
5	1PE	I	61	-	4,4,15	0.29	0	3,3,14	0.60	0
4	SO4	C	15	-	4,4,4	0.30	0	6,6,6	0.14	0
4	SO4	C	16	-	4,4,4	0.21	0	6,6,6	0.47	0
3	CO3	H	1002	-	3,3,3	0.46	0	2,3,3	1.33	0
5	1PE	A	57	-	5,5,15	0.69	0	4,4,14	0.58	0
3	CO3	K	1002	-	3,3,3	0.65	0	2,3,3	3.48	2 (100%)
5	1PE	J	2	-	10,10,15	0.55	0	9,9,14	1.20	1 (11%)
4	SO4	I	17	-	4,4,4	0.46	0	6,6,6	0.31	0
5	1PE	L	25	-	11,11,15	0.49	0	10,10,14	0.52	0
5	1PE	K	50	-	5,5,15	0.58	0	4,4,14	0.42	0
5	1PE	C	17	-	12,12,15	0.74	0	11,11,14	0.93	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	G	48	-	5,5,15	0.55	0	4,4,14	0.62	0
6	2PE	B	14	-	25,25,27	0.52	0	24,24,26	0.59	0
5	1PE	E	46	-	8,8,15	0.62	0	7,7,14	0.59	0
5	1PE	I	27	-	8,8,15	0.52	0	7,7,14	0.31	0
4	SO4	D	10	-	4,4,4	0.32	0	6,6,6	0.24	0
5	1PE	G	58	-	14,14,15	0.63	0	13,13,14	0.88	0
5	1PE	D	62	-	4,4,15	0.55	0	3,3,14	0.62	0
4	SO4	E	11	-	4,4,4	0.26	0	6,6,6	0.44	0
5	1PE	A	19	-	8,8,15	0.58	0	7,7,14	0.71	0
4	SO4	K	19	-	4,4,4	0.46	0	6,6,6	0.46	0
3	CO3	A	1002	-	3,3,3	0.48	0	2,3,3	2.22	2 (100%)
5	1PE	D	612	-	8,8,15	0.78	0	7,7,14	0.67	0
3	CO3	I	1002	-	3,3,3	1.27	0	2,3,3	2.06	2 (100%)
5	1PE	J	60	-	8,8,15	0.70	0	7,7,14	0.66	0
5	1PE	J	3	-	9,9,15	0.82	0	8,8,14	1.07	0
5	1PE	H	54	-	10,10,15	0.67	0	9,9,14	0.76	0
3	CO3	C	1002	-	3,3,3	1.01	0	2,3,3	1.75	1 (50%)
5	1PE	K	55	-	7,7,15	0.51	0	6,6,14	0.42	0
5	1PE	D	23	-	10,10,15	0.69	0	9,9,14	0.49	0
3	CO3	F	1002	-	3,3,3	0.93	0	2,3,3	0.63	0
4	SO4	D	5	-	4,4,4	0.31	0	6,6,6	0.65	0
5	1PE	K	4	-	11,11,15	1.05	0	10,10,14	1.33	1 (10%)

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
5	1PE	E	8	-	-	0/9/9/13	-
5	1PE	G	16	-	-	6/7/7/13	-
5	1PE	K	50	-	-	3/3/3/13	-
5	1PE	E	28	-	-	5/8/8/13	-
5	1PE	C	17	-	-	3/10/10/13	-
5	1PE	H	51	-	-	1/3/3/13	-
5	1PE	K	42	-	-	2/8/8/13	-
5	1PE	G	48	-	-	2/3/3/13	-
6	2PE	B	14	-	-	8/23/23/25	-
5	1PE	D	44	-	-	3/8/8/13	-
5	1PE	E	46	-	-	3/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	C	18	-	-	4/6/6/13	-
5	1PE	D	9	-	-	7/7/7/13	-
5	1PE	F	53	-	-	9/9/9/13	-
5	1PE	I	22	-	-	0/8/8/13	-
5	1PE	D	34	-	-	4/7/7/13	-
5	1PE	I	27	-	-	3/6/6/13	-
6	2PE	F	63	-	-	2/3/3/25	-
5	1PE	B	40	-	-	3/8/8/13	-
5	1PE	K	52	-	-	6/8/8/13	-
5	1PE	F	31	-	-	2/7/7/13	-
5	1PE	L	1	-	-	3/7/7/13	-
5	1PE	J	49	-	-	4/8/8/13	-
5	1PE	F	32	-	-	3/7/7/13	-
5	1PE	G	58	-	-	2/12/12/13	-
5	1PE	D	62	-	-	1/2/2/13	-
5	1PE	G	47	-	-	2/3/3/13	-
6	2PE	H	6	-	-	15/22/22/25	-
5	1PE	J	15	-	-	6/9/9/13	-
5	1PE	A	19	-	-	4/6/6/13	-
5	1PE	E	43	-	-	2/5/5/13	-
5	1PE	C	41	-	-	3/5/5/13	-
5	1PE	J	45	-	-	5/8/8/13	-
6	2PE	B	13	-	-	13/21/21/25	-
5	1PE	K	36	-	-	5/8/8/13	-
5	1PE	F	33	-	-	5/7/7/13	-
5	1PE	L	29	-	-	5/7/7/13	-
5	1PE	G	30	-	-	2/4/4/13	-
5	1PE	K	5	-	-	3/9/9/13	-
5	1PE	I	21	-	-	7/12/12/13	-
5	1PE	A	20	-	-	6/9/9/13	-
5	1PE	I	61	-	-	0/2/2/13	-
5	1PE	L	59	-	-	5/9/9/13	-
5	1PE	D	612	-	-	3/6/6/13	-
5	1PE	A	57	-	-	2/3/3/13	-
5	1PE	J	60	-	-	4/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	E	35	-	-	5/7/7/13	-
5	1PE	J	3	-	-	5/7/7/13	-
5	1PE	G	12	-	-	6/6/6/13	-
5	1PE	L	56	-	-	3/8/8/13	-
5	1PE	H	54	-	-	7/8/8/13	-
5	1PE	K	55	-	-	2/5/5/13	-
5	1PE	J	2	-	-	5/8/8/13	-
5	1PE	A	24	-	-	4/6/6/13	-
5	1PE	E	7	-	-	1/9/9/13	-
5	1PE	L	25	-	-	6/9/9/13	-
5	1PE	D	23	-	-	4/8/8/13	-
5	1PE	K	4	-	-	4/9/9/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1002	CO3	O1-C	3.29	1.37	1.25

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1002	CO3	O2-C-O1	-3.95	109.56	119.68
5	K	4	1PE	OH5-C14-C24	3.07	124.33	110.35
3	B	1002	CO3	O3-C-O1	-3.04	111.90	119.68
3	K	1002	CO3	O3-C-O1	2.94	127.20	119.68
3	G	1002	CO3	O2-C-O1	2.53	126.15	119.68

There are no chirality outliers.

5 of 238 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	52	1PE	C24-C14-OH5-C25
6	B	13	2PE	C12-C11-O10-C9
6	H	6	2PE	C24-C23-O22-C21
6	B	14	2PE	O13-C14-C15-O16
5	D	9	1PE	OH5-C14-C24-OH4

There are no ring outliers.

48 monomers are involved in 116 short contacts:

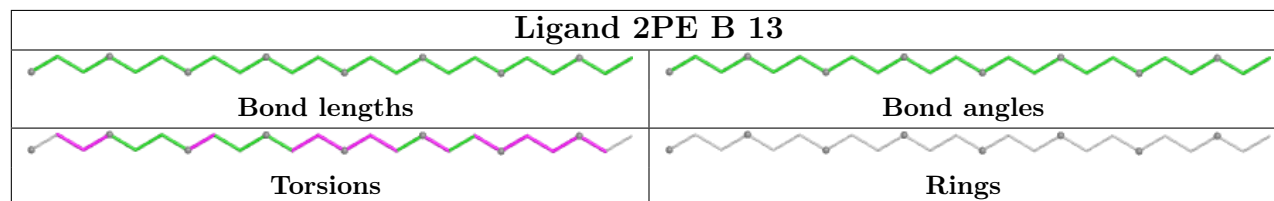
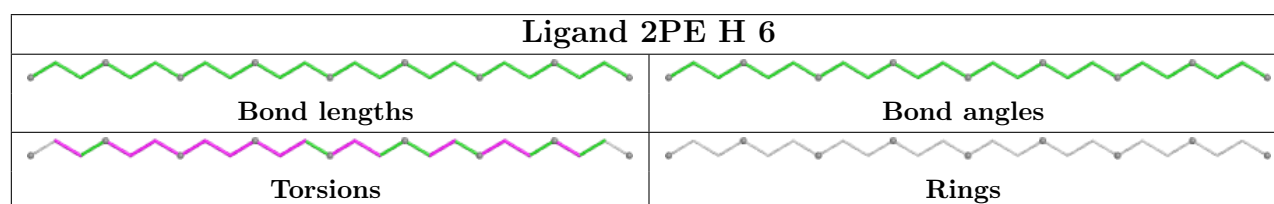
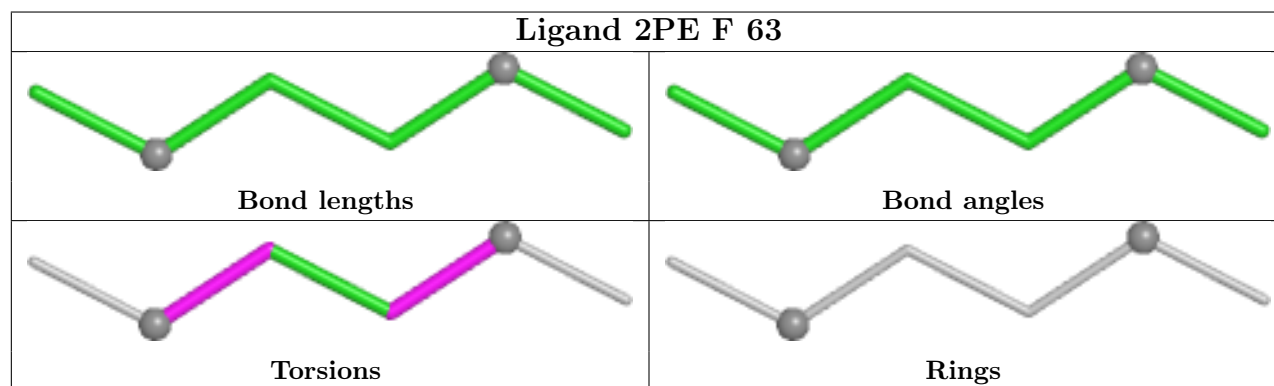
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	51	1PE	2	0
5	C	18	1PE	1	0
5	D	9	1PE	1	0
5	B	40	1PE	6	0
4	A	1	SO4	1	0
5	J	49	1PE	5	0
5	E	43	1PE	1	0
5	D	34	1PE	1	0
5	F	31	1PE	1	0
5	L	1	1PE	1	0
5	F	32	1PE	3	0
5	J	15	1PE	2	0
5	C	41	1PE	1	0
4	B	3	SO4	1	0
5	F	33	1PE	1	0
5	L	59	1PE	1	0
5	L	56	1PE	1	0
4	K	18	SO4	1	0
5	A	24	1PE	3	0
5	G	16	1PE	2	0
5	E	28	1PE	5	0
5	D	44	1PE	1	0
5	F	53	1PE	1	0
5	K	52	1PE	2	0
6	H	6	2PE	1	0
5	J	45	1PE	4	0
6	B	13	2PE	10	0
5	L	29	1PE	2	0
5	I	21	1PE	6	0
5	A	20	1PE	1	0
5	I	61	1PE	7	0
5	A	57	1PE	2	0
5	J	2	1PE	4	0
5	L	25	1PE	6	0
5	G	48	1PE	1	0
6	B	14	2PE	4	0
5	E	46	1PE	1	0
5	I	27	1PE	7	0
5	G	58	1PE	1	0
5	D	62	1PE	2	0
4	K	19	SO4	1	0
5	D	612	1PE	1	0
5	J	60	1PE	2	0

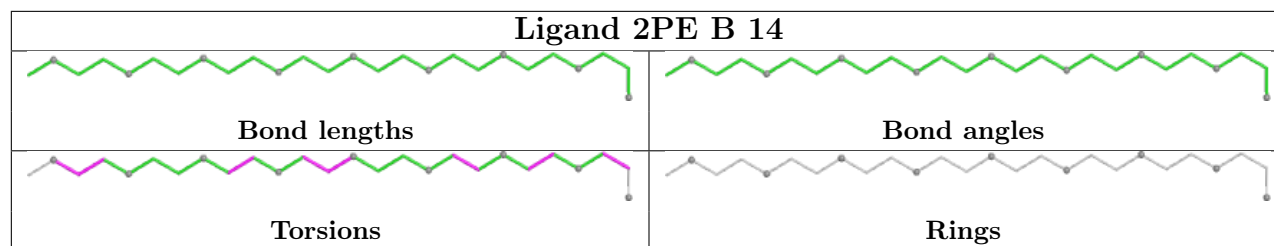
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	3	1PE	6	0
5	H	54	1PE	1	0
5	K	55	1PE	1	0
5	D	23	1PE	1	0
5	K	4	1PE	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	514/528 (97%)	-0.54	1 (0%)	91 90	5, 13, 30, 50	1 (0%)
1	B	510/528 (96%)	0.31	34 (6%)	24 22	5, 16, 49, 65	1 (0%)
1	C	518/528 (98%)	-0.38	3 (0%)	85 85	4, 13, 35, 54	1 (0%)
1	D	514/528 (97%)	-0.50	5 (0%)	79 79	5, 12, 30, 50	0
1	E	509/528 (96%)	-0.62	1 (0%)	91 90	5, 11, 25, 42	0
1	F	510/528 (96%)	0.32	29 (5%)	29 28	4, 15, 39, 56	0
1	G	514/528 (97%)	-0.55	4 (0%)	82 82	6, 12, 30, 51	0
1	H	510/528 (96%)	0.42	42 (8%)	17 16	5, 16, 49, 65	1 (0%)
1	I	515/528 (97%)	-0.19	7 (1%)	73 73	5, 13, 35, 50	0
1	J	514/528 (97%)	-0.52	3 (0%)	85 85	5, 12, 30, 53	0
1	K	509/528 (96%)	-0.54	2 (0%)	88 88	5, 11, 25, 42	0
1	L	508/528 (96%)	-0.14	10 (1%)	65 64	4, 12, 36, 47	0
All	All	6145/6336 (96%)	-0.25	141 (2%)	61 60	4, 13, 37, 65	4 (0%)

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	603	ASP	5.6
1	L	603	ASP	4.7
1	C	260	ASN	4.7
1	F	153	VAL	4.5
1	D	603	ASP	4.4

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 ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	2PE	B	13	24/28	0.56	0.35	98,109,127,128	0
2	ZN	J	1001	1/1	0.73	0.20	92,92,92,92	0
4	SO4	C	15	5/5	0.74	0.14	90,90,94,94	0
4	SO4	J	20	5/5	0.75	0.17	62,70,75,78	0
4	SO4	E	11	5/5	0.75	0.20	72,78,89,93	0
4	SO4	D	10	5/5	0.76	0.14	60,66,69,70	0
5	1PE	F	53	12/16	0.77	0.17	42,46,56,59	0
4	SO4	B	12	5/5	0.77	0.13	67,72,76,81	0
2	ZN	D	1001	1/1	0.79	0.22	71,71,71,71	0
5	1PE	D	44	11/16	0.79	0.16	26,33,44,54	0
6	2PE	F	63	6/28	0.79	0.17	37,39,45,46	0
5	1PE	A	20	12/16	0.80	0.15	19,39,49,50	0
2	ZN	F	1001	1/1	0.81	0.17	82,82,82,82	0
5	1PE	J	45	11/16	0.81	0.15	24,33,44,53	0
5	1PE	E	28	11/16	0.83	0.14	26,40,43,43	0
5	1PE	K	36	11/16	0.83	0.14	32,40,51,54	0
5	1PE	L	59	12/16	0.83	0.14	31,41,46,47	0
2	ZN	H	1001	1/1	0.83	0.23	73,73,73,73	0
5	1PE	H	51	6/16	0.83	0.16	32,39,43,50	0
5	1PE	C	17	13/16	0.84	0.12	18,36,44,45	0
4	SO4	C	16	5/5	0.84	0.15	52,59,75,85	0
5	1PE	J	15	12/16	0.84	0.15	26,35,42,44	0
5	1PE	B	40	11/16	0.84	0.15	35,39,53,54	0
5	1PE	L	56	11/16	0.85	0.14	39,45,52,59	0
5	1PE	E	46	9/16	0.85	0.15	18,37,43,46	0
5	1PE	D	612	9/16	0.86	0.12	23,30,38,42	0
5	1PE	F	32	10/16	0.86	0.12	37,43,46,48	0
4	SO4	G	23	5/5	0.86	0.11	49,50,60,67	0
5	1PE	A	57	6/16	0.86	0.11	28,32,42,50	0
5	1PE	H	54	11/16	0.86	0.14	24,41,47,49	0
5	1PE	I	21	15/16	0.86	0.13	24,33,58,58	0
5	1PE	I	27	9/16	0.86	0.13	29,41,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	1PE	K	50	6/16	0.87	0.13	29,33,39,39	0
5	1PE	K	52	11/16	0.87	0.13	38,46,54,56	0
5	1PE	K	55	8/16	0.87	0.15	19,44,50,53	0
5	1PE	D	34	10/16	0.87	0.11	33,39,46,47	0
5	1PE	E	7	12/16	0.87	0.11	24,31,38,40	0
5	1PE	G	58	15/16	0.87	0.12	20,34,50,51	0
5	1PE	I	22	11/16	0.87	0.13	20,26,37,39	0
5	1PE	D	23	11/16	0.88	0.16	29,42,58,65	0
5	1PE	G	16	10/16	0.88	0.12	37,41,45,49	0
5	1PE	G	48	6/16	0.88	0.13	27,32,36,37	0
5	1PE	C	18	9/16	0.88	0.11	16,24,32,40	0
5	1PE	A	24	9/16	0.88	0.13	30,38,42,44	0
5	1PE	D	62	5/16	0.88	0.12	31,31,34,49	0
5	1PE	K	42	11/16	0.88	0.12	29,37,42,45	0
4	SO4	K	19	5/5	0.89	0.14	34,54,58,61	0
5	1PE	K	4	12/16	0.89	0.11	14,29,42,46	0
5	1PE	G	12	9/16	0.89	0.11	10,16,31,32	0
4	SO4	D	5	5/5	0.89	0.12	43,55,68,70	0
5	1PE	J	60	9/16	0.89	0.10	30,35,41,45	0
5	1PE	J	49	11/16	0.90	0.11	27,35,43,45	0
5	1PE	E	35	10/16	0.90	0.10	24,39,42,49	0
5	1PE	C	41	8/16	0.90	0.12	33,41,44,46	0
5	1PE	J	3	10/16	0.90	0.10	29,34,41,43	0
4	SO4	A	2	5/5	0.90	0.14	35,37,52,57	0
6	2PE	B	14	26/28	0.90	0.11	23,40,47,51	0
5	1PE	F	33	10/16	0.90	0.10	19,31,46,47	0
5	1PE	E	43	8/16	0.91	0.10	24,31,34,38	0
5	1PE	L	25	12/16	0.91	0.09	20,33,39,44	0
5	1PE	L	29	10/16	0.91	0.11	37,42,50,55	0
5	1PE	J	2	11/16	0.91	0.11	12,33,44,49	0
5	1PE	D	9	10/16	0.92	0.10	21,29,40,42	0
5	1PE	G	30	7/16	0.92	0.10	34,41,45,49	0
5	1PE	F	31	10/16	0.92	0.10	20,33,41,42	0
5	1PE	A	19	9/16	0.92	0.09	22,28,31,33	0
4	SO4	C	6	5/5	0.92	0.16	23,25,33,36	0
2	ZN	B	1001	1/1	0.92	0.16	60,60,60,60	0
2	ZN	L	1001	1/1	0.92	0.26	65,65,65,65	0
6	2PE	H	6	25/28	0.92	0.10	20,37,50,52	0
5	1PE	G	47	6/16	0.93	0.09	20,27,30,51	0
3	CO3	G	1002	4/4	0.93	0.09	14,18,22,25	0
2	ZN	K	1001	1/1	0.94	0.18	60,60,60,60	0
5	1PE	I	61	5/16	0.94	0.08	15,24,28,33	0

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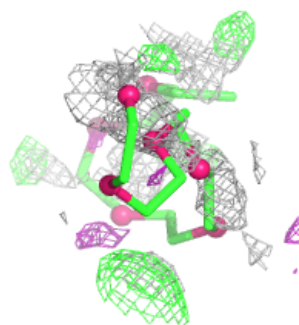
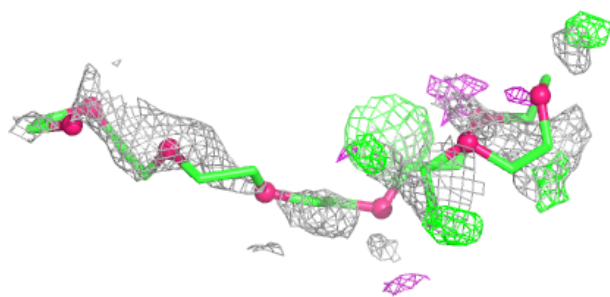
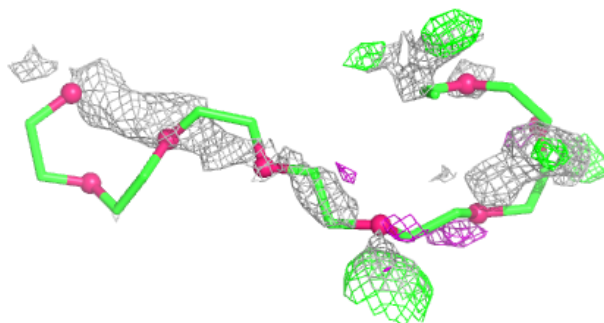
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1	5/5	0.95	0.10	39,51,58,63	0
5	1PE	K	5	12/16	0.95	0.09	18,25,40,41	0
2	ZN	C	1001	1/1	0.95	0.21	59,59,59,59	0
5	1PE	E	8	12/16	0.95	0.09	20,23,50,51	0
3	CO3	E	1002	4/4	0.95	0.06	16,20,22,22	0
3	CO3	F	1002	4/4	0.95	0.07	21,22,23,28	0
2	ZN	E	1001	1/1	0.95	0.19	67,67,67,67	0
2	ZN	I	1001	1/1	0.96	0.16	64,64,64,64	0
5	1PE	L	1	10/16	0.96	0.07	17,24,39,46	0
3	CO3	H	1002	4/4	0.96	0.05	13,13,16,17	0
3	CO3	J	1002	4/4	0.96	0.06	9,13,15,17	0
3	CO3	A	1002	4/4	0.96	0.07	14,16,17,24	0
3	CO3	B	1002	4/4	0.96	0.07	13,15,17,20	0
3	CO3	C	1002	4/4	0.96	0.06	14,14,19,20	0
3	CO3	D	1002	4/4	0.96	0.05	13,14,17,20	0
2	ZN	G	1001	1/1	0.96	0.17	74,74,74,74	0
2	ZN	A	1001	1/1	0.96	0.14	77,77,77,77	0
3	CO3	K	1002	4/4	0.97	0.06	10,12,17,17	0
3	CO3	L	1002	4/4	0.97	0.08	6,8,15,16	0
3	CO3	I	1002	4/4	0.97	0.05	11,12,13,18	0
4	SO4	D	7	5/5	0.98	0.06	12,15,17,18	0
4	SO4	K	18	5/5	0.99	0.05	8,12,14,15	0
4	SO4	I	17	5/5	0.99	0.04	10,11,14,16	0
4	SO4	B	3	5/5	0.99	0.03	11,12,12,13	0

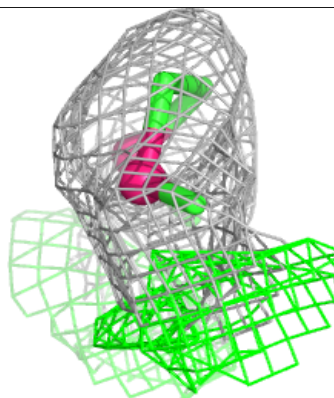
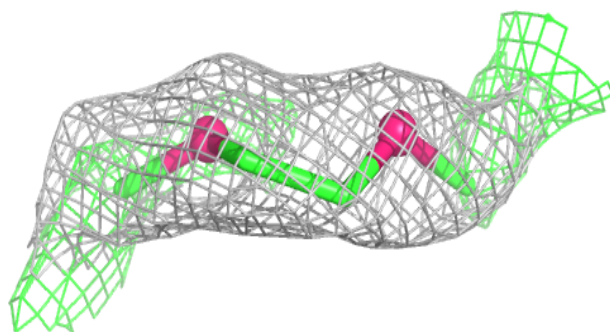
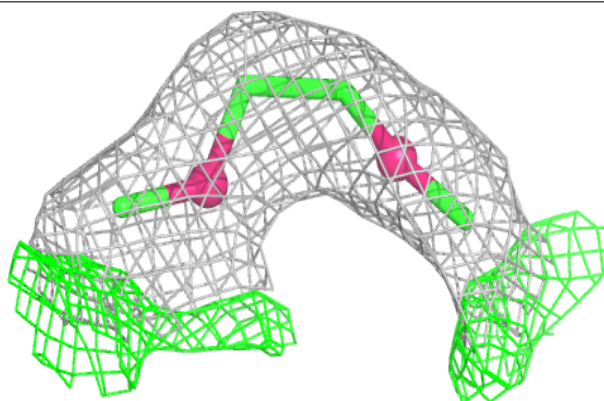
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PE B 13:

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

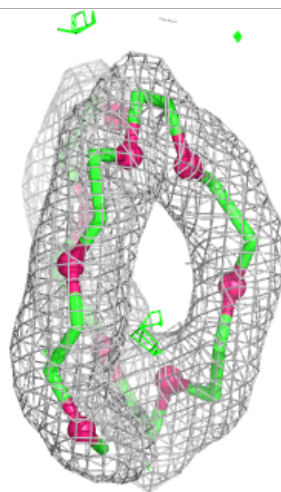
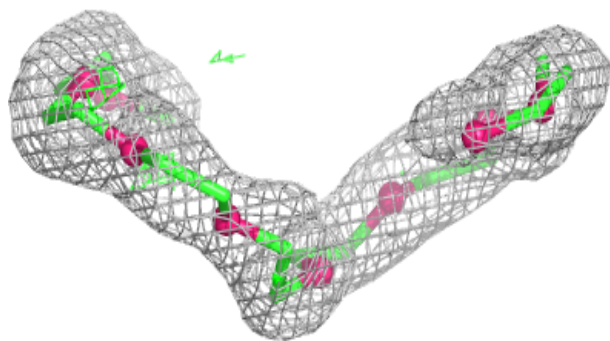
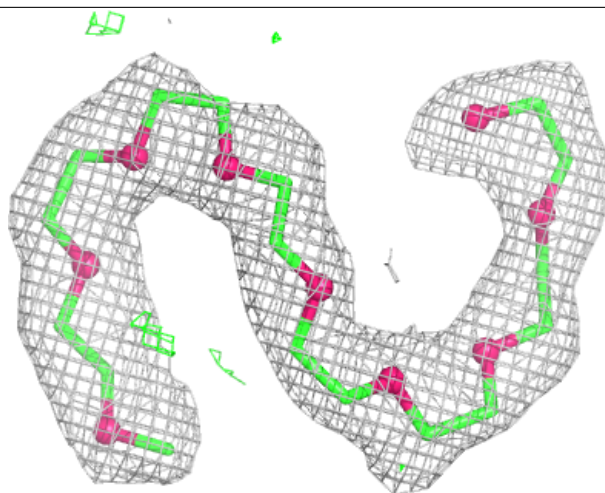
**Electron density around 2PE F 63:**

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



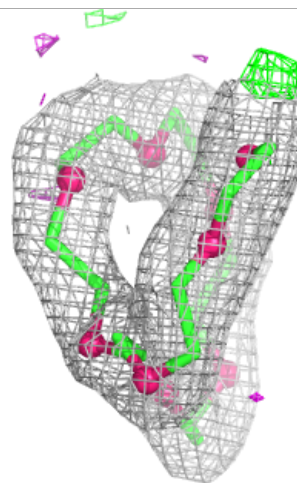
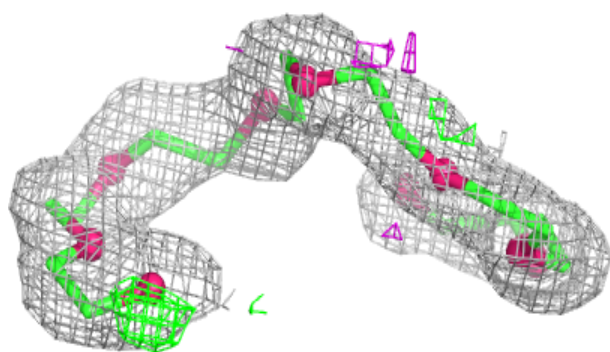
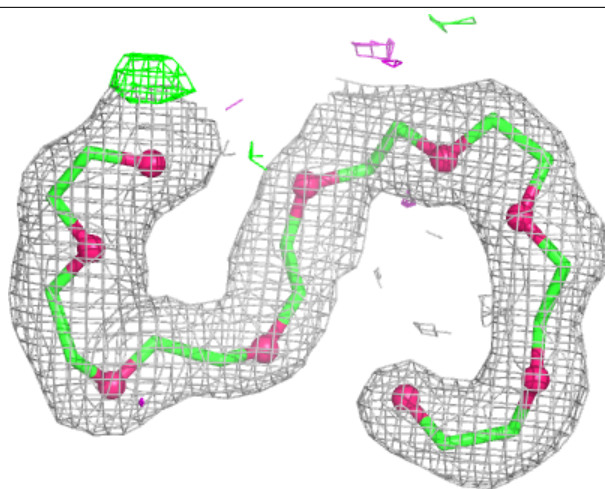
Electron density around 2PE B 14:

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



Electron density around 2PE H 6:

$2mF_o-DF_c$ (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.