



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 12:46 AM EDT

PDB ID : 3KQZ  
Title : Structure of a protease 2  
Authors : McGowan, S.; Whisstock, J.C.  
Deposited on : 2009-11-17  
Resolution : 2.39 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

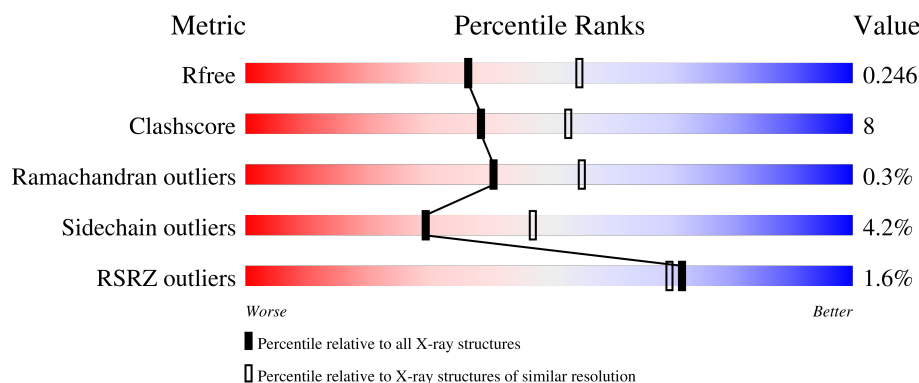
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	528	<div> <div>0%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	B	528	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	C	528	<div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	D	528	<div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	E	528	<div> <div>79%</div> <div>16%</div> <div>..</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	K	18	-	-	X	-
5	1PE	L	25	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50062 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	0	0	0
			3941	2534	632	756	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	0	0
			3952	2542	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
			3798	2445	612	722	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
			3866	2488	624	735	19			
1	I	515	Total	C	N	O	S	0	0	0
			3930	2529	633	749	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
			3891	2507	624	741	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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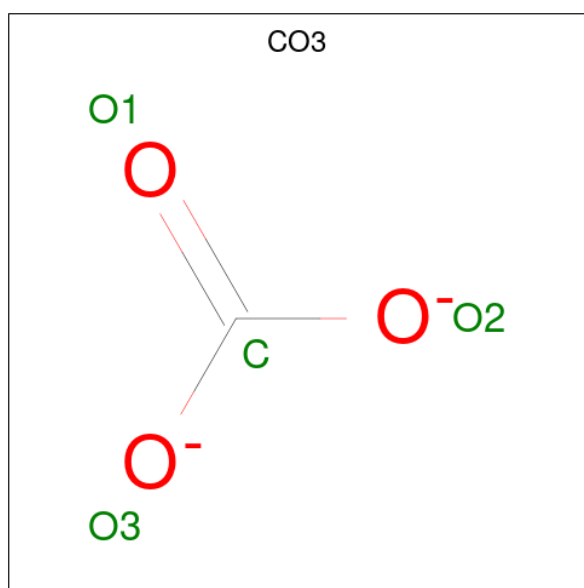
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression 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 CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

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

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

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

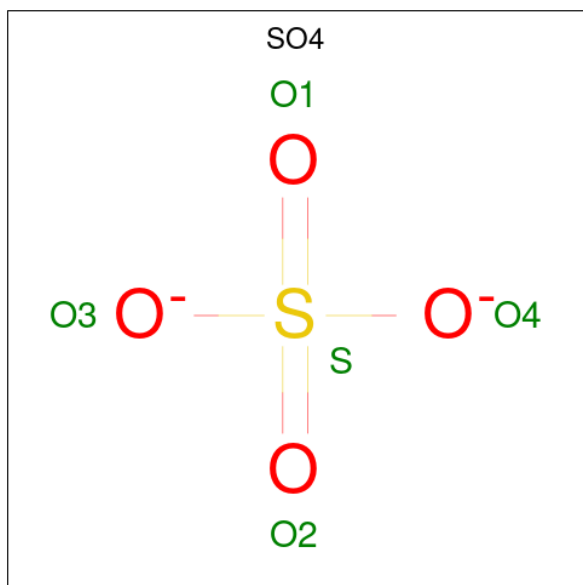
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	Zn	0	0
			2	2		
3	K	2	Total	Zn	0	0
			2	2		
3	L	2	Total	Zn	0	0
			2	2		

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



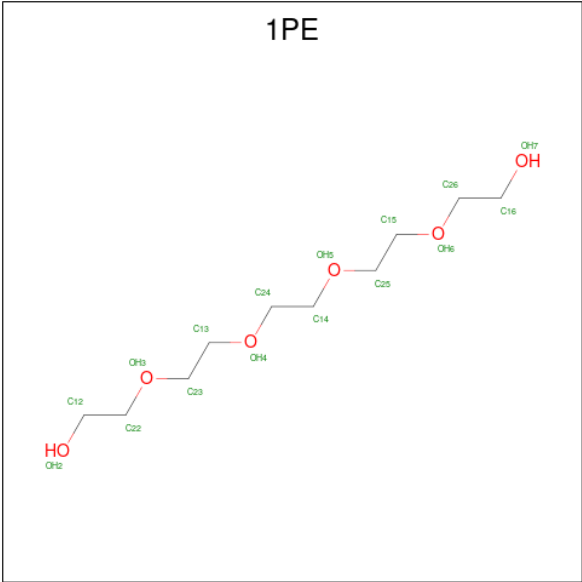
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
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	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	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		
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 (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



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		
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		

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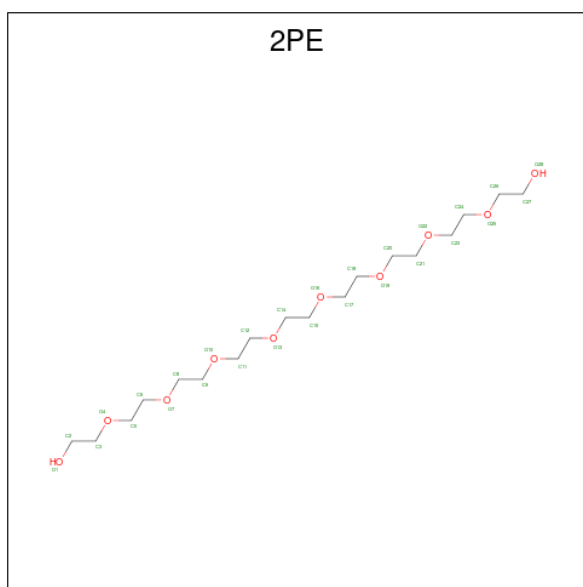
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			12	8	4		
5	E	1	Total	C	O	0	0
			12	8	4		
5	E	1	Total	C	O	0	0
			11	7	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			8	5	3		
5	E	1	Total	C	O	0	0
			9	6	3		
5	F	1	Total	C	O	0	0
			10	6	4		
5	F	1	Total	C	O	0	0
			10	6	4		
5	F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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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 (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 26	C 17	O 9	0	0
6	F	1	Total 6	C 4	O 2	0	0
6	H	1	Total 25	C 16	O 9	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	224	Total O 224 224	0	0
7	B	180	Total O 180 180	0	0
7	C	242	Total O 242 242	0	0
7	D	249	Total O 249 249	0	0
7	E	257	Total O 257 257	0	0
7	F	156	Total O 156 156	0	0
7	G	230	Total O 230 230	0	0
7	H	163	Total O 163 163	0	0
7	I	180	Total O 180 180	0	0

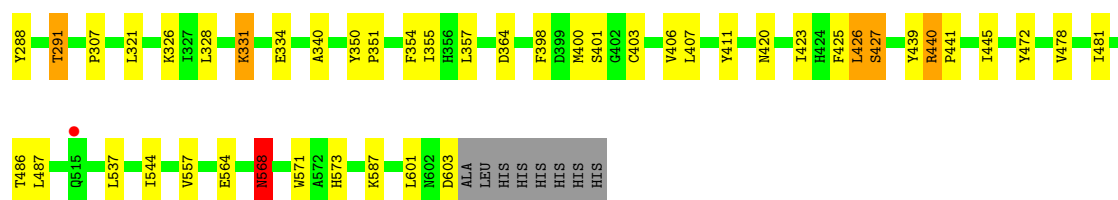
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	219	Total 219	O 219	0	0
7	K	237	Total 237	O 237	0	0
7	L	186	Total 186	O 186	0	0

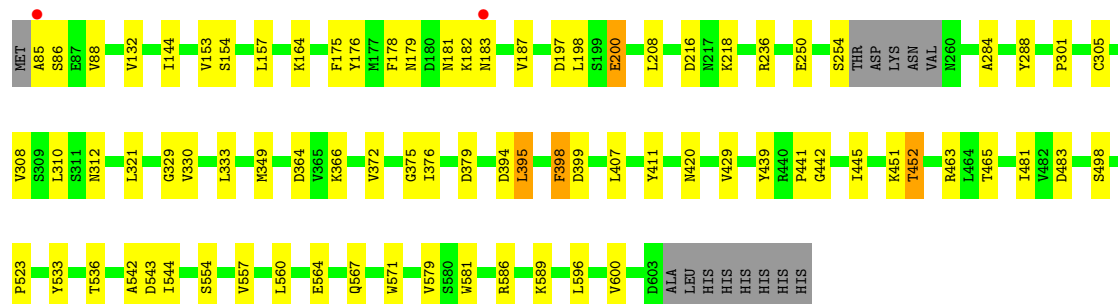






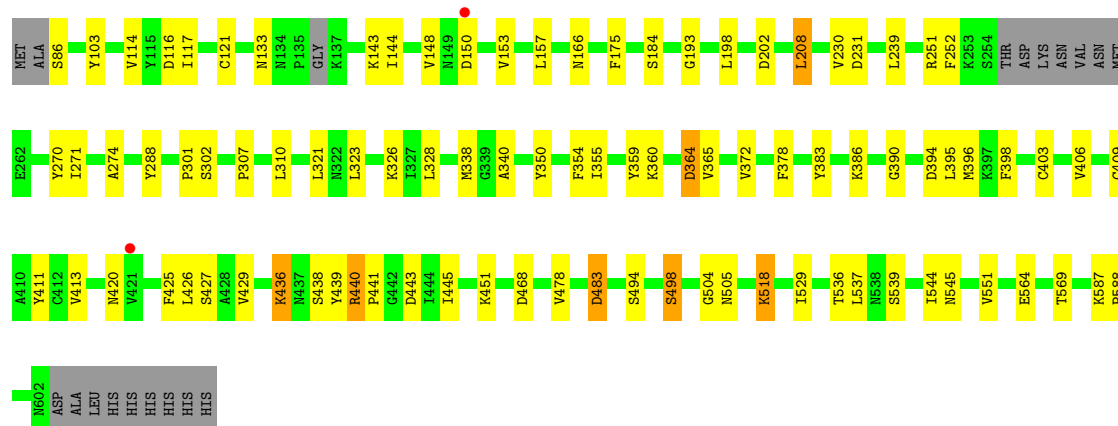
● Molecule 1: M17 leucyl aminopeptidase

Chain D: 82% 15% ..



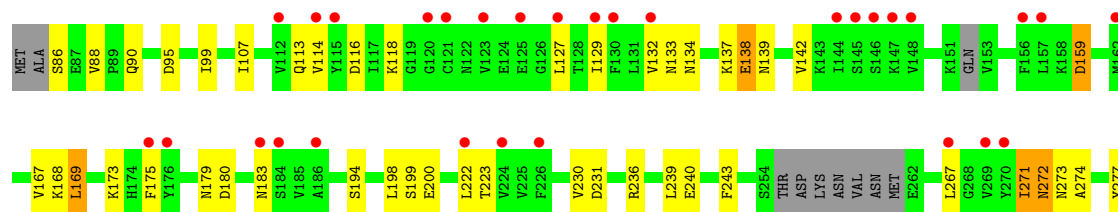
● Molecule 1: M17 leucyl aminopeptidase

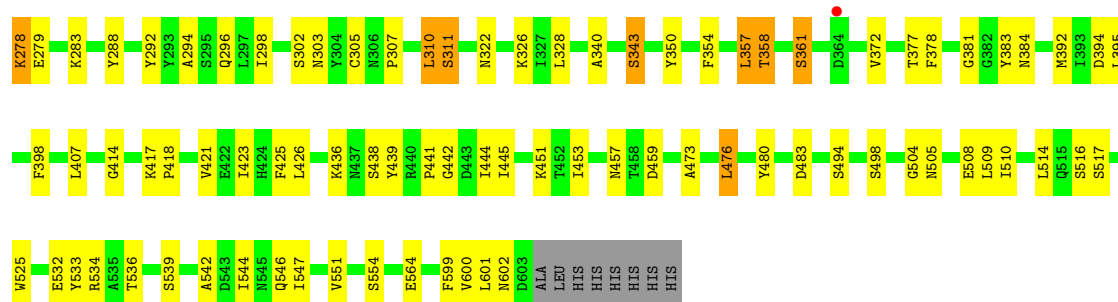
Chain E: 79% 16% ..



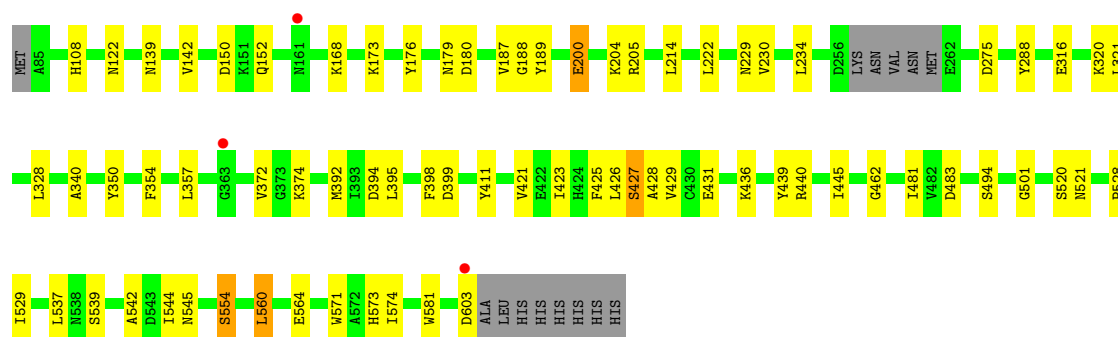
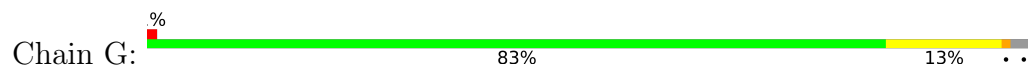
● Molecule 1: M17 leucyl aminopeptidase

Chain F: 6% 72% 22% ..

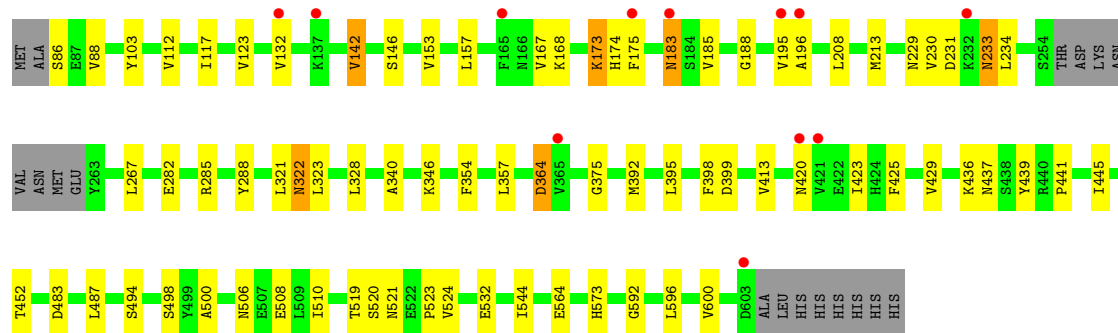
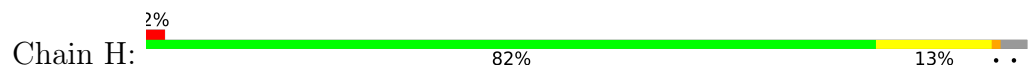




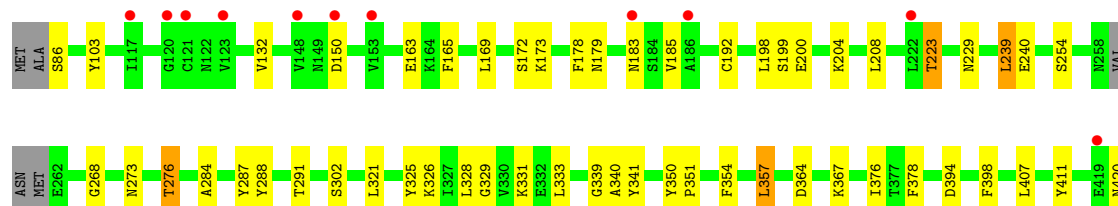
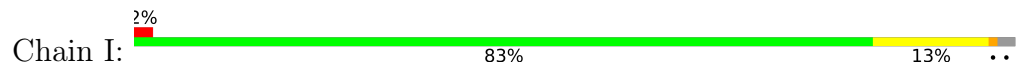
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



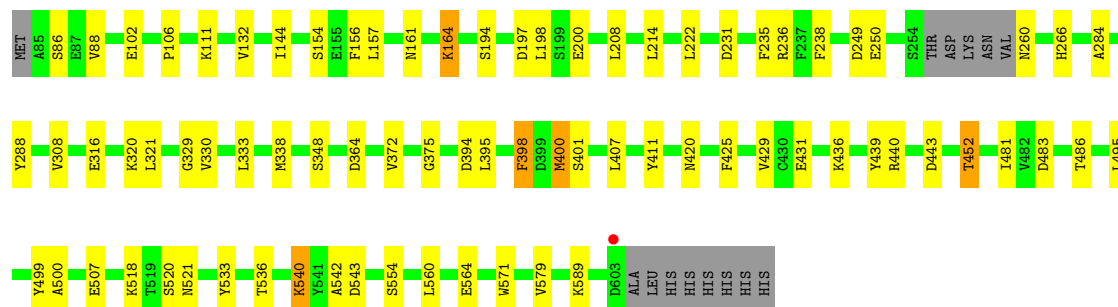
• Molecule 1: M17 leucyl aminopeptidase





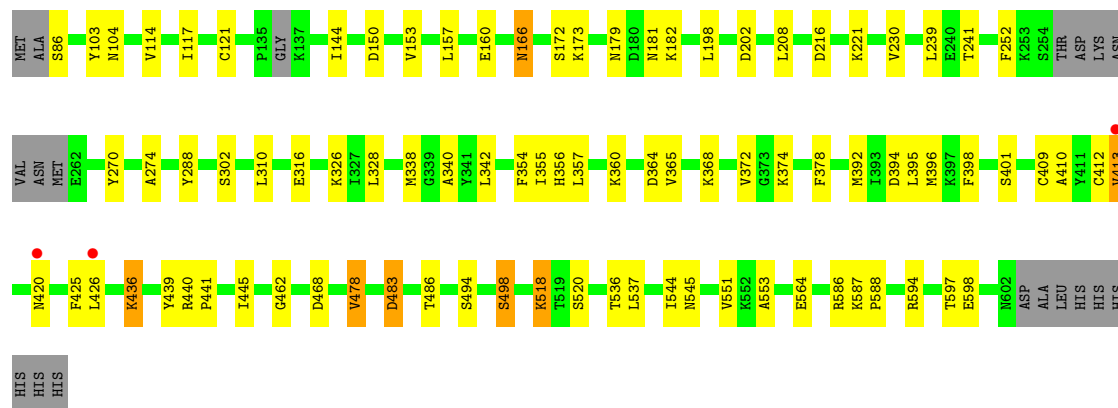
• Molecule 1: M17 leucyl aminopeptidase

Chain J: 83% 14% . .



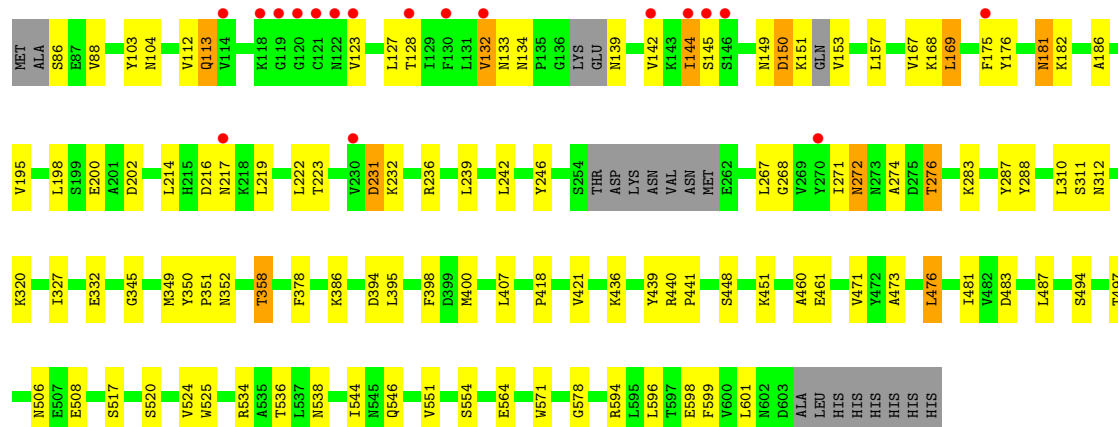
• Molecule 1: M17 leucyl aminopeptidase

Chain K: 80% 15% . .



• Molecule 1: M17 leucyl aminopeptidase

Chain L: 3% 75% 19% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.70Å 173.73Å 220.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.08 – 2.39 56.08 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (56.08-2.39) 99.1 (56.08-2.39)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.176 , 0.242 0.182 , 0.246	Depositor DCC
$R_{free}$ test set	12914 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	50062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 47.05 % 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 1.0488e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.84	0/4017	0.81	2/5448 (0.0%)
1	B	0.78	0/3944	0.79	0/5357
1	C	0.85	0/4030	0.79	0/5469
1	D	0.87	0/4008	0.83	2/5435 (0.0%)
1	E	0.89	0/3964	0.83	1/5378 (0.0%)
1	F	0.82	0/3874	0.86	2/5273 (0.0%)
1	G	0.83	0/4022	0.79	2/5455 (0.0%)
1	H	0.76	0/3943	0.77	1/5356 (0.0%)
1	I	0.84	0/4007	0.81	0/5437
1	J	0.88	0/4008	0.82	1/5435 (0.0%)
1	K	0.89	1/3967 (0.0%)	0.81	1/5382 (0.0%)
1	L	0.87	1/3883 (0.0%)	0.87	0/5279
All	All	0.84	2/47667 (0.0%)	0.81	12/64704 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	461	GLU	CD-OE1	5.98	1.32	1.25
1	K	121	CYS	CB-SG	-5.31	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	594	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	D	463	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	586	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	H	399	ASP	CB-CG-OD2	5.77	123.49	118.30
1	F	169	LEU	CA-CB-CG	5.42	127.77	115.30
1	G	399	ASP	CB-CG-OD2	5.40	123.16	118.30
1	F	534	ARG	NE-CZ-NH1	5.24	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	459	ASP	CB-CG-OD1	5.18	122.96	118.30
1	J	249	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	G	560	LEU	CA-CB-CG	5.11	127.05	115.30
1	E	251	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3941	0	3868	73	0
1	B	3867	0	3762	61	1
1	C	3952	0	3877	52	0
1	D	3931	0	3866	56	1
1	E	3888	0	3810	65	0
1	F	3798	0	3614	95	0
1	G	3945	0	3873	48	0
1	H	3866	0	3760	53	1
1	I	3930	0	3855	39	0
1	J	3931	0	3866	57	0
1	K	3891	0	3816	74	0
1	L	3809	0	3651	79	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	10	0	0	1	0
4	B	15	0	0	1	0
4	C	20	0	0	0	0
4	D	15	0	0	1	0
4	E	15	0	0	2	0
4	F	5	0	0	1	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	I	10	0	0	1	0
4	J	5	0	0	0	0
4	K	25	0	0	4	0
5	A	36	0	36	7	0
5	B	11	0	12	1	0
5	C	30	0	32	2	0
5	D	56	0	60	2	0
5	E	62	0	71	3	0
5	F	42	0	51	5	0
5	G	53	0	59	6	0
5	H	6	0	4	2	0
5	I	40	0	45	3	0
5	J	64	0	74	10	0
5	K	71	0	76	10	0
5	L	55	0	66	15	0
6	B	26	0	33	2	0
6	F	6	0	4	0	0
6	H	25	0	33	1	0
7	A	224	0	0	7	0
7	B	180	0	0	1	1
7	C	242	0	0	5	0
7	D	249	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	257	0	0	3	0
7	F	156	0	0	7	0
7	G	230	0	0	7	0
7	H	163	0	0	5	0
7	I	180	0	0	3	0
7	J	219	0	0	6	0
7	K	237	0	0	9	0
7	L	186	0	0	10	0
All	All	50062	0	46274	705	2

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 8.

All (705) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:395:LEU:HB2	5:K:55:1PE:OH6	1.26	1.31
1:B:216:ASP:CB	1:F:173:LYS:NZ	2.11	1.14
1:F:138:GLU:N	1:F:139:ASN:HA	1.50	1.14
1:J:452:THR:HG22	1:J:543:ASP:H	1.17	1.08
1:D:452:THR:HG22	1:D:543:ASP:H	1.18	1.08
1:L:451:LYS:HG2	5:L:25:1PE:H142	1.36	1.05
1:L:271:ILE:O	1:L:272:ASN:HB2	1.55	1.03
1:F:361:SER:HB2	1:F:421:VAL:O	1.58	1.01
1:B:216:ASP:CB	1:F:173:LYS:HZ3	1.72	0.96
1:E:395:LEU:HB2	7:E:3982:HOH:O	1.63	0.96
1:F:133:ASN:HA	1:F:167:VAL:HG11	1.46	0.96
1:F:138:GLU:H	1:F:139:ASN:HA	1.23	0.96
1:A:156:PHE:CD2	1:A:156:PHE:CZ	2.43	0.95
1:F:358:THR:HG22	7:F:1366:HOH:O	1.65	0.95
1:D:452:THR:HG21	1:E:252:PHE:O	1.66	0.94
1:K:409:CYS:O	1:K:413:VAL:HG22	1.65	0.94
1:J:452:THR:HG21	1:K:252:PHE:O	1.68	0.92
1:K:316:GLU:HG3	5:K:4:1PE:H152	1.52	0.92
1:E:409:CYS:O	1:E:413:VAL:HG23	1.69	0.91
1:B:216:ASP:CB	1:F:173:LYS:HZ2	1.83	0.90
1:D:179:ASN:ND2	1:D:183:ASN:HB2	1.87	0.89
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.56	0.87
1:K:395:LEU:CB	5:K:55:1PE:OH6	2.20	0.86
1:E:338:MET:HE2	1:E:468:ASP:HB3	1.59	0.85
1:A:498:SER:O	1:A:499:TYR:CD1	2.30	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:451:LYS:CG	5:L:25:1PE:H142	2.07	0.83
1:A:489:GLY:HA3	5:A:24:1PE:H252	1.58	0.83
1:K:413:VAL:HG21	1:K:425:PHE:HZ	1.42	0.83
1:B:515:GLN:HG2	7:B:2431:HOH:O	1.77	0.83
1:J:316:GLU:HG3	5:J:3:1PE:H141	1.61	0.83
1:D:178:PHE:CD1	1:D:182:LYS:O	2.32	0.82
1:E:150:ASP:HB3	1:E:153:VAL:HB	1.62	0.82
5:I:21:1PE:H262	7:I:3128:HOH:O	1.79	0.81
1:L:271:ILE:O	1:L:272:ASN:CB	2.29	0.81
1:K:338:MET:CE	1:K:468:ASP:HB3	2.11	0.80
1:I:440:ARG:HG3	1:I:440:ARG:HH11	1.46	0.80
1:D:178:PHE:HD1	1:D:182:LYS:O	1.65	0.80
1:F:271:ILE:O	1:F:272:ASN:HB2	1.82	0.79
1:E:338:MET:CE	1:E:468:ASP:HB3	2.12	0.79
1:F:138:GLU:N	1:F:139:ASN:CA	2.40	0.78
1:E:403:CYS:SG	1:E:427:SER:OG	2.38	0.78
1:J:452:THR:HG22	1:J:543:ASP:N	1.97	0.78
1:D:179:ASN:CG	1:D:183:ASN:HB2	2.05	0.77
1:K:394:ASP:OD2	5:K:55:1PE:C13	2.32	0.77
1:E:427:SER:O	1:E:429:VAL:HG23	1.84	0.76
1:A:529:ILE:HG22	1:A:560:LEU:HD13	1.69	0.75
1:L:133:ASN:HA	1:L:167:VAL:HG11	1.68	0.75
1:A:498:SER:C	1:A:499:TYR:HD1	1.88	0.75
1:G:122:ASN:OD1	5:G:48:1PE:H151	1.86	0.75
5:F:53:1PE:H242	7:F:4301:HOH:O	1.88	0.74
1:C:223:THR:HG23	7:C:2469:HOH:O	1.88	0.74
1:K:413:VAL:HG21	1:K:425:PHE:CZ	2.23	0.74
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.69	0.73
1:K:356:HIS:CD2	1:K:426:LEU:HD21	2.23	0.73
1:H:117:ILE:HD11	1:H:146:SER:OG	1.87	0.73
1:A:498:SER:OG	1:F:532:GLU:OE1	2.06	0.73
1:K:198:LEU:HD22	1:K:202:ASP:HB3	1.70	0.72
1:E:440:ARG:HH21	1:E:440:ARG:HG3	1.54	0.72
1:D:554:SER:HB3	7:D:875:HOH:O	1.89	0.72
1:A:498:SER:O	1:A:499:TYR:HD1	1.70	0.72
1:F:504:GLY:HA3	1:F:510:ILE:HD11	1.70	0.71
1:J:533:TYR:O	1:J:536:THR:HG22	1.91	0.71
1:G:374:LYS:HE3	1:G:462:GLY:HA3	1.73	0.71
1:J:320:LYS:HE2	5:J:3:1PE:H251	1.72	0.71
1:L:231:ASP:HB2	7:L:3184:HOH:O	1.89	0.70
1:L:86:SER:HB2	1:L:312:ASN:OD1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:332:GLU:HG3	7:L:2155:HOH:O	1.92	0.70
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.73	0.70
1:D:179:ASN:HD21	1:D:183:ASN:HB2	1.54	0.69
1:G:440:ARG:NH1	7:G:1234:HOH:O	2.24	0.69
1:B:320:LYS:HB3	6:B:14:2PE:H182	1.74	0.69
1:C:440:ARG:HH11	1:C:440:ARG:HG3	1.57	0.69
1:E:440:ARG:HH11	1:F:350:TYR:HE1	1.40	0.69
1:D:178:PHE:HA	1:D:183:ASN:O	1.93	0.69
1:A:529:ILE:CG2	1:A:560:LEU:HD13	2.23	0.68
1:I:178:PHE:HA	1:I:183:ASN:O	1.93	0.68
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.75	0.68
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.76	0.68
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.74	0.68
1:C:364:ASP:O	1:C:420:ASN:HA	1.94	0.67
1:J:411:TYR:CE1	5:J:2:1PE:H152	2.29	0.67
1:I:440:ARG:HG3	1:I:440:ARG:NH1	2.09	0.67
1:L:564:GLU:OE2	5:L:25:1PE:C12	2.43	0.67
1:K:356:HIS:CD2	1:K:426:LEU:CD2	2.78	0.67
1:L:451:LYS:HZ2	5:L:25:1PE:H141	1.60	0.67
1:K:518:LYS:NZ	5:K:52:1PE:H142	2.10	0.66
1:A:498:SER:O	1:A:523:PRO:HG2	1.95	0.66
1:L:232:LYS:HE3	1:L:276:THR:O	1.95	0.66
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.78	0.66
1:F:114:VAL:HG12	1:F:274:ALA:HB1	1.78	0.66
1:J:411:TYR:HE1	5:J:2:1PE:H152	1.60	0.66
1:L:104:ASN:HD22	5:L:1:1PE:H241	1.61	0.65
1:L:144:ILE:HG21	1:L:157:LEU:HD13	1.77	0.65
1:G:392:MET:HE3	1:G:395:LEU:HD22	1.78	0.65
1:B:216:ASP:CB	1:F:173:LYS:HD2	2.27	0.65
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.77	0.64
1:C:150:ASP:OD1	1:C:179:ASN:HB2	1.98	0.64
1:D:179:ASN:OD1	1:D:183:ASN:HB2	1.97	0.64
1:D:452:THR:HG22	1:D:543:ASP:N	2.02	0.64
1:F:451:LYS:HE2	5:F:612:1PE:H151	1.79	0.64
1:L:451:LYS:HG2	5:L:25:1PE:C14	2.23	0.64
1:I:364:ASP:O	1:I:420:ASN:HA	1.97	0.64
1:E:143:LYS:CG	7:E:3989:HOH:O	2.46	0.63
1:K:544:ILE:CD1	1:K:564:GLU:HG3	2.29	0.63
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.81	0.63
1:K:356:HIS:CG	1:K:426:LEU:CD2	2.82	0.63
1:I:172:SER:O	1:I:173:LYS:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.79	0.63
1:F:421:VAL:HG22	1:F:423:ILE:HG13	1.81	0.63
1:L:506:ASN:OD1	1:L:508:GLU:HG2	1.99	0.62
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.80	0.62
1:K:355:ILE:O	1:K:426:LEU:HA	1.99	0.62
1:B:413:VAL:HG11	1:B:423:ILE:HD12	1.81	0.62
1:K:181:ASN:O	1:K:182:LYS:HB2	1.99	0.62
1:L:104:ASN:ND2	5:L:1:1PE:H241	2.15	0.62
1:L:167:VAL:HG12	1:L:167:VAL:O	2.00	0.62
1:G:529:ILE:HG22	1:G:560:LEU:CD1	2.29	0.62
1:G:529:ILE:HG22	1:G:560:LEU:HD13	1.82	0.61
1:I:367:LYS:HG3	1:I:603:ASP:OD1	1.99	0.61
1:F:179:ASN:OD1	1:F:183:ASN:HB2	2.01	0.61
1:J:320:LYS:CE	5:J:3:1PE:H251	2.30	0.61
1:K:551:VAL:HG12	1:K:553:ALA:H	1.66	0.61
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.83	0.61
1:E:569:THR:HG23	7:E:1038:HOH:O	2.01	0.61
1:L:451:LYS:NZ	5:L:25:1PE:H222	2.16	0.61
1:D:301:PRO:CG	1:F:444:ILE:HG13	2.30	0.60
1:H:508:GLU:HG3	7:H:2499:HOH:O	2.00	0.60
1:H:233:ASN:ND2	1:H:519:THR:O	2.33	0.60
1:E:403:CYS:CB	1:E:427:SER:HG	2.14	0.60
1:F:272:ASN:O	1:F:273:ASN:HB2	2.00	0.60
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.83	0.60
1:A:498:SER:C	1:A:499:TYR:CD1	2.72	0.60
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.67	0.60
1:L:418:PRO:HB3	1:L:601:LEU:HD12	1.83	0.60
1:E:364:ASP:O	1:E:420:ASN:HA	2.02	0.60
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.84	0.59
1:G:427:SER:O	1:G:429:VAL:HG23	2.01	0.59
1:B:117:ILE:HD11	1:B:146:SER:OG	2.02	0.59
1:L:451:LYS:NZ	5:L:25:1PE:H141	2.17	0.59
1:A:451:LYS:HG2	5:A:57:1PE:H141	1.84	0.59
1:G:529:ILE:CG2	1:G:560:LEU:HD13	2.32	0.59
1:G:173:LYS:NZ	7:G:2988:HOH:O	2.36	0.59
1:F:361:SER:CB	1:F:421:VAL:O	2.44	0.59
1:A:341:TYR:CE1	1:A:428:ALA:HB1	2.39	0.58
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.38	0.58
1:B:282:GLU:OE2	1:B:285:ARG:HD2	2.03	0.58
1:B:436:LYS:HG2	4:B:3:SO4:O2	2.03	0.58
1:G:426:LEU:O	1:G:427:SER:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:SER:O	1:C:173:LYS:HD2	2.03	0.58
1:K:374:LYS:HE3	1:K:462:GLY:HA3	1.85	0.58
1:B:233:ASN:ND2	1:B:519:THR:O	2.31	0.58
1:D:301:PRO:HG3	1:F:444:ILE:HG13	1.86	0.58
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.85	0.58
1:G:350:TYR:HE1	1:I:440:ARG:HH21	1.52	0.58
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.85	0.58
1:L:544:ILE:CD1	1:L:564:GLU:HG3	2.34	0.57
1:L:214:LEU:HD21	1:L:222:LEU:HD22	1.85	0.57
5:K:50:1PE:H141	7:K:638:HOH:O	2.04	0.57
1:A:498:SER:HB2	1:F:533:TYR:CE2	2.39	0.57
1:B:498:SER:O	1:B:523:PRO:HG2	2.04	0.57
1:F:395:LEU:HG	1:F:395:LEU:O	2.04	0.57
1:H:498:SER:O	1:H:523:PRO:HG2	2.04	0.57
1:K:536:THR:HG21	1:K:551:VAL:HG23	1.86	0.57
1:D:181:ASN:O	1:D:182:LYS:HB2	2.03	0.57
1:A:427:SER:O	1:A:429:VAL:HG23	2.05	0.57
1:J:235:PHE:O	1:J:238:PHE:HB3	2.03	0.57
1:C:423:ILE:CG2	1:C:425:PHE:CZ	2.88	0.57
1:E:372:VAL:O	1:E:483:ASP:HA	2.04	0.57
1:H:413:VAL:HG11	1:H:423:ILE:HD12	1.87	0.57
1:I:150:ASP:OD1	1:I:179:ASN:HB2	2.05	0.57
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.86	0.57
1:F:271:ILE:HG23	1:F:272:ASN:H	1.69	0.57
1:A:431:GLU:OE2	1:C:440:ARG:NE	2.26	0.57
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.85	0.56
1:C:423:ILE:HG21	1:C:425:PHE:CZ	2.41	0.56
1:I:354:PHE:HE1	1:I:426:LEU:HD22	1.70	0.56
1:L:104:ASN:HB3	7:L:2365:HOH:O	2.03	0.56
1:D:85:ALA:HA	1:D:312:ASN:OD1	2.04	0.56
1:F:473:ALA:O	1:F:476:LEU:HB2	2.05	0.56
1:K:364:ASP:O	1:K:420:ASN:HA	2.06	0.56
1:C:273:ASN:O	1:C:276:THR:HG22	2.06	0.56
5:I:61:1PE:H142	1:J:499:TYR:OH	2.06	0.56
1:A:551:VAL:HG22	7:F:4143:HOH:O	2.05	0.56
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.41	0.56
1:I:544:ILE:CD1	1:I:564:GLU:HG3	2.36	0.56
1:J:540:LYS:HE2	7:K:1520:HOH:O	2.05	0.56
1:A:544:ILE:CD1	1:A:564:GLU:HG3	2.36	0.56
1:H:506:ASN:O	1:H:510:ILE:HG12	2.06	0.56
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:THR:CG2	7:C:2469:HOH:O	2.51	0.55
1:G:544:ILE:CD1	1:G:564:GLU:HG3	2.36	0.55
1:K:436:LYS:HG2	4:K:18:SO4:O4	2.07	0.55
1:G:395:LEU:HD11	1:G:581:TRP:CG	2.40	0.55
1:C:426:LEU:HD22	1:C:472:TYR:CE2	2.41	0.55
5:G:47:1PE:C24	5:G:48:1PE:C24	2.85	0.55
1:C:440:ARG:HG3	1:C:440:ARG:NH1	2.19	0.55
1:F:372:VAL:HG22	1:F:426:LEU:HD12	1.87	0.55
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.87	0.55
1:J:564:GLU:OE1	5:J:45:1PE:C23	2.54	0.55
1:D:579:VAL:O	1:D:589:LYS:HD2	2.07	0.55
1:A:451:LYS:CG	5:A:57:1PE:H141	2.37	0.55
1:D:533:TYR:O	1:D:536:THR:HG22	2.06	0.55
1:L:149:ASN:O	1:L:150:ASP:HB2	2.07	0.55
1:J:520:SER:O	1:J:521:ASN:HB2	2.07	0.55
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.39	0.55
1:K:518:LYS:HZ2	5:K:52:1PE:H142	1.72	0.55
1:L:112:VAL:HG22	1:L:267:LEU:HB3	1.89	0.55
1:I:273:ASN:O	1:I:276:THR:HG22	2.07	0.54
1:C:355:ILE:O	1:C:426:LEU:HA	2.07	0.54
1:L:451:LYS:HZ2	5:L:25:1PE:H222	1.71	0.54
1:E:103:TYR:N	4:E:25:SO4:O4	2.27	0.54
1:J:401:SER:HB2	1:J:486:THR:HG23	1.90	0.54
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.90	0.54
1:G:374:LYS:HE3	1:G:462:GLY:CA	2.37	0.54
1:A:350:TYR:HE1	1:C:440:ARG:HH21	1.55	0.54
1:F:602:ASN:CB	7:F:1958:HOH:O	2.54	0.54
1:C:481:ILE:O	1:C:571:TRP:HA	2.07	0.53
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.88	0.53
1:F:516:SER:OG	1:F:599:PHE:HA	2.08	0.53
1:B:395:LEU:O	1:B:395:LEU:HG	2.07	0.53
1:F:536:THR:HG21	1:F:551:VAL:HG23	1.90	0.53
1:E:544:ILE:CD1	1:E:564:GLU:HG3	2.38	0.53
1:I:329:GLY:O	1:I:333:LEU:HG	2.09	0.53
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.91	0.53
1:J:375:GLY:O	1:J:429:VAL:HA	2.08	0.53
1:B:132:VAL:HG21	1:B:142:VAL:HB	1.91	0.53
1:F:307:PRO:O	1:F:311:SER:OG	2.19	0.53
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.90	0.53
1:F:127:LEU:HD11	1:F:129:ILE:HD11	1.91	0.53
1:J:102:GLU:HG3	7:J:649:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:VAL:HG13	1:L:128:THR:OG1	2.09	0.53
1:A:529:ILE:HG22	1:A:560:LEU:CD1	2.37	0.52
1:E:440:ARG:HG3	1:E:440:ARG:NH2	2.22	0.52
1:A:341:TYR:CD1	1:A:428:ALA:HB1	2.44	0.52
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.92	0.52
1:G:204:LYS:HD3	7:G:3689:HOH:O	2.09	0.52
1:C:215:HIS:O	1:C:216:ASP:HB2	2.09	0.52
1:G:205:ARG:NE	7:G:3229:HOH:O	2.43	0.52
1:F:381:GLY:HA2	1:F:459:ASP:OD1	2.10	0.52
1:G:392:MET:HE2	5:G:16:1PE:H141	1.92	0.52
1:L:311:SER:HB2	1:L:327:ILE:HD12	1.91	0.52
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.92	0.52
1:A:328:LEU:HD12	1:A:328:LEU:N	2.25	0.52
1:E:133:ASN:HB2	1:E:193:GLY:O	2.09	0.52
1:F:139:ASN:CB	7:F:3095:HOH:O	2.58	0.52
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.91	0.52
1:J:260:ASN:N	7:J:3827:HOH:O	2.43	0.52
1:K:172:SER:O	1:K:173:LYS:HG2	2.10	0.52
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.92	0.52
1:L:395:LEU:HB2	7:L:3292:HOH:O	2.09	0.52
1:D:305:CYS:SG	1:D:310:LEU:HD12	2.51	0.51
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.93	0.51
1:E:587:LYS:HB2	1:E:588:PRO:CD	2.40	0.51
1:H:392:MET:HE2	5:H:51:1PE:H242	1.93	0.51
1:K:440:ARG:NH1	7:K:647:HOH:O	2.43	0.51
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.91	0.51
1:J:533:TYR:HB2	1:J:560:LEU:HD11	1.92	0.51
1:B:494:SER:HB3	1:E:494:SER:CB	2.40	0.51
1:C:426:LEU:O	1:C:427:SER:HB2	2.09	0.51
1:F:230:VAL:O	1:F:277:TYR:OH	2.23	0.51
1:L:349:MET:HG2	7:L:1003:HOH:O	2.11	0.51
1:L:473:ALA:O	1:L:476:LEU:HB2	2.11	0.51
1:B:240:GLU:OE2	1:B:287:TYR:HD2	1.93	0.51
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.93	0.51
1:C:440:ARG:O	1:C:441:PRO:C	2.47	0.51
1:L:127:LEU:HB2	1:L:219:LEU:HD22	1.93	0.51
1:J:102:GLU:CG	7:J:649:HOH:O	2.59	0.51
1:C:403:CYS:HG	1:C:427:SER:HG	1.58	0.51
1:F:294:ALA:O	1:F:298:ILE:HG13	2.11	0.51
1:E:390:GLY:N	4:E:28:SO4:O4	2.42	0.50
1:I:239:LEU:HB3	1:I:284:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:GLU:HB3	7:I:2574:HOH:O	2.10	0.50
1:A:133:ASN:HB2	1:A:193:GLY:O	2.11	0.50
1:C:423:ILE:HG21	1:C:425:PHE:CE1	2.47	0.50
1:F:451:LYS:HG3	5:F:612:1PE:H141	1.92	0.50
1:K:150:ASP:OD2	1:K:153:VAL:HG23	2.12	0.50
1:L:520:SER:CB	1:L:598:GLU:HG3	2.40	0.50
1:B:112:VAL:HA	1:B:267:LEU:O	2.12	0.50
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.92	0.50
1:D:395:LEU:O	1:D:395:LEU:HG	2.12	0.50
1:K:117:ILE:HG12	1:K:270:TYR:HB3	1.93	0.50
1:A:494:SER:HB3	1:F:494:SER:HB3	1.92	0.50
1:E:383:TYR:HE2	1:E:438:SER:HB2	1.76	0.50
1:A:384:ASN:OD1	1:A:457:ASN:HA	2.11	0.50
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.93	0.50
4:D:7:SO4:O4	1:E:436:LYS:HG2	2.11	0.50
1:A:262:GLU:HA	7:A:3272:HOH:O	2.12	0.50
1:B:544:ILE:CD1	1:B:564:GLU:HG3	2.42	0.50
1:E:386:LYS:HE3	1:E:396:MET:SD	2.52	0.50
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.12	0.50
1:J:106:PRO:HD3	7:J:3022:HOH:O	2.12	0.50
1:J:398:PHE:C	1:J:398:PHE:CD2	2.85	0.50
1:H:195:VAL:HA	7:H:1602:HOH:O	2.12	0.50
1:L:451:LYS:HZ2	5:L:25:1PE:C14	2.24	0.50
1:L:508:GLU:HG2	7:L:3277:HOH:O	2.11	0.50
1:B:483:ASP:OD2	1:B:573:HIS:HB2	2.12	0.49
1:D:236:ARG:HG3	1:D:284:ALA:HB2	1.93	0.49
1:F:133:ASN:HA	1:F:167:VAL:CG1	2.32	0.49
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.94	0.49
1:K:441:PRO:HD2	1:L:378:PHE:CZ	2.48	0.49
1:D:394:ASP:HA	1:F:441:PRO:CB	2.42	0.49
1:H:173:LYS:HE2	1:L:217:ASN:ND2	2.27	0.49
1:G:529:ILE:CG2	1:G:560:LEU:CD1	2.88	0.49
1:D:442:GLY:O	1:E:301:PRO:HB3	2.13	0.49
1:L:320:LYS:HE3	5:L:56:1PE:OH7	2.12	0.49
1:A:426:LEU:O	1:A:427:SER:HB2	2.12	0.49
1:G:275:ASP:HB2	7:G:3761:HOH:O	2.12	0.49
1:J:436:LYS:HG2	4:K:18:SO4:O1	2.13	0.49
1:B:346:LYS:HB3	1:B:437:ASN:O	2.13	0.49
1:E:539:SER:HB2	1:E:545:ASN:OD1	2.12	0.49
1:F:310:LEU:HD12	1:F:377:THR:HG22	1.93	0.49
1:H:544:ILE:CD1	1:H:564:GLU:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.94	0.49
1:G:152:GLN:HG2	1:G:180:ASP:OD1	2.12	0.49
1:C:160:GLU:O	1:C:163:GLU:HG2	2.12	0.49
1:D:452:THR:HG23	1:D:542:ALA:HB1	1.94	0.49
1:H:132:VAL:HG21	1:H:142:VAL:HB	1.95	0.49
1:J:452:THR:CG2	1:J:543:ASP:H	2.07	0.49
1:K:410:ALA:HA	1:K:413:VAL:CG2	2.43	0.49
1:D:86:SER:HB2	1:D:308:VAL:HG13	1.95	0.49
1:E:326:LYS:HD2	1:E:328:LEU:HD11	1.94	0.49
1:J:395:LEU:HG	1:J:395:LEU:O	2.13	0.49
1:A:489:GLY:CA	5:A:24:1PE:H252	2.36	0.48
1:G:554:SER:HA	7:G:3237:HOH:O	2.13	0.48
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.95	0.48
1:K:357:LEU:HB2	1:K:425:PHE:HB2	1.95	0.48
5:K:55:1PE:H252	7:K:4241:HOH:O	2.13	0.48
1:D:179:ASN:HD21	1:D:183:ASN:CB	2.25	0.48
5:L:29:1PE:H251	7:L:2855:HOH:O	2.13	0.48
1:H:167:VAL:O	1:H:168:LYS:C	2.51	0.48
1:I:325:TYR:HB2	1:I:357:LEU:HD12	1.95	0.48
1:K:372:VAL:O	1:K:483:ASP:HA	2.12	0.48
1:C:423:ILE:HB	1:C:425:PHE:CZ	2.48	0.48
5:D:34:1PE:H161	7:D:1405:HOH:O	2.14	0.48
1:F:107:ILE:HG21	1:F:243:PHE:HB3	1.94	0.48
1:A:103:TYR:CD1	5:A:20:1PE:H251	2.49	0.48
1:C:287:TYR:O	1:C:291:THR:CG2	2.62	0.48
1:H:423:ILE:HD11	1:H:600:VAL:CG1	2.44	0.48
1:L:139:ASN:HA	7:L:2918:HOH:O	2.14	0.48
1:A:104:ASN:ND2	4:A:1:SO4:O4	2.45	0.48
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.95	0.48
1:J:316:GLU:CD	5:J:3:1PE:H252	2.34	0.48
1:B:532:GLU:OE2	1:E:498:SER:OG	2.31	0.48
1:G:316:GLU:HG3	5:G:58:1PE:H231	1.95	0.48
1:D:301:PRO:HG2	1:F:444:ILE:HG13	1.96	0.48
1:E:441:PRO:HD2	1:F:378:PHE:CZ	2.49	0.48
1:H:500:ALA:HB3	1:H:524:VAL:HG22	1.96	0.48
1:L:175:PHE:O	1:L:186:ALA:HA	2.14	0.48
1:J:543:ASP:HB3	5:J:45:1PE:H242	1.96	0.47
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.96	0.47
1:C:331:LYS:HE2	1:C:334:GLU:OE1	2.14	0.47
1:H:592:GLY:O	1:H:596:LEU:HG	2.13	0.47
1:I:326:LYS:HE3	1:I:328:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.96	0.47
1:H:153:VAL:O	1:H:157:LEU:HG	2.14	0.47
1:H:452:THR:HG23	1:I:254:SER:HB2	1.95	0.47
1:I:440:ARG:O	1:I:441:PRO:C	2.53	0.47
1:K:356:HIS:HA	1:K:426:LEU:HD23	1.95	0.47
1:L:169:LEU:HD11	1:L:202:ASP:HB3	1.95	0.47
1:L:534:ARG:NH1	1:L:538:ASN:OD1	2.44	0.47
1:B:179:ASN:OD1	1:B:183:ASN:HB2	2.14	0.47
1:C:544:ILE:CD1	1:C:564:GLU:HG3	2.44	0.47
1:D:452:THR:CG2	1:D:543:ASP:H	2.08	0.47
1:E:355:ILE:O	1:E:426:LEU:HA	2.14	0.47
1:F:167:VAL:O	1:F:168:LYS:C	2.52	0.47
1:K:374:LYS:HE3	1:K:462:GLY:CA	2.44	0.47
1:L:223:THR:HA	1:L:268:GLY:O	2.15	0.47
1:D:372:VAL:O	1:D:483:ASP:HA	2.14	0.47
1:D:557:VAL:HA	1:D:560:LEU:HD12	1.97	0.47
1:E:451:LYS:HE3	1:E:564:GLU:O	2.15	0.47
1:F:167:VAL:O	1:F:167:VAL:HG12	2.15	0.47
1:J:481:ILE:O	1:J:571:TRP:HA	2.13	0.47
1:J:500:ALA:HB2	1:J:579:VAL:HG21	1.97	0.47
1:K:103:TYR:HB2	4:K:19:SO4:O1	2.15	0.47
1:K:166:ASN:C	1:K:166:ASN:HD22	2.18	0.47
1:K:360:LYS:HE3	1:K:365:VAL:HG21	1.97	0.47
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.97	0.47
1:D:451:LYS:HE3	1:D:564:GLU:O	2.15	0.47
1:E:406:VAL:CG1	1:E:425:PHE:HB3	2.45	0.47
1:C:568:ASN:HB2	7:C:3888:HOH:O	2.14	0.47
1:H:494:SER:HB3	1:K:494:SER:CB	2.45	0.47
1:J:372:VAL:O	1:J:483:ASP:HA	2.14	0.47
1:B:108:HIS:NE2	6:B:14:2PE:H242	2.30	0.47
1:B:138:GLU:C	1:B:139:ASN:HD22	2.19	0.47
1:C:326:LYS:HE3	1:C:328:LEU:HD21	1.96	0.47
1:H:282:GLU:OE2	1:H:285:ARG:HD2	2.15	0.47
1:L:103:TYR:HB2	5:L:56:1PE:H161	1.97	0.47
1:A:256:ASP:CB	7:A:4367:HOH:O	2.63	0.46
5:C:18:1PE:H231	7:C:997:HOH:O	2.15	0.46
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.98	0.46
1:H:375:GLY:O	1:H:429:VAL:HA	2.15	0.46
1:A:556:ILE:O	1:A:559:SER:HB2	2.15	0.46
1:C:354:PHE:CE1	1:C:426:LEU:HB3	2.50	0.46
1:D:179:ASN:ND2	1:D:183:ASN:CB	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:544:ILE:HD12	1:H:564:GLU:HG3	1.98	0.46
1:I:354:PHE:CE1	1:I:426:LEU:HD22	2.50	0.46
1:J:507:GLU:CG	7:J:3451:HOH:O	2.63	0.46
1:A:523:PRO:HA	7:A:2235:HOH:O	2.15	0.46
1:G:494:SER:CB	1:L:494:SER:HB3	2.45	0.46
1:A:372:VAL:O	1:A:483:ASP:HA	2.16	0.46
1:B:123:VAL:HG11	1:B:185:VAL:HG21	1.96	0.46
1:C:307:PRO:HD2	1:C:350:TYR:CB	2.45	0.46
1:D:132:VAL:HG11	1:D:144:ILE:HD13	1.96	0.46
1:D:200:GLU:CB	7:D:2566:HOH:O	2.64	0.46
1:G:501:GLY:O	1:G:574:ILE:HA	2.16	0.46
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.97	0.46
1:I:481:ILE:O	1:I:571:TRP:HA	2.15	0.46
1:B:153:VAL:O	1:B:157:LEU:HG	2.15	0.46
1:K:150:ASP:HB3	1:K:153:VAL:HB	1.98	0.46
1:K:356:HIS:CG	1:K:426:LEU:HD23	2.50	0.46
1:C:117:ILE:HD11	1:C:146:SER:OG	2.16	0.46
1:K:587:LYS:HB2	1:K:588:PRO:CD	2.45	0.46
1:G:320:LYS:HG3	5:G:58:1PE:H221	1.97	0.46
1:B:165:PHE:HB3	1:B:189:TYR:OH	2.16	0.46
1:E:150:ASP:OD2	1:E:153:VAL:HG23	2.15	0.46
1:F:137:LYS:CB	1:F:194:SER:OG	2.64	0.46
1:F:372:VAL:O	1:F:483:ASP:HA	2.16	0.46
1:G:200:GLU:HB3	7:G:2334:HOH:O	2.15	0.46
1:I:199:SER:HB2	7:I:1704:HOH:O	2.16	0.46
1:L:181:ASN:O	1:L:182:LYS:CB	2.62	0.46
1:L:358:THR:HG22	7:L:665:HOH:O	2.15	0.46
1:E:443:ASP:CG	1:F:303:ASN:HB3	2.36	0.46
1:L:287:TYR:CD2	1:L:594:ARG:HG2	2.51	0.46
1:L:517:SER:HB2	1:L:524:VAL:HB	1.98	0.46
1:D:375:GLY:O	1:D:429:VAL:HA	2.14	0.46
1:E:360:LYS:HE3	1:E:365:VAL:HG21	1.98	0.46
5:K:52:1PE:H251	5:K:52:1PE:H241	1.65	0.46
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.96	0.46
1:C:177:MET:HG2	1:C:185:VAL:HG12	1.97	0.45
1:H:364:ASP:O	1:H:420:ASN:HA	2.15	0.45
1:K:410:ALA:HA	1:K:425:PHE:CZ	2.50	0.45
1:L:86:SER:CB	1:L:312:ASN:OD1	2.61	0.45
1:L:236:ARG:HD3	1:L:283:LYS:HD3	1.99	0.45
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.97	0.45
1:B:178:PHE:HA	1:B:183:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:SER:O	1:D:523:PRO:HG2	2.16	0.45
1:F:236:ARG:HD3	1:F:283:LYS:HD3	1.99	0.45
1:A:567:GLN:CG	7:A:1408:HOH:O	2.64	0.45
1:C:423:ILE:HB	1:C:425:PHE:CE2	2.51	0.45
1:D:254:SER:OG	5:F:612:1PE:H142	2.17	0.45
1:H:123:VAL:HG11	1:H:185:VAL:HG21	1.97	0.45
1:H:532:GLU:OE2	1:K:498:SER:OG	2.35	0.45
1:K:356:HIS:CD2	1:K:426:LEU:HD23	2.52	0.45
1:L:345:GLY:HA3	1:L:352:ASN:OD1	2.17	0.45
1:A:516:SER:OG	1:A:599:PHE:HA	2.16	0.45
1:B:423:ILE:HD11	1:B:600:VAL:CG1	2.47	0.45
1:C:106:PRO:HD2	1:C:247:MET:SD	2.57	0.45
1:L:536:THR:HG21	1:L:551:VAL:HG23	1.97	0.45
1:D:301:PRO:HB3	1:F:442:GLY:O	2.17	0.45
1:E:537:LEU:HA	1:E:545:ASN:HB2	1.98	0.45
1:F:383:TYR:HE2	1:F:438:SER:HB2	1.82	0.45
1:J:364:ASP:O	1:J:420:ASN:HA	2.17	0.45
1:K:401:SER:HB2	1:K:486:THR:HG23	1.99	0.45
1:A:451:LYS:CE	7:A:4147:HOH:O	2.65	0.45
1:C:537:LEU:HD21	1:C:557:VAL:CG1	2.47	0.45
1:D:379:ASP:HB2	1:D:399:ASP:OD2	2.17	0.45
1:D:544:ILE:CD1	1:D:564:GLU:HG3	2.46	0.45
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.99	0.45
1:B:132:VAL:HG23	1:B:132:VAL:O	2.16	0.45
1:D:481:ILE:O	1:D:571:TRP:HA	2.17	0.45
5:H:51:1PE:C25	7:H:4259:HOH:O	2.65	0.45
1:J:348:SER:OG	1:J:431:GLU:HB3	2.17	0.45
1:K:520:SER:HB3	1:K:598:GLU:HG3	1.99	0.45
1:A:139:ASN:HD21	1:A:168:LYS:HD2	1.82	0.44
1:A:355:ILE:CG2	1:A:357:LEU:HD13	2.47	0.44
1:F:198:LEU:HD12	1:F:198:LEU:HA	1.84	0.44
1:F:514:LEU:O	1:F:517:SER:HB3	2.17	0.44
1:G:230:VAL:HB	1:G:234:LEU:HB3	1.99	0.44
1:H:183:ASN:HD22	1:H:183:ASN:HA	1.57	0.44
1:K:360:LYS:HE2	7:K:2116:HOH:O	2.16	0.44
1:K:587:LYS:NZ	7:K:1642:HOH:O	2.41	0.44
1:L:128:THR:HG23	1:L:223:THR:OG1	2.17	0.44
1:I:350:TYR:HA	1:I:351:PRO:HD3	1.83	0.44
1:K:160:GLU:CD	1:K:160:GLU:H	2.19	0.44
1:F:99:ILE:CD1	1:F:305:CYS:HB2	2.47	0.44
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:544:ILE:HD12	1:F:564:GLU:HG3	1.99	0.44
1:K:326:LYS:HD2	1:K:328:LEU:HD11	1.99	0.44
1:B:506:ASN:O	1:B:510:ILE:HG12	2.17	0.44
1:E:323:LEU:HD22	1:E:359:TYR:HB2	2.00	0.44
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.00	0.44
1:L:460:ALA:HB3	1:L:546:GLN:NE2	2.32	0.44
1:G:483:ASP:OD1	1:G:573:HIS:ND1	2.34	0.44
1:K:302:SER:OG	1:K:378:PHE:HB2	2.18	0.44
1:K:441:PRO:HB2	1:L:394:ASP:HA	2.00	0.44
1:A:307:PRO:HA	1:A:429:VAL:CG1	2.48	0.44
1:G:372:VAL:O	1:G:483:ASP:HA	2.18	0.44
1:I:287:TYR:CD2	1:I:594:ARG:HG2	2.53	0.44
1:K:396:MET:CE	5:K:36:1PE:H252	2.47	0.44
1:L:216:ASP:OD1	1:L:216:ASP:O	2.36	0.44
1:A:451:LYS:HE3	7:A:4147:HOH:O	2.16	0.44
1:B:183:ASN:HB3	1:B:184:SER:H	1.62	0.44
1:C:406:VAL:CG1	1:C:425:PHE:HB3	2.48	0.44
1:H:357:LEU:HB2	1:H:425:PHE:HB2	2.00	0.44
1:A:412:CYS:HB3	1:A:597:THR:HG21	2.00	0.44
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.98	0.44
1:E:505:ASN:OD1	1:E:505:ASN:C	2.55	0.44
1:F:292:TYR:O	1:F:296:GLN:HG3	2.18	0.44
1:F:539:SER:HB3	1:F:542:ALA:O	2.18	0.44
1:H:423:ILE:HD11	1:H:600:VAL:HG13	1.99	0.44
1:K:586:ARG:HD2	4:K:20:SO4:O1	2.17	0.44
1:A:407:LEU:O	1:A:410:ALA:HB3	2.18	0.44
1:A:529:ILE:CG2	1:A:560:LEU:CD1	2.94	0.44
1:B:541:TYR:OH	1:C:587:LYS:HB2	2.17	0.44
1:F:322:ASN:HB3	1:K:160:GLU:OE1	2.18	0.44
1:K:241:THR:HG23	7:K:1539:HOH:O	2.18	0.44
1:L:481:ILE:O	1:L:571:TRP:HA	2.18	0.44
1:A:536:THR:HG21	1:A:551:VAL:HG23	2.00	0.43
1:C:287:TYR:O	1:C:291:THR:HG23	2.18	0.43
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.50	0.43
1:H:483:ASP:OD1	1:H:573:HIS:ND1	2.35	0.43
1:L:596:LEU:O	1:L:599:PHE:HB3	2.18	0.43
1:A:394:ASP:CG	7:A:1379:HOH:O	2.56	0.43
1:H:321:LEU:HB2	1:H:323:LEU:HG	2.01	0.43
1:E:121:CYS:HA	1:E:270:TYR:CE2	2.53	0.43
1:E:231:ASP:O	1:E:231:ASP:OD2	2.37	0.43
1:G:139:ASN:HD21	1:G:168:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:ASN:OD1	1:K:179:ASN:C	2.57	0.43
1:F:99:ILE:HD13	1:F:305:CYS:HB2	2.00	0.43
1:H:112:VAL:HA	1:H:267:LEU:O	2.19	0.43
1:F:137:LYS:O	1:F:138:GLU:CB	2.67	0.43
1:G:431:GLU:OE2	1:I:440:ARG:NE	2.32	0.43
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.53	0.43
1:H:508:GLU:CG	7:H:2499:HOH:O	2.63	0.43
1:A:494:SER:CB	1:F:494:SER:HB3	2.48	0.43
1:A:497:THR:O	1:A:497:THR:OG1	2.33	0.43
1:B:494:SER:HB3	1:E:494:SER:HB3	1.99	0.43
1:D:567:GLN:NE2	5:D:44:1PE:C16	2.81	0.43
1:G:187:VAL:HG12	1:G:188:GLY:N	2.33	0.43
1:H:436:LYS:HG2	4:I:17:SO4:O2	2.18	0.43
1:H:520:SER:O	1:H:521:ASN:HB2	2.18	0.43
1:I:487:LEU:HD22	1:I:573:HIS:CE1	2.53	0.43
1:J:236:ARG:HG3	1:J:284:ALA:HB2	2.00	0.43
1:K:392:MET:HE3	1:K:395:LEU:HD23	2.01	0.43
1:C:487:LEU:HD22	1:C:573:HIS:CE1	2.53	0.43
1:F:222:LEU:HD23	1:F:267:LEU:HD13	2.00	0.43
1:G:539:SER:HB3	1:G:542:ALA:O	2.17	0.43
1:K:144:ILE:HG13	1:K:157:LEU:HD22	2.00	0.43
1:B:461:GLU:HG2	1:B:462:GLY:N	2.34	0.43
1:J:86:SER:HB2	1:J:308:VAL:HG13	2.01	0.43
1:J:231:ASP:OD2	1:J:231:ASP:C	2.56	0.43
1:J:452:THR:HG23	1:J:542:ALA:HB1	2.01	0.43
1:A:396:MET:HE3	5:A:24:1PE:H131	2.01	0.43
1:B:326:LYS:HE3	1:B:328:LEU:HD11	2.01	0.43
1:E:116:ASP:HA	1:E:271:ILE:O	2.19	0.43
1:I:192:CYS:O	1:I:198:LEU:HD21	2.19	0.43
1:J:425:PHE:CD2	1:J:425:PHE:N	2.87	0.43
1:B:216:ASP:CB	1:F:173:LYS:CD	2.96	0.43
1:D:441:PRO:HB2	1:E:394:ASP:HA	2.00	0.43
1:K:356:HIS:NE2	1:K:426:LEU:HD21	2.34	0.43
1:B:242:LEU:O	1:B:246:TYR:HB2	2.18	0.42
1:D:544:ILE:HD12	1:D:564:GLU:HG3	2.01	0.42
1:E:396:MET:CE	5:E:612:1PE:H152	2.49	0.42
1:F:116:ASP:C	1:F:118:LYS:N	2.73	0.42
1:G:520:SER:O	1:G:521:ASN:HB2	2.19	0.42
1:A:440:ARG:HB2	1:A:443:ASP:OD1	2.19	0.42
1:A:537:LEU:HD22	1:A:545:ASN:O	2.19	0.42
1:E:117:ILE:HG12	1:E:270:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:PRO:HB3	1:F:601:LEU:HD12	2.01	0.42
1:H:174:HIS:CE1	1:H:213:MET:HG2	2.53	0.42
1:I:165:PHE:CE2	1:I:173:LYS:HG2	2.53	0.42
1:C:350:TYR:HA	1:C:351:PRO:HD3	1.92	0.42
1:D:395:LEU:HD11	1:D:581:TRP:CG	2.54	0.42
1:L:358:THR:CG2	7:L:665:HOH:O	2.67	0.42
1:A:208:LEU:O	1:A:212:THR:HG23	2.20	0.42
1:C:401:SER:HB2	1:C:486:THR:HG23	2.01	0.42
1:F:546:GLN:HG2	1:F:547:ILE:HG23	2.00	0.42
1:I:376:ILE:HA	1:I:430:CYS:O	2.20	0.42
1:F:384:ASN:OD1	1:F:457:ASN:HA	2.20	0.42
1:G:142:VAL:HG21	1:G:189:TYR:CZ	2.54	0.42
1:H:483:ASP:OD2	1:H:573:HIS:HB2	2.20	0.42
1:K:338:MET:HE2	1:K:338:MET:HB3	1.92	0.42
1:K:440:ARG:O	1:K:441:PRO:C	2.57	0.42
1:L:133:ASN:HA	1:L:167:VAL:CG1	2.42	0.42
1:A:499:TYR:HE1	7:F:1147:HOH:O	2.03	0.42
1:E:302:SER:OG	1:E:378:PHE:HB2	2.20	0.42
1:E:440:ARG:HD2	1:F:302:SER:HB2	2.00	0.42
1:H:395:LEU:HG	1:H:395:LEU:O	2.19	0.42
1:I:533:TYR:OH	1:J:495:LEU:O	2.35	0.42
1:J:518:LYS:NZ	5:J:60:1PE:H241	2.34	0.42
1:B:181:ASN:O	1:B:182:LYS:C	2.58	0.42
1:F:392:MET:HG3	4:F:33:SO4:O3	2.20	0.42
1:L:242:LEU:O	1:L:246:TYR:HB2	2.20	0.42
1:B:144:ILE:HG23	1:B:227:GLU:OE2	2.20	0.42
1:D:349:MET:HG2	7:D:710:HOH:O	2.19	0.42
1:F:343:SER:OG	1:F:445:ILE:HG21	2.20	0.42
1:G:214:LEU:HD21	1:G:222:LEU:HD22	2.01	0.42
1:H:494:SER:HB3	1:K:494:SER:HB3	2.00	0.42
1:I:103:TYR:CD1	5:I:21:1PE:H251	2.55	0.42
1:J:338:MET:HB3	1:J:338:MET:HE2	1.99	0.42
1:A:512:LYS:NZ	1:A:603:ASP:OD1	2.45	0.42
1:D:398:PHE:C	1:D:398:PHE:CD2	2.91	0.42
1:H:231:ASP:OD2	1:H:231:ASP:N	2.52	0.42
1:A:489:GLY:HA3	5:A:24:1PE:C25	2.41	0.42
1:J:518:LYS:HZ1	5:J:60:1PE:H241	1.85	0.42
1:K:342:LEU:HD23	1:K:342:LEU:HA	1.94	0.42
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.02	0.41
1:C:95:ASP:HA	1:C:96:PRO:HD3	1.92	0.41
1:H:117:ILE:HD11	1:H:146:SER:HG	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:333:LEU:HD13	1:I:341:TYR:CE2	2.55	0.41
1:J:554:SER:HB2	7:J:793:HOH:O	2.19	0.41
1:K:104:ASN:HB3	7:K:2992:HOH:O	2.19	0.41
1:K:412:CYS:HB3	1:K:597:THR:HG21	2.02	0.41
1:B:174:HIS:CE1	1:B:213:MET:HG2	2.55	0.41
1:B:208:LEU:HD13	1:B:208:LEU:HA	1.94	0.41
1:B:216:ASP:CB	1:F:173:LYS:CE	2.96	0.41
1:B:364:ASP:O	1:B:420:ASN:HA	2.19	0.41
1:E:148:VAL:HG12	1:E:150:ASP:H	1.85	0.41
1:F:277:TYR:O	1:F:278:LYS:C	2.58	0.41
1:G:481:ILE:O	1:G:571:TRP:HA	2.20	0.41
1:I:223:THR:HA	1:I:268:GLY:O	2.20	0.41
1:I:339:GLY:HA3	1:I:446:THR:O	2.20	0.41
1:J:579:VAL:O	1:J:589:LYS:HD2	2.20	0.41
1:K:537:LEU:HA	1:K:545:ASN:HB2	2.01	0.41
1:L:151:LYS:O	1:L:153:VAL:N	2.53	0.41
1:C:223:THR:HG21	7:C:3325:HOH:O	2.21	0.41
1:H:346:LYS:HB3	1:H:437:ASN:O	2.20	0.41
1:B:174:HIS:HB3	1:F:175:PHE:CD1	2.55	0.41
1:B:383:TYR:HE2	1:B:438:SER:HB2	1.85	0.41
1:C:199:SER:O	1:C:200:GLU:C	2.58	0.41
1:D:153:VAL:HG13	1:D:187:VAL:HG21	2.01	0.41
1:F:480:TYR:CD1	1:F:509:LEU:HD13	2.56	0.41
1:G:108:HIS:NE2	5:G:12:1PE:H142	2.34	0.41
1:J:111:LYS:HD2	1:J:266:HIS:CE1	2.55	0.41
1:K:410:ALA:O	1:K:413:VAL:HG23	2.20	0.41
1:A:374:LYS:HE3	1:A:462:GLY:HA3	2.02	0.41
1:B:190:VAL:HG11	1:B:206:VAL:HG13	2.02	0.41
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.85	0.41
1:E:307:PRO:HD2	1:E:350:TYR:CB	2.51	0.41
1:F:236:ARG:NE	1:F:240:GLU:OE2	2.47	0.41
1:F:277:TYR:O	1:F:279:GLU:N	2.53	0.41
1:A:307:PRO:HA	1:A:429:VAL:HG11	2.03	0.41
1:C:178:PHE:HA	1:C:183:ASN:O	2.20	0.41
1:C:411:TYR:HE1	5:C:18:1PE:H231	1.85	0.41
1:G:421:VAL:HG22	1:G:423:ILE:CD1	2.51	0.41
1:H:173:LYS:O	1:H:188:GLY:HA3	2.20	0.41
1:J:400:MET:HE2	1:J:400:MET:O	2.21	0.41
1:B:110:ILE:O	1:B:285:ARG:NH2	2.50	0.41
1:F:505:ASN:OD1	1:F:505:ASN:C	2.58	0.41
1:H:103:TYR:HB3	6:H:6:2PE:H272	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:VAL:HG22	1:H:267:LEU:HB3	2.03	0.41
1:H:196:ALA:N	7:H:1602:HOH:O	2.44	0.41
1:L:350:TYR:HA	1:L:351:PRO:HD3	1.80	0.41
1:L:448:SER:OG	1:L:471:VAL:HG22	2.21	0.41
1:A:173:LYS:HD2	1:D:176:TYR:CE1	2.55	0.41
1:B:293:TYR:CE2	1:B:297:LEU:HD11	2.56	0.41
1:C:174:HIS:HB3	1:E:175:PHE:CD2	2.56	0.41
1:E:441:PRO:HB2	1:F:394:ASP:HA	2.03	0.41
1:G:176:TYR:CE2	1:J:156:PHE:HB2	2.56	0.41
1:K:368:LYS:C	1:K:478:VAL:HG22	2.40	0.41
1:A:528:PRO:HB3	1:F:525:TRP:CZ3	2.56	0.41
1:B:302:SER:OG	1:B:378:PHE:HB2	2.21	0.41
1:D:329:GLY:O	1:D:333:LEU:HG	2.21	0.41
1:E:504:GLY:O	1:E:529:ILE:HD12	2.21	0.41
1:G:537:LEU:HD22	1:G:545:ASN:O	2.21	0.41
1:J:499:TYR:C	1:J:579:VAL:HG11	2.41	0.41
1:K:221:LYS:HE3	7:K:3233:HOH:O	2.20	0.41
1:L:113:GLN:HE21	1:L:113:GLN:HB3	1.65	0.41
1:L:440:ARG:HE	1:L:440:ARG:HB2	1.80	0.41
5:L:25:1PE:H222	5:L:25:1PE:H131	1.65	0.41
1:E:518:LYS:HZ1	5:E:35:1PE:H161	1.86	0.41
1:F:137:LYS:CB	1:F:139:ASN:HA	2.50	0.41
1:F:451:LYS:CG	5:F:612:1PE:H141	2.51	0.41
1:H:441:PRO:HB2	1:I:394:ASP:HA	2.02	0.41
1:L:497:THR:HA	1:L:578:GLY:O	2.21	0.41
1:A:107:ILE:HA	1:A:110:ILE:HD12	2.02	0.40
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.97	0.40
1:A:426:LEU:O	1:A:427:SER:CB	2.69	0.40
1:B:321:LEU:HB2	1:B:323:LEU:HG	2.03	0.40
1:B:372:VAL:O	1:B:483:ASP:HA	2.20	0.40
1:B:487:LEU:HD12	1:B:487:LEU:HA	1.90	0.40
1:B:544:ILE:HD12	1:B:564:GLU:HG3	2.03	0.40
1:F:90:GLN:HG2	1:F:95:ASP:HB2	2.03	0.40
1:F:159:ASP:OD1	1:F:159:ASP:N	2.54	0.40
1:I:302:SER:OG	1:I:378:PHE:HB2	2.21	0.40
1:I:510:ILE:HD13	1:I:526:TRP:NE1	2.36	0.40
1:L:487:LEU:HD12	1:L:487:LEU:HA	1.81	0.40
1:A:383:TYR:HE2	1:A:438:SER:HB2	1.85	0.40
1:D:376:ILE:HD11	1:D:465:THR:HG21	2.04	0.40
1:F:414:GLY:O	1:F:417:LYS:HE3	2.21	0.40
1:J:533:TYR:HB2	1:J:560:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:217:ASN:HB2	1:L:219:LEU:HD11	2.01	0.40
1:B:174:HIS:HB3	1:F:175:PHE:CE1	2.56	0.40
1:B:392:MET:HE2	5:B:40:1PE:C24	2.52	0.40
1:C:112:VAL:HG22	1:C:267:LEU:HB3	2.04	0.40
1:C:239:LEU:HB3	1:C:284:ALA:HB1	2.02	0.40
1:D:364:ASP:O	1:D:420:ASN:HA	2.21	0.40
1:E:440:ARG:NH2	1:E:440:ARG:CG	2.83	0.40
1:F:444:ILE:HA	1:F:453:ILE:O	2.21	0.40
1:H:423:ILE:CD1	1:H:600:VAL:HG11	2.51	0.40
1:J:161:ASN:OD1	1:J:164:LYS:HE2	2.21	0.40
1:A:152:GLN:HG2	1:A:180:ASP:OD1	2.20	0.40
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.57	0.40
1:B:231:ASP:OD2	1:B:231:ASP:N	2.53	0.40
1:D:596:LEU:O	1:D:600:VAL:HG13	2.20	0.40
1:E:518:LYS:HE2	5:E:35:1PE:H161	2.03	0.40
1:F:326:LYS:HE3	1:F:328:LEU:HD11	2.03	0.40
1:H:487:LEU:HD12	1:H:487:LEU:HA	1.79	0.40
1:J:440:ARG:HB2	1:J:443:ASP:OD1	2.22	0.40
1:L:222:LEU:O	1:L:267:LEU:HD12	2.21	0.40
1:A:544:ILE:HD12	1:A:564:GLU:HG3	2.04	0.40
1:D:144:ILE:HG13	1:D:157:LEU:HD22	2.04	0.40
1:F:138:GLU:H	1:F:139:ASN:CA	2.11	0.40
1:F:358:THR:CG2	7:F:1366:HOH:O	2.46	0.40
1:J:329:GLY:O	1:J:333:LEU:HG	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASN:ND2	1:H:322:ASN:ND2[2_664]	1.92	0.28
1:D:366:LYS:CE	7:B:895:HOH:O[4_455]	2.06	0.14

## 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	510/528 (97%)	495 (97%)	12 (2%)	3 (1%)	25	36
1	B	506/528 (96%)	482 (95%)	24 (5%)	0	100	100
1	C	516/528 (98%)	496 (96%)	18 (4%)	2 (0%)	34	48
1	D	510/528 (97%)	491 (96%)	19 (4%)	0	100	100
1	E	503/528 (95%)	480 (95%)	23 (5%)	0	100	100
1	F	504/528 (96%)	473 (94%)	24 (5%)	7 (1%)	11	15
1	G	510/528 (97%)	497 (98%)	11 (2%)	2 (0%)	34	48
1	H	506/528 (96%)	485 (96%)	21 (4%)	0	100	100
1	I	511/528 (97%)	501 (98%)	10 (2%)	0	100	100
1	J	510/528 (97%)	494 (97%)	16 (3%)	0	100	100
1	K	503/528 (95%)	487 (97%)	16 (3%)	0	100	100
1	L	500/528 (95%)	476 (95%)	19 (4%)	5 (1%)	15	23
All	All	6089/6336 (96%)	5857 (96%)	213 (4%)	19 (0%)	41	55

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	SER
1	F	272	ASN
1	G	427	SER
1	L	272	ASN
1	A	498	SER
1	C	427	SER
1	F	138	GLU
1	L	150	ASP
1	A	428	ALA
1	F	180	ASP
1	F	200	GLU
1	F	278	LYS
1	G	428	ALA
1	C	568	ASN
1	L	231	ASP
1	L	274	ALA
1	L	386	LYS
1	F	231	ASP
1	F	271	ILE

### 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	420/455 (92%)	411 (98%)	9 (2%)	53	72
1	B	405/455 (89%)	393 (97%)	12 (3%)	41	61
1	C	419/455 (92%)	395 (94%)	24 (6%)	20	33
1	D	416/455 (91%)	398 (96%)	18 (4%)	29	46
1	E	412/455 (90%)	395 (96%)	17 (4%)	30	48
1	F	385/455 (85%)	360 (94%)	25 (6%)	17	27
1	G	421/455 (92%)	413 (98%)	8 (2%)	57	75
1	H	405/455 (89%)	392 (97%)	13 (3%)	39	59
1	I	417/455 (92%)	393 (94%)	24 (6%)	20	32
1	J	416/455 (91%)	399 (96%)	17 (4%)	30	48
1	K	413/455 (91%)	397 (96%)	16 (4%)	32	50
1	L	391/455 (86%)	365 (93%)	26 (7%)	16	26
All	All	4920/5460 (90%)	4711 (96%)	209 (4%)	30	47

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	GLU
1	A	229	ASN
1	A	288	TYR
1	A	398	PHE
1	A	436	LYS
1	A	439	TYR
1	A	498	SER
1	A	554	SER
1	A	603	ASP
1	B	86	SER
1	B	88	VAL
1	B	142	VAL
1	B	173	LYS
1	B	229	ASN

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Mol	Chain	Res	Type
1	B	233	ASN
1	B	288	TYR
1	B	322	ASN
1	B	368	LYS
1	B	398	PHE
1	B	439	TYR
1	B	483	ASP
1	C	86	SER
1	C	132	VAL
1	C	163	GLU
1	C	169	LEU
1	C	185	VAL
1	C	200	GLU
1	C	208	LEU
1	C	223	THR
1	C	239	LEU
1	C	276	THR
1	C	288	TYR
1	C	291	THR
1	C	331	LYS
1	C	357	LEU
1	C	398	PHE
1	C	400	MET
1	C	407	LEU
1	C	426	LEU
1	C	439	TYR
1	C	440	ARG
1	C	478	VAL
1	C	568	ASN
1	C	601	LEU
1	C	603	ASP
1	D	88	VAL
1	D	154	SER
1	D	164	LYS
1	D	197	ASP
1	D	198	LEU
1	D	200	GLU
1	D	208	LEU
1	D	216	ASP
1	D	218	LYS
1	D	250	GLU
1	D	288	TYR

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Mol	Chain	Res	Type
1	D	330	VAL
1	D	395	LEU
1	D	398	PHE
1	D	407	LEU
1	D	439	TYR
1	D	445	ILE
1	D	452	THR
1	E	86	SER
1	E	166	ASN
1	E	184	SER
1	E	208	LEU
1	E	230	VAL
1	E	239	LEU
1	E	288	TYR
1	E	310	LEU
1	E	364	ASP
1	E	398	PHE
1	E	436	LYS
1	E	439	TYR
1	E	440	ARG
1	E	478	VAL
1	E	483	ASP
1	E	498	SER
1	E	518	LYS
1	F	86	SER
1	F	88	VAL
1	F	113	GLN
1	F	134	ASN
1	F	159	ASP
1	F	169	LEU
1	F	199	SER
1	F	223	THR
1	F	239	LEU
1	F	288	TYR
1	F	310	LEU
1	F	311	SER
1	F	343	SER
1	F	357	LEU
1	F	358	THR
1	F	361	SER
1	F	398	PHE
1	F	407	LEU

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Mol	Chain	Res	Type
1	F	436	LYS
1	F	439	TYR
1	F	476	LEU
1	F	498	SER
1	F	508	GLU
1	F	554	SER
1	F	600	VAL
1	G	200	GLU
1	G	229	ASN
1	G	288	TYR
1	G	398	PHE
1	G	436	LYS
1	G	439	TYR
1	G	554	SER
1	G	603	ASP
1	H	86	SER
1	H	88	VAL
1	H	142	VAL
1	H	173	LYS
1	H	183	ASN
1	H	208	LEU
1	H	229	ASN
1	H	233	ASN
1	H	288	TYR
1	H	322	ASN
1	H	364	ASP
1	H	398	PHE
1	H	439	TYR
1	I	86	SER
1	I	132	VAL
1	I	163	GLU
1	I	169	LEU
1	I	185	VAL
1	I	200	GLU
1	I	204	LYS
1	I	208	LEU
1	I	223	THR
1	I	229	ASN
1	I	239	LEU
1	I	276	THR
1	I	288	TYR
1	I	291	THR

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Mol	Chain	Res	Type
1	I	331	LYS
1	I	357	LEU
1	I	398	PHE
1	I	407	LEU
1	I	439	TYR
1	I	440	ARG
1	I	478	VAL
1	I	568	ASN
1	I	601	LEU
1	I	603	ASP
1	J	88	VAL
1	J	154	SER
1	J	164	LYS
1	J	194	SER
1	J	197	ASP
1	J	198	LEU
1	J	200	GLU
1	J	208	LEU
1	J	250	GLU
1	J	288	TYR
1	J	330	VAL
1	J	398	PHE
1	J	400	MET
1	J	407	LEU
1	J	439	TYR
1	J	452	THR
1	J	540	LYS
1	K	86	SER
1	K	166	ASN
1	K	208	LEU
1	K	216	ASP
1	K	230	VAL
1	K	239	LEU
1	K	288	TYR
1	K	310	LEU
1	K	398	PHE
1	K	413	VAL
1	K	436	LYS
1	K	439	TYR
1	K	478	VAL
1	K	483	ASP
1	K	498	SER

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Mol	Chain	Res	Type
1	K	518	LYS
1	L	88	VAL
1	L	113	GLN
1	L	132	VAL
1	L	134	ASN
1	L	144	ILE
1	L	145	SER
1	L	168	LYS
1	L	169	LEU
1	L	181	ASN
1	L	195	VAL
1	L	198	LEU
1	L	200	GLU
1	L	239	LEU
1	L	276	THR
1	L	288	TYR
1	L	310	LEU
1	L	358	THR
1	L	398	PHE
1	L	400	MET
1	L	407	LEU
1	L	421	VAL
1	L	436	LYS
1	L	439	TYR
1	L	476	LEU
1	L	483	ASP
1	L	554	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	B	139	ASN
1	B	174	HIS
1	B	319	GLN
1	C	113	GLN
1	D	139	ASN
1	E	166	ASN
1	E	181	ASN
1	E	437	ASN
1	F	134	ASN
1	F	322	ASN

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Mol	Chain	Res	Type
1	G	272	ASN
1	H	139	ASN
1	H	174	HIS
1	H	183	ASN
1	H	319	GLN
1	I	113	GLN
1	J	139	ASN
1	J	183	ASN
1	J	273	ASN
1	J	437	ASN
1	K	166	ASN
1	L	104	ASN
1	L	113	GLN
1	L	134	ASN
1	L	183	ASN
1	L	217	ASN
1	L	322	ASN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 24 are monoatomic - leaving 95 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	E	8	-	11,11,15	0.64	0	10,10,14	0.49	0
2	CO3	L	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	K	50	-	5,5,15	0.55	0	4,4,14	0.25	0
2	CO3	A	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	L	1	-	9,9,15	0.54	0	8,8,14	0.47	0
5	1PE	L	59	-	11,11,15	0.81	0	10,10,14	0.84	0
5	1PE	C	18	-	8,8,15	0.69	0	7,7,14	0.72	0
5	1PE	D	23	-	10,10,15	0.69	0	9,9,14	0.89	0
2	CO3	F	1002	-	0,3,3	-	-	0,3,3	-	-
2	CO3	J	1002	-	0,3,3	-	-	0,3,3	-	-
4	SO4	B	12	-	4,4,4	0.28	0	6,6,6	0.26	0
5	1PE	L	56	-	10,10,15	0.67	0	9,9,14	0.37	0
2	CO3	K	1002	-	0,3,3	-	-	0,3,3	-	-
4	SO4	I	34	-	4,4,4	0.36	0	6,6,6	0.64	0
4	SO4	K	31	-	4,4,4	0.19	0	6,6,6	0.28	0
5	1PE	G	16	-	9,9,15	0.66	0	8,8,14	0.83	0
5	1PE	D	34	-	9,9,15	0.52	0	8,8,14	0.58	0
5	1PE	C	41	-	7,7,15	0.89	0	6,6,14	0.82	0
5	1PE	E	43	-	7,7,15	0.58	0	6,6,14	0.39	0
6	2PE	B	14	-	25,25,27	0.53	0	24,24,26	0.33	0
4	SO4	G	27	-	4,4,4	0.13	0	6,6,6	0.75	0
6	2PE	H	6	-	24,24,27	0.47	0	23,23,26	0.44	0
4	SO4	B	29	-	4,4,4	0.22	0	6,6,6	0.48	0
4	SO4	H	26	-	4,4,4	0.18	0	6,6,6	0.49	0
5	1PE	E	35	-	9,9,15	0.54	0	8,8,14	0.23	0
5	1PE	K	36	-	10,10,15	0.80	0	9,9,14	0.70	0
2	CO3	C	1002	-	0,3,3	-	-	0,3,3	-	-
2	CO3	E	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	A	24	-	8,8,15	0.68	0	7,7,14	0.99	0
5	1PE	L	29	-	9,9,15	0.42	0	8,8,14	0.50	0
2	CO3	I	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	K	4	-	11,11,15	0.74	0	10,10,14	0.86	0
5	1PE	K	42	-	10,10,15	0.62	0	9,9,14	0.37	0
2	CO3	H	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	J	2	-	10,10,15	0.63	0	9,9,14	0.57	0
5	1PE	J	49	-	10,10,15	0.56	0	9,9,14	0.39	0
4	SO4	A	1	-	4,4,4	0.15	0	6,6,6	0.43	0
5	1PE	F	612	-	9,9,15	0.63	0	8,8,14	0.70	0
4	SO4	J	32	-	4,4,4	0.20	0	6,6,6	0.45	0
5	1PE	L	25	-	11,11,15	0.51	0	10,10,14	0.39	0
4	SO4	A	2	-	4,4,4	0.07	0	6,6,6	0.42	0
5	1PE	J	45	-	10,10,15	0.65	0	9,9,14	0.47	0
5	1PE	K	52	-	10,10,15	0.64	0	9,9,14	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	1PE	F	32	-	9,9,15	0.63	0	8,8,14	0.31	0
4	SO4	K	18	-	4,4,4	0.44	0	6,6,6	0.45	0
5	1PE	H	51	-	5,5,15	0.86	0	4,4,14	0.69	0
5	1PE	J	3	-	9,9,15	0.65	0	8,8,14	0.56	0
5	1PE	K	55	-	7,7,15	0.50	0	6,6,14	0.50	0
4	SO4	C	16	-	4,4,4	0.14	0	6,6,6	0.43	0
2	CO3	D	1002	-	0,3,3	-	-	0,3,3	-	-
4	SO4	C	24	-	4,4,4	0.14	0	6,6,6	0.31	0
4	SO4	E	11	-	4,4,4	0.12	0	6,6,6	0.22	0
4	SO4	C	6	-	4,4,4	0.33	0	6,6,6	0.27	0
5	1PE	G	48	-	5,5,15	0.70	0	4,4,14	0.77	0
5	1PE	E	7	-	11,11,15	0.72	0	10,10,14	0.67	0
4	SO4	F	33	-	4,4,4	0.40	0	6,6,6	0.34	0
5	1PE	F	53	-	11,11,15	0.74	0	10,10,14	0.43	0
4	SO4	K	19	-	4,4,4	0.24	0	6,6,6	0.32	0
4	SO4	E	28	-	4,4,4	0.36	0	6,6,6	0.35	0
5	1PE	G	47	-	5,5,15	0.52	0	4,4,14	0.31	0
4	SO4	K	20	-	4,4,4	0.16	0	6,6,6	0.29	0
5	1PE	G	12	-	8,8,15	0.70	0	7,7,14	0.62	0
5	1PE	A	19	-	8,8,15	0.56	0	7,7,14	0.65	0
6	2PE	F	63	-	5,5,27	1.03	0	4,4,26	1.07	0
5	1PE	D	612	-	8,8,15	0.83	0	7,7,14	0.81	0
5	1PE	E	612	-	10,10,15	0.52	0	9,9,14	0.31	0
5	1PE	D	9	-	9,9,15	0.61	0	8,8,14	0.52	0
5	1PE	D	44	-	10,10,15	0.72	0	9,9,14	0.66	0
4	SO4	D	5	-	4,4,4	0.10	0	6,6,6	0.55	0
4	SO4	K	30	-	4,4,4	0.17	0	6,6,6	0.53	0
4	SO4	B	3	-	4,4,4	0.16	0	6,6,6	0.75	0
4	SO4	D	10	-	4,4,4	0.15	0	6,6,6	0.31	0
5	1PE	E	46	-	8,8,15	0.61	0	7,7,14	0.59	0
5	1PE	C	17	-	12,12,15	0.71	0	11,11,14	0.50	0
5	1PE	I	61	-	4,4,15	0.53	0	3,3,14	0.46	0
4	SO4	C	15	-	4,4,4	0.13	0	6,6,6	0.37	0
5	1PE	D	62	-	4,4,15	0.81	0	3,3,14	0.27	0
5	1PE	F	31	-	9,9,15	0.61	0	8,8,14	0.59	0
5	1PE	A	57	-	5,5,15	0.76	0	4,4,14	0.46	0
5	1PE	J	15	-	11,11,15	0.58	0	10,10,14	1.10	1 (10%)
5	1PE	A	20	-	11,11,15	0.90	0	10,10,14	0.85	0
4	SO4	E	25	-	4,4,4	0.22	0	6,6,6	0.39	0
5	1PE	I	27	-	8,8,15	0.75	0	7,7,14	0.61	0
4	SO4	I	17	-	4,4,4	0.34	0	6,6,6	0.56	0
5	1PE	G	58	-	14,14,15	0.65	0	13,13,14	0.62	0
5	1PE	I	22	-	10,10,15	0.76	0	9,9,14	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	7	-	4,4,4	0.36	0	6,6,6	0.18	0
5	1PE	G	30	-	6,6,15	0.40	0	5,5,14	0.65	0
2	CO3	B	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	I	21	-	14,14,15	0.66	0	13,13,14	0.57	0
5	1PE	J	60	-	8,8,15	0.73	0	7,7,14	0.59	0
4	SO4	G	23	-	4,4,4	0.17	0	6,6,6	0.38	0
5	1PE	B	40	-	10,10,15	0.56	0	9,9,14	0.95	0
2	CO3	G	1002	-	0,3,3	-	-	0,3,3	-	-
5	1PE	K	5	-	11,11,15	0.60	0	10,10,14	0.37	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
5	1PE	E	8	-	-	2/9/9/13	-
5	1PE	K	4	-	-	4/9/9/13	-
5	1PE	K	42	-	-	2/8/8/13	-
5	1PE	K	50	-	-	3/3/3/13	-
5	1PE	E	46	-	-	2/6/6/13	-
5	1PE	J	2	-	-	4/8/8/13	-
5	1PE	L	1	-	-	3/7/7/13	-
5	1PE	C	17	-	-	5/10/10/13	-
5	1PE	I	61	-	-	1/2/2/13	-
5	1PE	J	49	-	-	4/8/8/13	-
5	1PE	F	53	-	-	8/9/9/13	-
5	1PE	L	59	-	-	5/9/9/13	-
5	1PE	C	18	-	-	4/6/6/13	-
5	1PE	D	23	-	-	2/8/8/13	-
5	1PE	D	62	-	-	2/2/2/13	-
5	1PE	F	31	-	-	5/7/7/13	-
5	1PE	A	57	-	-	3/3/3/13	-
5	1PE	J	15	-	-	3/9/9/13	-
5	1PE	A	20	-	-	4/9/9/13	-
5	1PE	F	612	-	-	6/7/7/13	-
5	1PE	L	56	-	-	2/8/8/13	-
5	1PE	G	47	-	-	2/3/3/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	I	27	-	-	1/6/6/13	-
5	1PE	L	25	-	-	4/9/9/13	-
5	1PE	G	58	-	-	3/12/12/13	-
5	1PE	I	22	-	-	3/8/8/13	-
5	1PE	G	30	-	-	3/4/4/13	-
5	1PE	G	16	-	-	3/7/7/13	-
5	1PE	D	34	-	-	2/7/7/13	-
5	1PE	C	41	-	-	1/5/5/13	-
5	1PE	E	43	-	-	1/5/5/13	-
5	1PE	J	45	-	-	6/8/8/13	-
6	2PE	B	14	-	-	9/23/23/25	-
5	1PE	K	52	-	-	6/8/8/13	-
5	1PE	F	32	-	-	2/7/7/13	-
5	1PE	H	51	-	-	1/3/3/13	-
5	1PE	G	12	-	-	6/6/6/13	-
5	1PE	J	3	-	-	4/7/7/13	-
6	2PE	H	6	-	-	13/22/22/25	-
5	1PE	K	55	-	-	4/5/5/13	-
5	1PE	A	19	-	-	2/6/6/13	-
5	1PE	E	35	-	-	4/7/7/13	-
6	2PE	F	63	-	-	2/3/3/25	-
5	1PE	D	612	-	-	6/6/6/13	-
5	1PE	E	612	-	-	4/8/8/13	-
5	1PE	I	21	-	-	6/12/12/13	-
5	1PE	J	60	-	-	5/6/6/13	-
5	1PE	D	9	-	-	6/7/7/13	-
5	1PE	D	44	-	-	1/8/8/13	-
5	1PE	K	36	-	-	5/8/8/13	-
5	1PE	A	24	-	-	5/6/6/13	-
5	1PE	G	48	-	-	2/3/3/13	-
5	1PE	L	29	-	-	4/7/7/13	-
5	1PE	B	40	-	-	4/8/8/13	-
5	1PE	E	7	-	-	2/9/9/13	-
5	1PE	K	5	-	-	1/9/9/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	15	1PE	OH4-C13-C23	-2.30	100.00	110.39

There are no chirality outliers.

All (207) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	59	1PE	C13-C23-OH3-C22
5	L	59	1PE	C15-C25-OH5-C14
5	K	52	1PE	C24-C14-OH5-C25
5	A	19	1PE	OH4-C13-C23-OH3
5	J	15	1PE	OH4-C13-C23-OH3
5	D	9	1PE	OH4-C13-C23-OH3
5	I	21	1PE	OH4-C13-C23-OH3
5	K	52	1PE	OH4-C13-C23-OH3
5	L	1	1PE	OH6-C15-C25-OH5
5	G	12	1PE	OH4-C13-C23-OH3
5	K	36	1PE	OH5-C14-C24-OH4
5	K	50	1PE	OH5-C14-C24-OH4
6	H	6	2PE	O13-C14-C15-O16
5	D	9	1PE	OH5-C14-C24-OH4
5	K	55	1PE	OH5-C14-C24-OH4
5	L	25	1PE	OH5-C14-C24-OH4
5	D	612	1PE	OH5-C14-C24-OH4
5	G	12	1PE	OH5-C14-C24-OH4
5	D	23	1PE	OH5-C14-C24-OH4
5	L	56	1PE	OH6-C15-C25-OH5
5	F	53	1PE	OH6-C15-C25-OH5
5	F	31	1PE	OH6-C15-C25-OH5
5	C	18	1PE	OH4-C13-C23-OH3
5	C	17	1PE	OH5-C14-C24-OH4
5	J	45	1PE	OH6-C15-C25-OH5
5	C	17	1PE	OH4-C13-C23-OH3
6	H	6	2PE	O7-C8-C9-O10
5	C	18	1PE	OH5-C14-C24-OH4
5	G	16	1PE	OH6-C15-C25-OH5
5	J	3	1PE	OH5-C14-C24-OH4
5	J	49	1PE	OH6-C15-C25-OH5
5	K	36	1PE	OH6-C15-C25-OH5
5	K	4	1PE	OH6-C15-C25-OH5
5	L	25	1PE	OH4-C13-C23-OH3
5	A	24	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
5	F	53	1PE	OH5-C14-C24-OH4
5	K	55	1PE	C14-C24-OH4-C13
5	F	612	1PE	OH6-C15-C25-OH5
5	L	59	1PE	OH5-C14-C24-OH4
5	A	19	1PE	OH5-C14-C24-OH4
5	F	31	1PE	OH5-C14-C24-OH4
5	F	31	1PE	OH7-C16-C26-OH6
5	F	32	1PE	OH5-C14-C24-OH4
5	F	612	1PE	OH7-C16-C26-OH6
5	I	21	1PE	OH7-C16-C26-OH6
5	J	3	1PE	OH7-C16-C26-OH6
5	K	55	1PE	OH6-C15-C25-OH5
5	L	29	1PE	OH4-C13-C23-OH3
5	L	29	1PE	OH6-C15-C25-OH5
6	B	14	2PE	O22-C23-C24-O25
5	J	60	1PE	OH5-C14-C24-OH4
5	J	3	1PE	OH6-C15-C25-OH5
5	I	22	1PE	OH4-C13-C23-OH3
5	E	43	1PE	OH4-C13-C23-OH3
6	H	6	2PE	O25-C26-C27-O28
5	D	612	1PE	OH4-C13-C23-OH3
6	H	6	2PE	O19-C20-C21-O22
5	E	46	1PE	C23-C13-OH4-C24
5	G	47	1PE	OH6-C15-C25-OH5
5	G	48	1PE	OH6-C15-C25-OH5
5	K	36	1PE	OH4-C13-C23-OH3
6	H	6	2PE	O22-C23-C24-O25
5	D	44	1PE	OH5-C14-C24-OH4
5	J	2	1PE	OH6-C15-C25-OH5
6	B	14	2PE	O7-C8-C9-O10
5	A	57	1PE	OH5-C14-C24-OH4
6	F	63	2PE	O19-C20-C21-O22
5	A	24	1PE	OH4-C13-C23-OH3
5	E	612	1PE	OH6-C15-C25-OH5
5	G	30	1PE	OH5-C14-C24-OH4
5	G	30	1PE	OH6-C15-C25-OH5
5	E	35	1PE	OH6-C15-C25-OH5
5	E	35	1PE	OH5-C14-C24-OH4
5	F	612	1PE	OH5-C14-C24-OH4
5	K	52	1PE	OH5-C14-C24-OH4
5	J	60	1PE	C15-C25-OH5-C14
5	I	21	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
5	C	17	1PE	C12-C22-OH3-C23
6	H	6	2PE	O16-C17-C18-O19
5	B	40	1PE	OH5-C14-C24-OH4
5	F	53	1PE	C25-C15-OH6-C26
5	A	57	1PE	C24-C14-OH5-C25
5	G	12	1PE	C13-C23-OH3-C22
5	G	12	1PE	C24-C14-OH5-C25
5	C	17	1PE	C25-C15-OH6-C26
5	D	23	1PE	C15-C25-OH5-C14
5	K	4	1PE	C12-C22-OH3-C23
5	E	8	1PE	C12-C22-OH3-C23
5	E	612	1PE	OH4-C13-C23-OH3
5	K	42	1PE	OH5-C14-C24-OH4
5	J	2	1PE	C14-C24-OH4-C13
5	J	49	1PE	OH5-C14-C24-OH4
5	D	62	1PE	C16-C26-OH6-C15
5	C	17	1PE	OH6-C15-C25-OH5
5	K	4	1PE	OH5-C14-C24-OH4
5	E	7	1PE	OH6-C15-C25-OH5
5	J	2	1PE	OH7-C16-C26-OH6
5	G	48	1PE	C15-C25-OH5-C14
5	L	25	1PE	C13-C23-OH3-C22
5	F	53	1PE	OH4-C13-C23-OH3
5	F	53	1PE	C24-C14-OH5-C25
5	I	21	1PE	C12-C22-OH3-C23
5	J	45	1PE	C15-C25-OH5-C14
5	K	52	1PE	C15-C25-OH5-C14
6	B	14	2PE	C18-C17-O16-C15
5	K	4	1PE	OH4-C13-C23-OH3
5	L	29	1PE	C24-C14-OH5-C25
5	C	18	1PE	C23-C13-OH4-C24
5	E	35	1PE	C16-C26-OH6-C15
5	F	612	1PE	C16-C26-OH6-C15
5	F	53	1PE	C23-C13-OH4-C24
5	G	30	1PE	C24-C14-OH5-C25
5	A	20	1PE	C25-C15-OH6-C26
5	B	40	1PE	C23-C13-OH4-C24
5	D	9	1PE	C23-C13-OH4-C24
5	J	3	1PE	C25-C15-OH6-C26
5	G	12	1PE	C23-C13-OH4-C24
5	G	58	1PE	C23-C13-OH4-C24
5	K	52	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
5	L	59	1PE	C23-C13-OH4-C24
5	I	22	1PE	C13-C23-OH3-C22
5	E	612	1PE	OH5-C14-C24-OH4
5	J	45	1PE	C24-C14-OH5-C25
5	A	24	1PE	C24-C14-OH5-C25
6	H	6	2PE	C5-C6-O7-C8
5	I	61	1PE	C24-C14-OH5-C25
5	I	21	1PE	C25-C15-OH6-C26
5	K	55	1PE	C24-C14-OH5-C25
5	J	60	1PE	C24-C14-OH5-C25
5	L	29	1PE	C14-C24-OH4-C13
5	E	7	1PE	C12-C22-OH3-C23
5	F	53	1PE	C15-C25-OH5-C14
5	B	40	1PE	C14-C24-OH4-C13
5	G	47	1PE	C24-C14-OH5-C25
5	L	59	1PE	C14-C24-OH4-C13
6	H	6	2PE	C17-C18-O19-C20
5	L	1	1PE	C24-C14-OH5-C25
6	H	6	2PE	C23-C24-O25-C26
6	B	14	2PE	O1-C2-C3-O4
6	H	6	2PE	O4-C5-C6-O7
5	B	40	1PE	C15-C25-OH5-C14
5	A	24	1PE	C23-C13-OH4-C24
5	K	52	1PE	C23-C13-OH4-C24
5	F	612	1PE	C15-C25-OH5-C14
5	G	12	1PE	C14-C24-OH4-C13
6	H	6	2PE	C14-C15-O16-C17
5	A	57	1PE	C14-C24-OH4-C13
5	D	9	1PE	C13-C23-OH3-C22
5	A	20	1PE	C14-C24-OH4-C13
5	F	32	1PE	C15-C25-OH5-C14
5	K	50	1PE	C24-C14-OH5-C25
5	J	60	1PE	C23-C13-OH4-C24
5	E	8	1PE	OH4-C13-C23-OH3
5	K	42	1PE	C15-C25-OH5-C14
6	B	14	2PE	C15-C14-O13-C12
5	L	25	1PE	C15-C25-OH5-C14
5	I	21	1PE	C16-C26-OH6-C15
5	G	58	1PE	C16-C26-OH6-C15
5	E	46	1PE	C15-C25-OH5-C14
5	J	15	1PE	C15-C25-OH5-C14
5	C	18	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
6	B	14	2PE	O19-C20-C21-O22
5	D	612	1PE	C24-C14-OH5-C25
5	F	31	1PE	C25-C15-OH6-C26
5	G	16	1PE	OH4-C13-C23-OH3
6	H	6	2PE	C8-C9-O10-C11
5	F	53	1PE	C14-C24-OH4-C13
5	E	35	1PE	C15-C25-OH5-C14
5	K	5	1PE	C15-C25-OH5-C14
6	B	14	2PE	C5-C6-O7-C8
5	J	60	1PE	C14-C24-OH4-C13
5	A	20	1PE	C13-C23-OH3-C22
5	J	45	1PE	C25-C15-OH6-C26
5	K	36	1PE	C23-C13-OH4-C24
5	J	49	1PE	OH4-C13-C23-OH3
5	I	27	1PE	C15-C25-OH5-C14
5	G	16	1PE	C14-C24-OH4-C13
5	K	50	1PE	C14-C24-OH4-C13
6	B	14	2PE	C23-C24-O25-C26
5	J	2	1PE	C15-C25-OH5-C14
5	C	41	1PE	C24-C14-OH5-C25
5	D	612	1PE	C13-C23-OH3-C22
5	F	31	1PE	C15-C25-OH5-C14
6	B	14	2PE	O10-C11-C12-O13
5	F	612	1PE	C25-C15-OH6-C26
5	H	51	1PE	C14-C24-OH4-C13
5	J	45	1PE	C23-C13-OH4-C24
5	I	22	1PE	C24-C14-OH5-C25
5	D	9	1PE	C24-C14-OH5-C25
5	J	15	1PE	C14-C24-OH4-C13
5	L	1	1PE	C16-C26-OH6-C15
5	A	24	1PE	C15-C25-OH5-C14
6	H	6	2PE	C18-C17-O16-C15
5	J	45	1PE	OH5-C14-C24-OH4
5	D	612	1PE	C23-C13-OH4-C24
5	D	34	1PE	C25-C15-OH6-C26
5	J	49	1PE	C13-C23-OH3-C22
5	G	58	1PE	C13-C23-OH3-C22
6	F	63	2PE	C21-C20-O19-C18
5	L	56	1PE	OH5-C14-C24-OH4
5	E	612	1PE	C23-C13-OH4-C24
5	D	612	1PE	C14-C24-OH4-C13
5	D	34	1PE	OH7-C16-C26-OH6

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Mol	Chain	Res	Type	Atoms
5	D	62	1PE	OH7-C16-C26-OH6
5	D	9	1PE	C12-C22-OH3-C23
5	A	20	1PE	OH5-C14-C24-OH4
5	K	36	1PE	C15-C25-OH5-C14

There are no ring outliers.

44 monomers are involved in 80 short contacts:

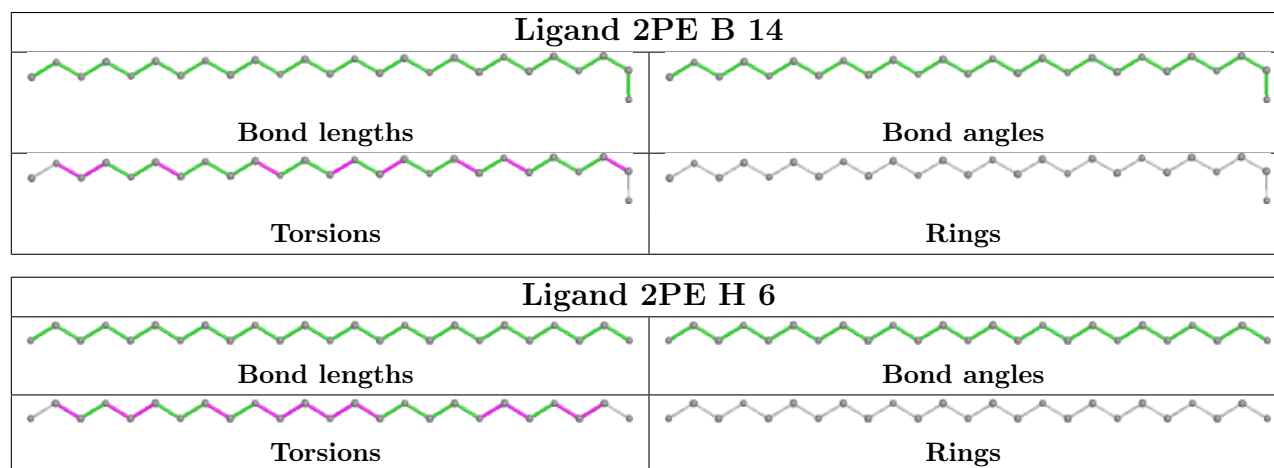
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	50	1PE	1	0
5	L	1	1PE	2	0
5	C	18	1PE	2	0
5	L	56	1PE	2	0
5	G	16	1PE	1	0
5	D	34	1PE	1	0
6	B	14	2PE	2	0
6	H	6	2PE	1	0
5	E	35	1PE	2	0
5	K	36	1PE	1	0
5	A	24	1PE	4	0
5	L	29	1PE	1	0
5	K	4	1PE	1	0
5	J	2	1PE	2	0
4	A	1	SO4	1	0
5	F	612	1PE	4	0
5	L	25	1PE	10	0
5	J	45	1PE	2	0
5	K	52	1PE	3	0
4	K	18	SO4	2	0
5	H	51	1PE	2	0
5	J	3	1PE	4	0
5	K	55	1PE	4	0
5	G	48	1PE	2	0
4	F	33	SO4	1	0
5	F	53	1PE	1	0
4	K	19	SO4	1	0
4	E	28	SO4	1	0
5	G	47	1PE	1	0
4	K	20	SO4	1	0
5	G	12	1PE	1	0
5	E	612	1PE	1	0
5	D	44	1PE	1	0

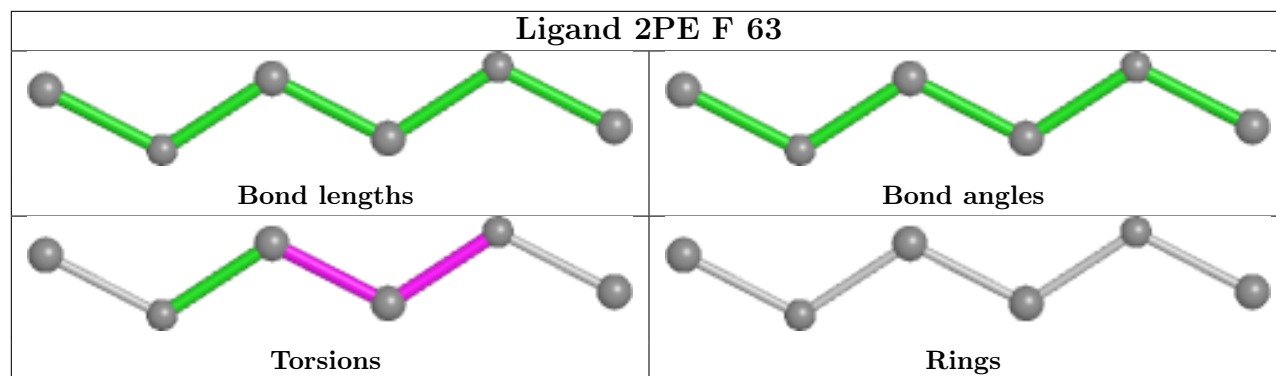
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3	SO4	1	0
5	I	61	1PE	1	0
5	A	57	1PE	2	0
5	A	20	1PE	1	0
4	E	25	SO4	1	0
4	I	17	SO4	1	0
5	G	58	1PE	2	0
4	D	7	SO4	1	0
5	I	21	1PE	2	0
5	J	60	1PE	2	0
5	B	40	1PE	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	514/528 (97%)	-0.17	5 (0%)	82 80	20, 30, 52, 74	0
1	B	510/528 (96%)	0.04	12 (2%)	59 57	20, 35, 79, 99	1 (0%)
1	C	518/528 (98%)	-0.10	1 (0%)	95 94	19, 30, 58, 68	0
1	D	514/528 (97%)	-0.20	2 (0%)	92 91	19, 30, 50, 67	0
1	E	509/528 (96%)	-0.22	2 (0%)	92 91	19, 28, 44, 61	0
1	F	510/528 (96%)	0.10	31 (6%)	21 20	20, 36, 73, 82	0
1	G	514/528 (97%)	-0.15	3 (0%)	89 88	20, 29, 51, 72	0
1	H	510/528 (96%)	0.03	12 (2%)	59 57	21, 36, 80, 102	1 (0%)
1	I	515/528 (97%)	0.04	11 (2%)	63 61	19, 32, 63, 76	0
1	J	514/528 (97%)	-0.23	1 (0%)	95 94	19, 29, 51, 68	0
1	K	509/528 (96%)	-0.20	3 (0%)	89 88	19, 29, 48, 68	0
1	L	508/528 (96%)	0.02	18 (3%)	44 43	18, 31, 64, 80	0
All	All	6145/6336 (96%)	-0.09	101 (1%)	72 70	18, 31, 64, 102	2 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	128	THR	5.0
1	F	156	PHE	4.9
1	F	123	VAL	4.8
1	F	114	VAL	4.6
1	L	119	GLY	4.6
1	F	148	VAL	4.6
1	F	121	CYS	4.6
1	F	146	SER	4.5
1	L	123	VAL	4.4
1	F	120	GLY	4.4
1	F	269	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	I	120	GLY	4.3
1	F	186	ALA	4.2
1	F	130	PHE	4.0
1	F	129	ILE	3.8
1	I	121	CYS	3.7
1	I	153	VAL	3.6
1	D	85	ALA	3.5
1	L	130	PHE	3.5
1	F	270	TYR	3.5
1	F	176	TYR	3.5
1	L	270	TYR	3.5
1	I	183	ASN	3.4
1	F	112	VAL	3.4
1	L	121	CYS	3.4
1	A	603	ASP	3.2
1	B	178	PHE	3.1
1	A	427	SER	3.1
1	B	183	ASN	3.1
1	F	115	TYR	3.0
1	F	183	ASN	3.0
1	H	421	VAL	3.0
1	K	426	LEU	3.0
1	F	127	LEU	2.9
1	J	603	ASP	2.9
1	H	183	ASN	2.9
1	F	145	SER	2.8
1	G	603	ASP	2.8
1	L	120	GLY	2.8
1	I	148	VAL	2.8
1	K	420	ASN	2.8
1	E	421	VAL	2.8
1	I	117	ILE	2.8
1	F	184	SER	2.7
1	B	421	VAL	2.7
1	B	136	GLY	2.7
1	I	186	ALA	2.7
1	A	497	THR	2.6
1	A	499	TYR	2.6
1	F	157	LEU	2.6
1	K	413	VAL	2.6
1	B	228	ILE	2.6
1	E	150	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	515	GLN	2.6
1	L	146	SER	2.6
1	B	177	MET	2.6
1	H	175	PHE	2.6
1	B	195	VAL	2.5
1	F	226	PHE	2.5
1	L	114	VAL	2.4
1	L	144	ILE	2.4
1	L	132	VAL	2.4
1	B	363	GLY	2.4
1	L	118	LYS	2.4
1	F	175	PHE	2.4
1	B	420	ASN	2.4
1	F	364	ASP	2.3
1	F	162	MET	2.3
1	H	603	ASP	2.3
1	F	144	ILE	2.3
1	H	196	ALA	2.3
1	F	224	VAL	2.3
1	H	195	VAL	2.3
1	L	122	ASN	2.3
1	H	137	LYS	2.2
1	I	150	ASP	2.2
1	G	363	GLY	2.2
1	I	222	LEU	2.2
1	G	161	ASN	2.2
1	B	603	ASP	2.2
1	D	183	ASN	2.2
1	L	230	VAL	2.2
1	F	222	LEU	2.2
1	L	145	SER	2.2
1	A	498	SER	2.1
1	H	132	VAL	2.1
1	F	147	LYS	2.1
1	H	365	VAL	2.1
1	H	165	PHE	2.1
1	L	142	VAL	2.1
1	F	125	GLU	2.1
1	B	225	VAL	2.1
1	F	132	VAL	2.1
1	I	123	VAL	2.1
1	H	232	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	420	ASN	2.0
1	I	419	GLU	2.0
1	B	479	ASP	2.0
1	L	217	ASN	2.0
1	L	175	PHE	2.0
1	F	267	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	16	5/5	0.71	0.36	94,103,106,110	0
4	SO4	E	11	5/5	0.74	0.24	105,107,109,112	0
5	1PE	F	53	12/16	0.80	0.17	64,70,81,85	0
6	2PE	F	63	6/28	0.80	0.34	31,41,53,57	0
5	1PE	I	27	9/16	0.81	0.31	38,42,50,52	0
5	1PE	D	612	9/16	0.82	0.19	46,54,69,75	0
5	1PE	K	55	8/16	0.83	0.26	46,68,77,84	0
5	1PE	A	57	6/16	0.83	0.20	31,44,52,54	0
5	1PE	K	52	11/16	0.84	0.19	57,63,73,74	0
5	1PE	A	20	12/16	0.85	0.17	32,50,57,57	0
5	1PE	H	51	6/16	0.86	0.26	29,45,54,56	0
5	1PE	J	3	10/16	0.87	0.17	43,49,52,52	0
5	1PE	D	62	5/16	0.87	0.25	35,41,56,66	0
5	1PE	J	45	11/16	0.88	0.22	40,56,73,77	0
5	1PE	L	59	12/16	0.88	0.26	34,50,60,60	0
5	1PE	D	44	11/16	0.88	0.24	38,56,64,65	0
5	1PE	E	46	9/16	0.89	0.21	30,43,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	1PE	F	31	10/16	0.89	0.16	35,44,53,55	0
5	1PE	J	60	9/16	0.89	0.17	38,48,56,58	0
5	1PE	K	4	12/16	0.89	0.16	33,46,57,60	0
5	1PE	F	32	10/16	0.89	0.17	44,63,69,73	0
5	1PE	D	34	10/16	0.89	0.16	45,56,64,64	0
5	1PE	B	40	11/16	0.89	0.24	35,50,57,58	0
5	1PE	A	24	9/16	0.89	0.29	29,41,53,61	0
5	1PE	G	16	10/16	0.90	0.26	29,40,63,63	0
5	1PE	G	58	15/16	0.90	0.16	39,49,60,63	0
4	SO4	B	12	5/5	0.90	0.23	75,79,85,86	0
5	1PE	C	41	8/16	0.90	0.23	23,43,46,48	0
5	1PE	F	612	10/16	0.91	0.18	31,44,57,61	0
5	1PE	J	49	11/16	0.91	0.26	43,74,78,80	0
5	1PE	J	15	12/16	0.92	0.31	24,36,58,61	0
5	1PE	I	22	11/16	0.92	0.17	33,46,57,63	0
5	1PE	E	7	12/16	0.92	0.18	40,49,56,57	0
5	1PE	G	48	6/16	0.92	0.12	30,35,38,48	0
6	2PE	B	14	26/28	0.92	0.15	36,57,77,82	0
5	1PE	K	36	11/16	0.92	0.22	33,42,55,56	0
5	1PE	E	8	12/16	0.93	0.15	33,41,51,51	0
5	1PE	L	56	11/16	0.93	0.17	44,58,76,77	0
5	1PE	E	35	10/16	0.93	0.15	48,59,65,66	0
5	1PE	K	50	6/16	0.93	0.13	53,55,56,58	0
5	1PE	C	17	13/16	0.93	0.17	33,47,60,60	0
5	1PE	G	47	6/16	0.94	0.16	39,47,50,61	0
5	1PE	A	19	9/16	0.94	0.13	17,39,41,52	0
4	SO4	D	5	5/5	0.94	0.14	60,60,65,67	0
5	1PE	L	29	10/16	0.94	0.14	44,56,65,68	0
5	1PE	G	12	9/16	0.94	0.16	23,31,44,46	0
5	1PE	I	21	15/16	0.94	0.20	30,51,64,69	0
5	1PE	D	23	11/16	0.94	0.25	18,35,45,47	0
5	1PE	G	30	7/16	0.94	0.30	45,56,62,66	0
6	2PE	H	6	25/28	0.94	0.14	33,62,78,83	0
5	1PE	J	2	11/16	0.95	0.21	29,44,63,75	0
5	1PE	L	1	10/16	0.95	0.16	19,38,54,60	0
5	1PE	L	25	12/16	0.95	0.14	32,43,49,52	0
5	1PE	C	18	9/16	0.95	0.11	28,34,47,48	0
4	SO4	C	15	5/5	0.95	0.12	73,74,78,79	0
5	1PE	K	5	12/16	0.95	0.17	23,35,58,59	0
5	1PE	K	42	11/16	0.95	0.17	39,42,58,63	0
4	SO4	K	30	5/5	0.95	0.10	63,67,74,75	0
5	1PE	E	612	11/16	0.95	0.17	31,38,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	1PE	D	9	10/16	0.96	0.14	30,44,52,54	0
4	SO4	E	28	5/5	0.96	0.15	54,56,64,72	0
5	1PE	E	43	8/16	0.96	0.15	42,50,55,58	0
4	SO4	K	31	5/5	0.97	0.12	48,60,63,64	0
2	CO3	F	1002	4/4	0.97	0.13	24,25,26,29	0
4	SO4	D	10	5/5	0.97	0.13	52,58,67,71	0
4	SO4	B	29	5/5	0.97	0.13	52,62,71,72	0
2	CO3	H	1002	4/4	0.97	0.12	25,26,26,26	0
4	SO4	K	20	5/5	0.97	0.13	56,65,70,76	0
2	CO3	J	1002	4/4	0.97	0.14	19,21,22,23	0
2	CO3	A	1002	4/4	0.98	0.12	29,30,30,31	0
2	CO3	G	1002	4/4	0.98	0.15	26,28,29,32	0
2	CO3	B	1002	4/4	0.98	0.19	25,25,26,28	0
4	SO4	C	24	5/5	0.98	0.16	54,62,62,64	0
2	CO3	C	1002	4/4	0.98	0.14	27,29,30,32	0
2	CO3	K	1002	4/4	0.98	0.13	22,23,24,27	0
2	CO3	L	1002	4/4	0.98	0.12	18,21,23,26	0
4	SO4	E	25	5/5	0.98	0.13	46,50,53,56	0
3	ZN	J	1004	1/1	0.98	0.13	32,32,32,32	0
4	SO4	F	33	5/5	0.98	0.10	50,53,57,64	0
4	SO4	G	23	5/5	0.98	0.13	49,60,70,72	0
4	SO4	H	26	5/5	0.98	0.11	46,50,60,61	0
4	SO4	I	34	5/5	0.98	0.18	42,48,51,52	0
4	SO4	J	32	5/5	0.98	0.25	53,55,61,69	0
4	SO4	K	19	5/5	0.98	0.10	47,54,56,62	0
3	ZN	K	1004	1/1	0.98	0.12	36,36,36,36	0
5	1PE	I	61	5/16	0.98	0.12	26,27,38,40	0
4	SO4	A	2	5/5	0.98	0.12	49,58,59,64	0
2	CO3	E	1002	4/4	0.98	0.13	27,28,31,32	0
3	ZN	D	1001	1/1	0.99	0.12	28,28,28,28	0
3	ZN	D	1004	1/1	0.99	0.12	29,29,29,29	0
3	ZN	E	1001	1/1	0.99	0.14	27,27,27,27	0
3	ZN	E	1004	1/1	0.99	0.12	31,31,31,31	0
3	ZN	F	1004	1/1	0.99	0.11	26,26,26,26	0
3	ZN	G	1001	1/1	0.99	0.14	32,32,32,32	0
3	ZN	G	1004	1/1	0.99	0.10	29,29,29,29	0
3	ZN	H	1001	1/1	0.99	0.12	37,37,37,37	0
4	SO4	G	27	5/5	0.99	0.10	43,46,48,57	0
3	ZN	H	1004	1/1	0.99	0.12	33,33,33,33	0
3	ZN	I	1001	1/1	0.99	0.11	27,27,27,27	0
3	ZN	J	1001	1/1	0.99	0.13	28,28,28,28	0
2	CO3	I	1002	4/4	0.99	0.14	23,24,24,28	0

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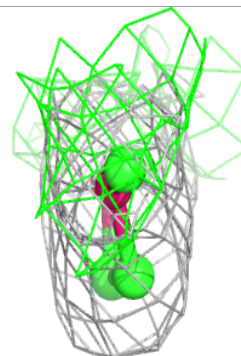
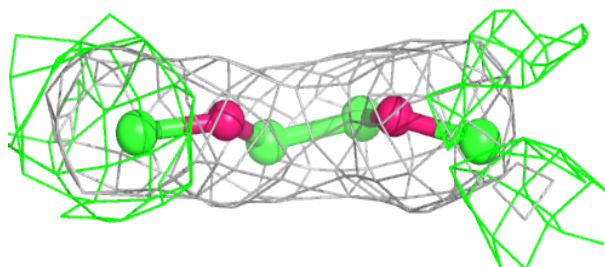
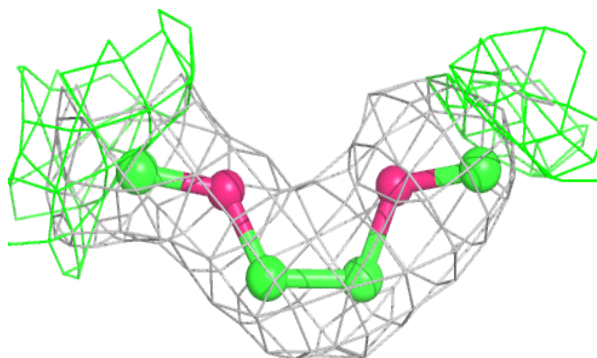
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	K	1001	1/1	0.99	0.14	32,32,32,32	0
2	CO3	D	1002	4/4	0.99	0.13	23,25,26,27	0
3	ZN	L	1001	1/1	0.99	0.10	30,30,30,30	0
4	SO4	A	1	5/5	0.99	0.11	47,47,58,59	0
3	ZN	A	1004	1/1	0.99	0.12	27,27,27,27	0
4	SO4	B	3	5/5	0.99	0.12	20,23,25,27	0
3	ZN	A	1001	1/1	0.99	0.13	29,29,29,29	0
3	ZN	B	1004	1/1	0.99	0.12	26,26,26,26	0
4	SO4	C	6	5/5	0.99	0.10	32,40,47,56	0
3	ZN	B	1001	1/1	0.99	0.14	27,27,27,27	0
3	ZN	C	1004	1/1	0.99	0.12	25,25,25,25	0
3	ZN	C	1001	1/1	1.00	0.11	23,23,23,23	0
4	SO4	D	7	5/5	1.00	0.09	23,23,24,32	0
4	SO4	K	18	5/5	1.00	0.15	25,28,32,33	0
3	ZN	I	1004	1/1	1.00	0.12	29,29,29,29	0
3	ZN	L	1004	1/1	1.00	0.12	26,26,26,26	0
3	ZN	F	1001	1/1	1.00	0.14	26,26,26,26	0
4	SO4	I	17	5/5	1.00	0.13	25,26,28,28	0

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

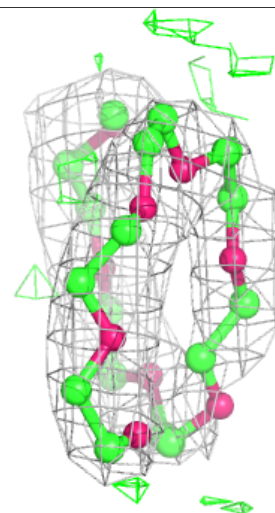
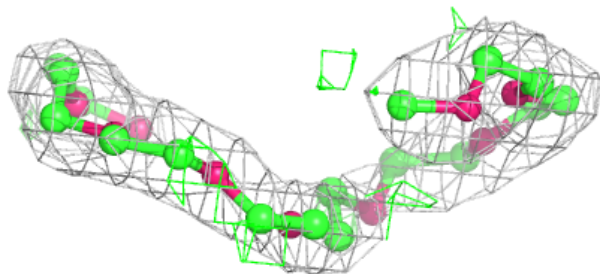
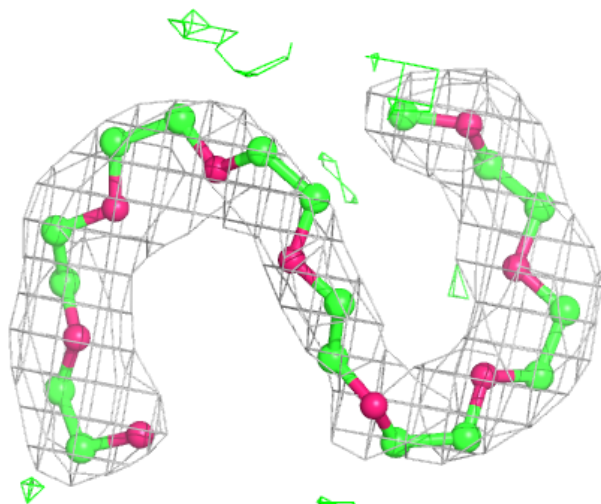
**Electron density around 2PE F 63:**

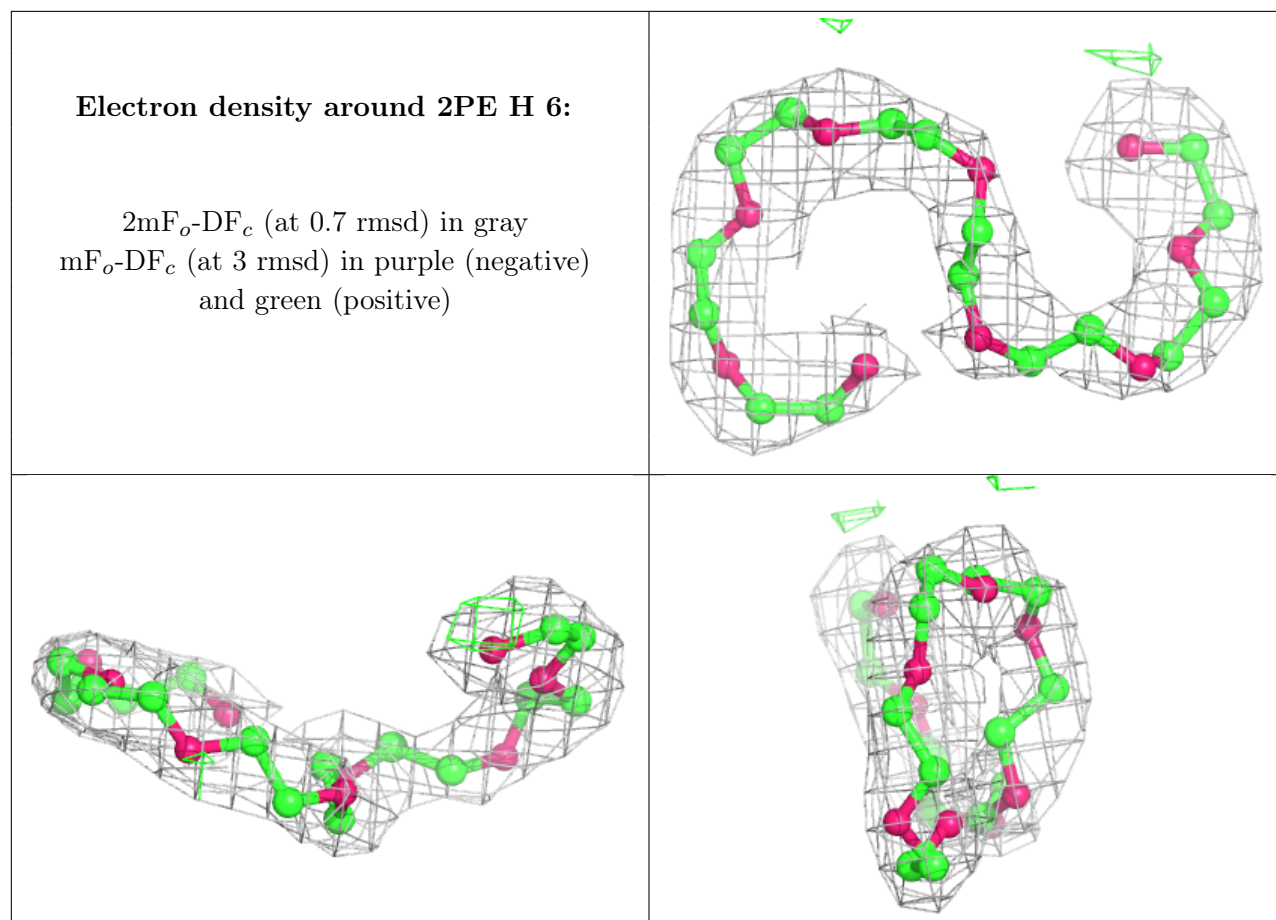
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.