Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 PM GMT

PDB ID	:	3T8W
Title	:	A bestatin-based chemical biology strategy reveals distinct roles for malaria M1- and M17-family aminopeptidases
Authors	:	McGowan, S.; Klemba, M.; Greebaum, D.C.
Deposited on	:	2011-08-01
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

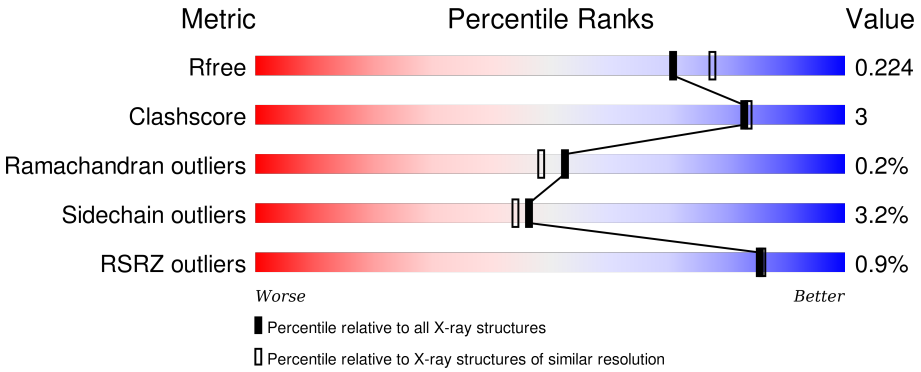
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	93% 5%
1	B	528	2% 90% 7%
1	C	528	91% 6%
1	D	528	90% 7%
1	E	528	90% 6%

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Mol	Chain	Length	Quality of chain
1	F	528	2% 87% 9%
1	G	528	91% 6%
1	H	528	90% 7%
1	I	528	92% 5%
1	J	528	89% 8%
1	K	528	89% 7%
1	L	528	88% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	A	612	-	-	-	X
2	CO3	B	612	-	-	-	X
2	CO3	C	612	-	-	-	X
2	CO3	D	612	-	-	-	X
2	CO3	E	612	-	-	-	X
2	CO3	F	612	-	-	-	X
2	CO3	G	612	-	-	-	X
2	CO3	H	612	-	-	-	X
2	CO3	I	612	-	-	-	X
2	CO3	J	612	-	-	-	X
2	CO3	K	612	-	-	-	X
2	CO3	L	612	-	-	-	X
5	SO4	A	617	-	-	-	X
5	SO4	C	617	-	-	-	X
5	SO4	C	618	-	-	-	X
5	SO4	C	619	-	-	-	X
5	SO4	C	620	-	-	-	X
5	SO4	E	616	-	-	-	X
5	SO4	E	618	-	-	-	X
5	SO4	G	617	-	-	-	X
5	SO4	G	618	-	-	-	X
5	SO4	G	619	-	-	-	X
5	SO4	H	617	-	-	-	X
5	SO4	H	618	-	-	-	X
5	SO4	I	617	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	I	618	-	-	-	X
5	SO4	I	619	-	-	-	X
5	SO4	J	618	-	-	-	X
5	SO4	L	616	-	-	-	X
6	1PE	D	618	-	-	-	X
6	1PE	D	619	-	-	-	X
6	1PE	D	620	-	-	-	X
6	1PE	D	621	-	X	-	X
6	1PE	E	620	-	X	-	X
6	1PE	E	621	-	-	-	X
6	1PE	F	616	-	-	-	X
6	1PE	F	618	-	-	-	X
6	1PE	G	621	-	-	-	X
6	1PE	G	623	-	-	X	X
6	1PE	I	623	-	-	-	X
6	1PE	J	621	-	-	-	X
6	1PE	J	622	-	-	-	X
6	1PE	K	618	-	-	-	X
6	1PE	K	619	-	X	-	X
6	1PE	K	620	-	-	-	X
6	1PE	L	618	-	-	-	X
6	1PE	L	619	-	-	-	X
6	1PE	L	620	-	X	-	-
7	2PE	B	616	-	-	-	X
7	2PE	H	619	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 53295 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	519	Total	C	N	O	S	0	0	0
			3973	2550	638	766	19			
1	B	517	Total	C	N	O	S	0	0	0
			3916	2515	636	746	19			
1	C	516	Total	C	N	O	S	0	0	0
			3942	2533	635	755	19			
1	D	514	Total	C	N	O	S	0	0	0
			3928	2529	633	746	20			
1	E	509	Total	C	N	O	S	0	0	0
			3900	2512	625	744	19			
1	F	511	Total	C	N	O	S	0	0	0
			3847	2473	621	734	19			
1	G	517	Total	C	N	O	S	0	0	0
			3978	2553	638	767	20			
1	H	518	Total	C	N	O	S	0	0	0
			3927	2521	636	750	20			
1	I	518	Total	C	N	O	S	0	0	0
			3955	2543	637	755	20			
1	J	514	Total	C	N	O	S	0	0	0
			3925	2527	632	746	20			
1	K	509	Total	C	N	O	S	0	0	0
			3897	2509	624	745	19			
1	L	511	Total	C	N	O	S	0	0	0
			3844	2469	621	735	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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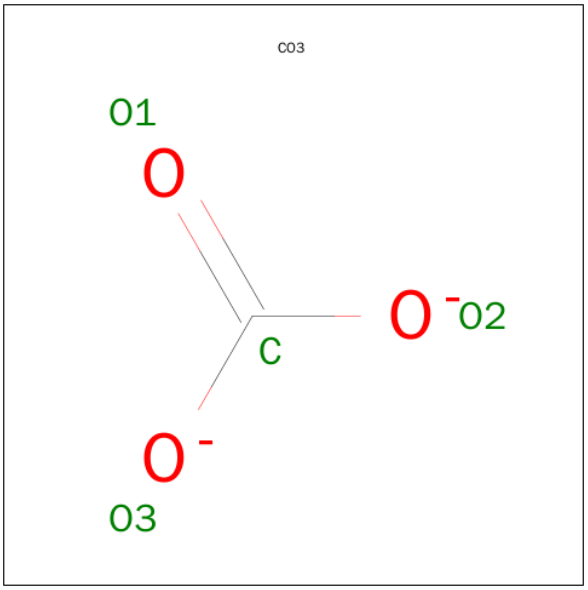
Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	608	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_3).



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

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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	G	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0

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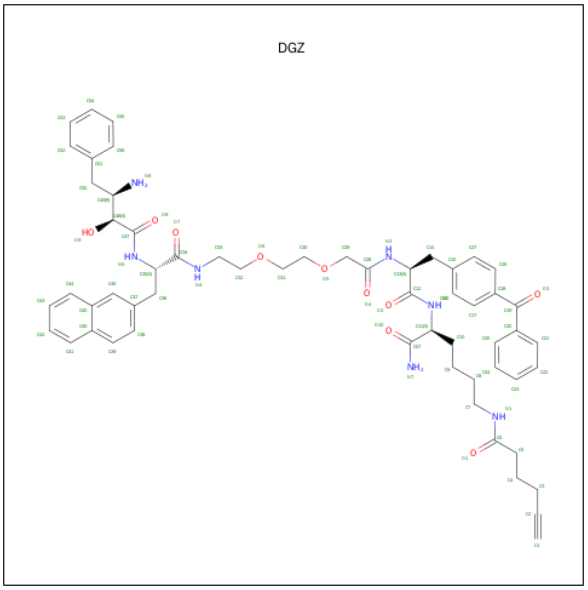
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	L	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0

- Molecule 4 is N-((2R,3S,6S,18S,21S)-2-AMINO-18-(4-BENZOYLBENZYL)-21-CARBAMOYL-3-HYDROXY-6-(NAPHTHALEN-2-YLMETHYL)-4,7,16,19-TETRAOXO-1-PHENYL-11,14-DIOXA-5,8,17,20-TETRAAZAPENTACOSAN-25-YL)HEX-5-YNAMIDE (three-letter code: DGZ) (formula: $C_{57}H_{67}N_7O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 74 57 7 10	0	0
4	B	1	Total C N O 74 57 7 10	0	0
4	C	1	Total C N O 74 57 7 10	0	0
4	D	1	Total C N O 74 57 7 10	0	0
4	E	1	Total C N O 74 57 7 10	0	0
4	F	1	Total C N O 74 57 7 10	0	0
4	G	1	Total C N O 74 57 7 10	0	0

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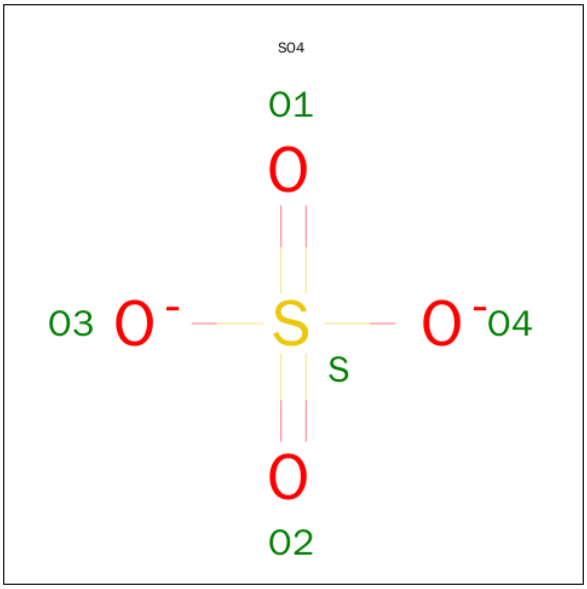
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 74 57 7 10	0	0
4	I	1	Total C N O 74 57 7 10	0	0
4	J	1	Total C N O 74 57 7 10	0	0
4	K	1	Total C N O 74 57 7 10	0	0
4	L	1	Total C N O 74 57 7 10	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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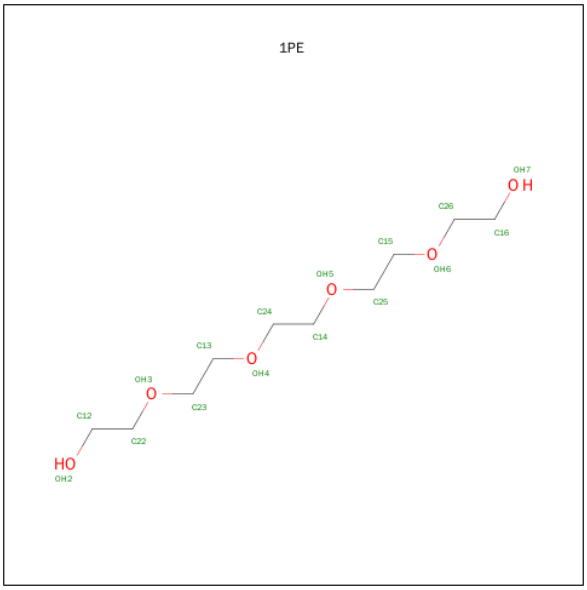
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0

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



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

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

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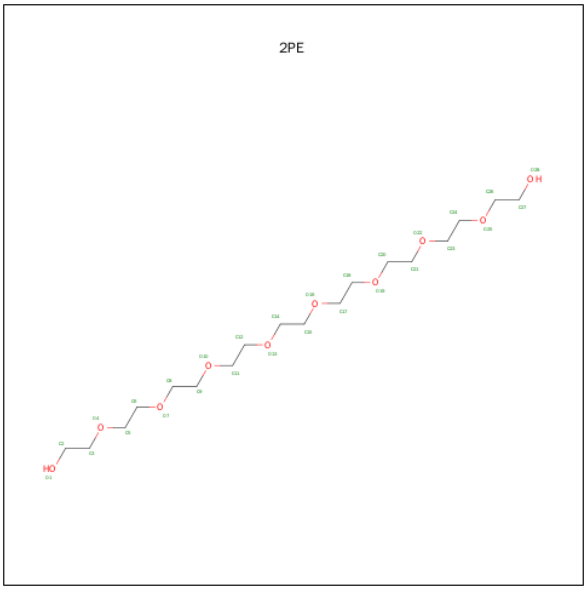
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 12 8 4	0	0
6	L	1	Total C O 7 4 3	0	0
6	L	1	Total C O 11 7 4	0	0

- Molecule 7 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 26 17 9	0	0
7	H	1	Total C O 25 16 9	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	421	Total O 421 421	0	0
8	B	351	Total O 351 351	0	0
8	C	431	Total O 431 431	0	0
8	D	424	Total O 424 424	0	0

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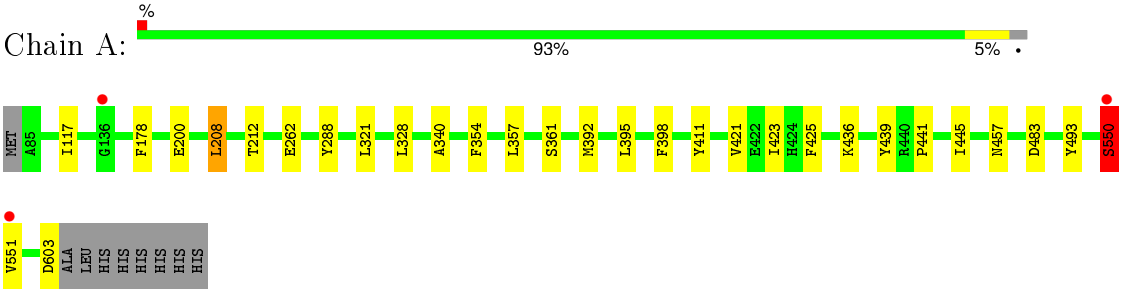
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	445	Total O 445 445	0	0
8	F	364	Total O 364 364	0	0
8	G	431	Total O 431 431	0	0
8	H	334	Total O 334 334	0	0
8	I	391	Total O 391 391	0	0
8	J	406	Total O 406 406	0	0
8	K	408	Total O 408 408	0	0
8	L	389	Total O 389 389	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

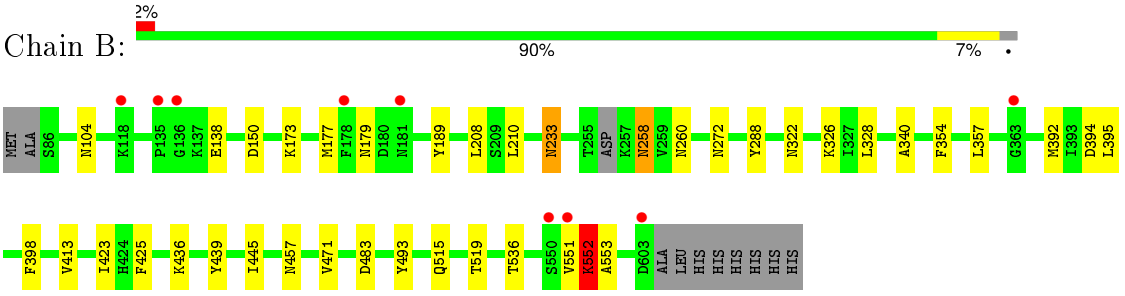
- Molecule 1: M17 leucyl aminopeptidase

Chain A:



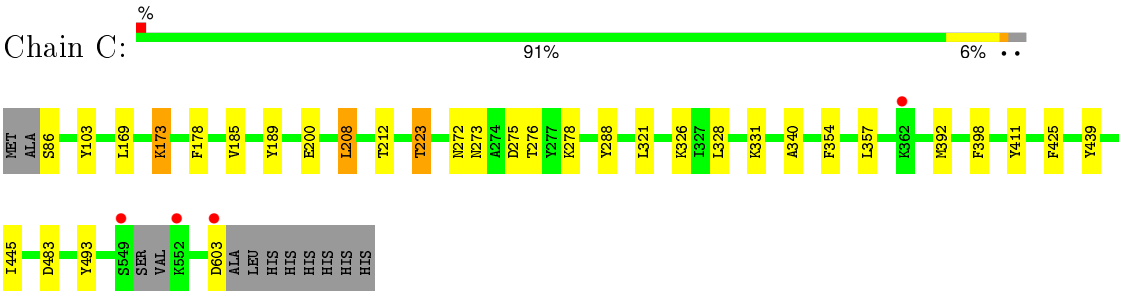
- Molecule 1: M17 leucyl aminopeptidase

Chain B:



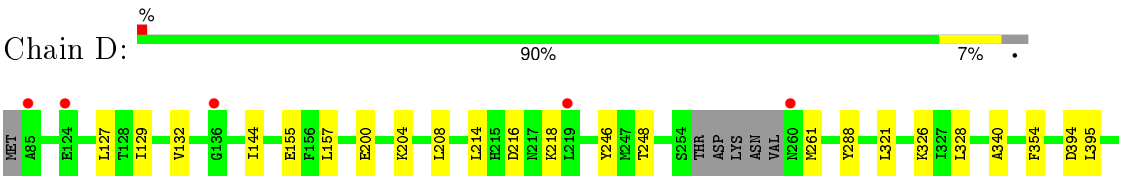
- Molecule 1: M17 leucyl aminopeptidase

Chain C:



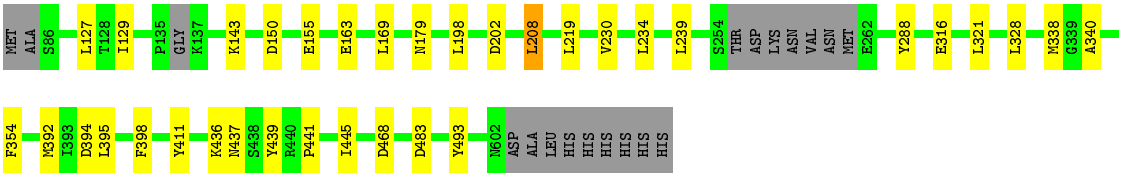
- Molecule 1: M17 leucyl aminopeptidase

Chain D:



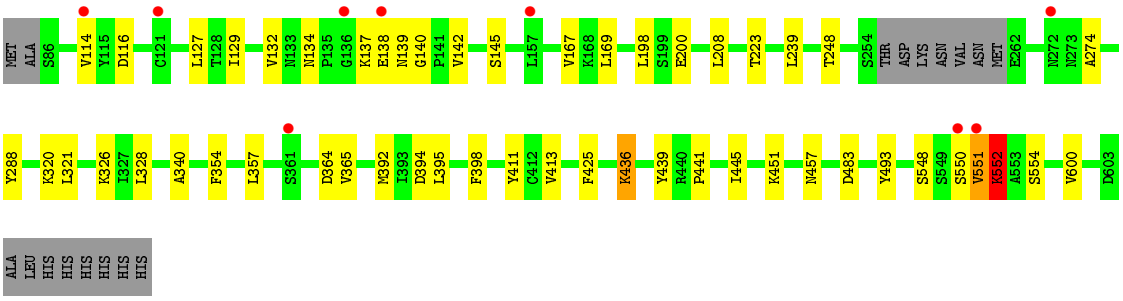
• Molecule 1: M17 leucyl aminopeptidase

Chain E:



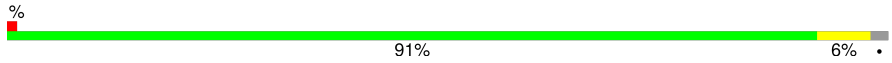
• Molecule 1: M17 leucyl aminopeptidase

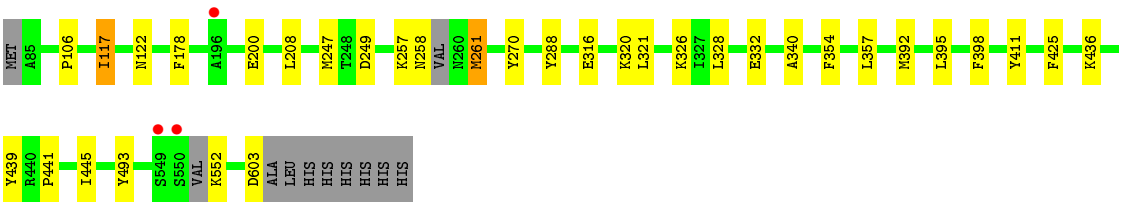
Chain F:



• Molecule 1: M17 leucyl aminopeptidase

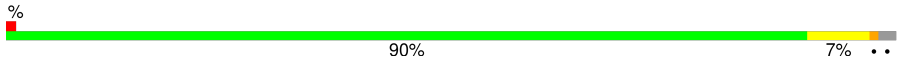
Chain G:

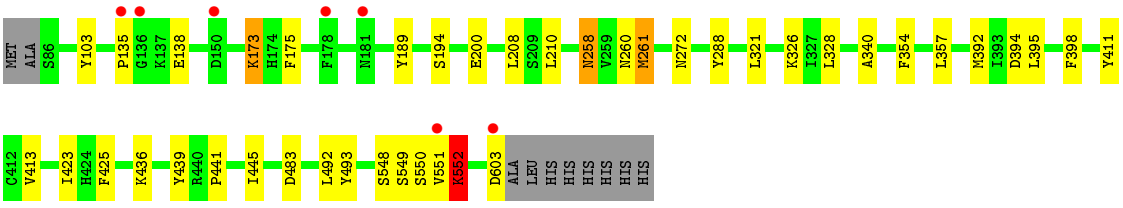




• Molecule 1: M17 leucyl aminopeptidase

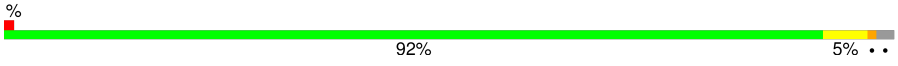
Chain H:

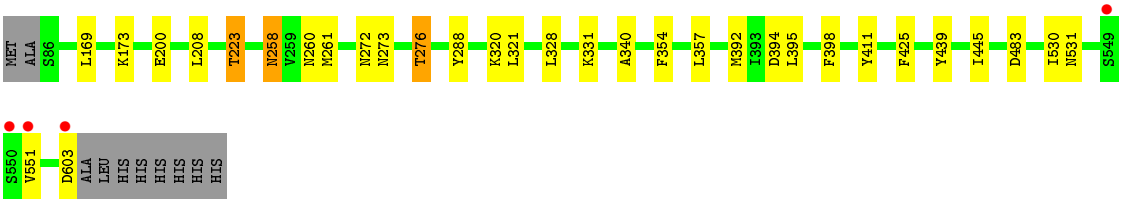




• Molecule 1: M17 leucyl aminopeptidase

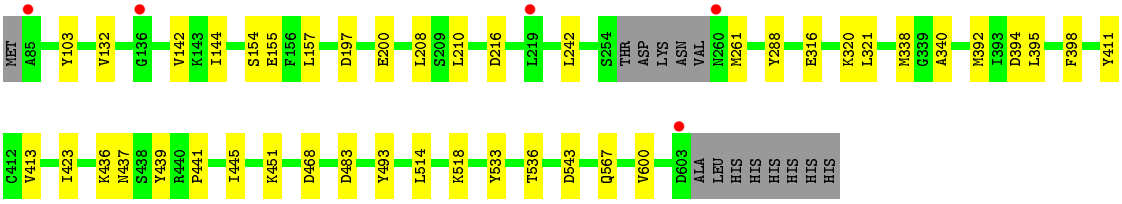
Chain I:





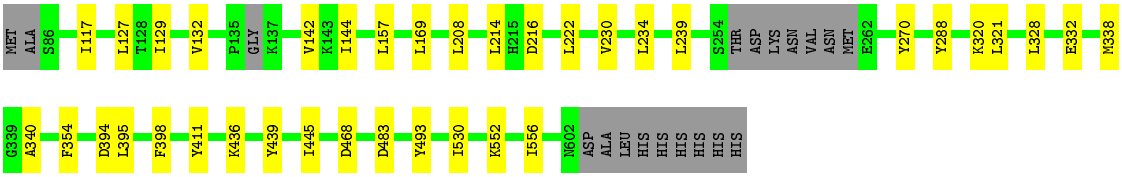
• Molecule 1: M17 leucyl aminopeptidase

Chain J:



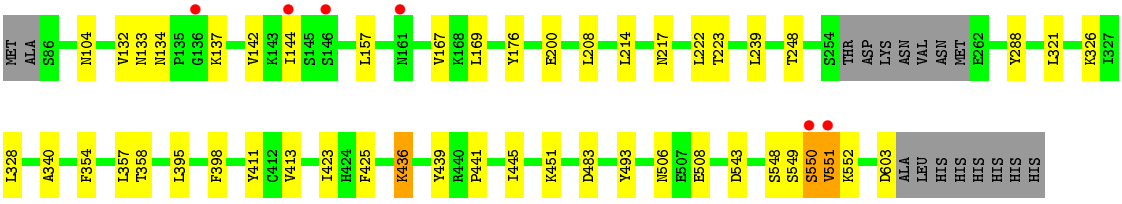
• Molecule 1: M17 leucyl aminopeptidase

Chain K:



• Molecule 1: M17 leucyl aminopeptidase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.75Å 177.06Å 231.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.32 – 2.00 81.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (81.32-2.00) 99.7 (81.32-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.164 , 0.200 0.185 , 0.224	Depositor DCC
R_{free} test set	23969 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 477144 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	53295	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 45.29 % 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 1.3495e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.49	0/4051	0.63	1/5498 (0.0%)
1	B	0.48	0/3993	0.66	1/5424 (0.0%)
1	C	0.50	0/4019	0.63	0/5453
1	D	0.52	1/4005 (0.0%)	0.64	0/5431
1	E	0.50	0/3976	0.63	0/5391
1	F	0.49	0/3924	0.66	1/5336 (0.0%)
1	G	0.49	0/4054	0.62	1/5494 (0.0%)
1	H	0.49	0/4005	0.64	0/5440
1	I	0.49	0/4033	0.64	0/5473
1	J	0.49	0/4002	0.63	0/5428
1	K	0.50	0/3973	0.63	0/5389
1	L	0.50	0/3921	0.66	1/5332 (0.0%)
All	All	0.50	1/47956 (0.0%)	0.64	5/65089 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	547	ILE	C-N	-8.24	1.15	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	550	SER	C-N-CA	5.82	136.24	121.70
1	F	552	LYS	N-CA-C	-5.77	95.41	111.00
1	G	257	LYS	C-N-CA	5.48	135.40	121.70
1	B	552	LYS	N-CA-C	-5.46	96.26	111.00
1	L	549	SER	C-N-CA	5.02	134.26	121.70

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	3973	0	3875	16	0
1	B	3916	0	3799	26	0
1	C	3942	0	3849	17	0
1	D	3928	0	3856	25	0
1	E	3900	0	3831	22	0
1	F	3847	0	3710	33	0
1	G	3978	0	3903	19	0
1	H	3927	0	3812	27	0
1	I	3955	0	3877	16	0
1	J	3925	0	3848	30	0
1	K	3897	0	3817	18	0
1	L	3844	0	3687	27	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	1	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	1	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	74	0	66	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	74	0	66	9	0
4	C	74	0	66	5	0
4	D	74	0	66	3	0
4	E	74	0	66	5	0
4	F	74	0	66	9	0
4	G	74	0	66	5	0
4	H	74	0	66	8	0
4	I	74	0	66	4	0
4	J	74	0	66	5	0
4	K	74	0	66	4	0
4	L	74	0	66	6	0
5	A	10	0	0	0	0
5	C	25	0	0	0	0
5	D	10	0	0	0	0
5	E	15	0	0	0	0
5	G	20	0	0	1	0
5	H	15	0	0	0	0
5	I	25	0	0	1	0
5	J	15	0	0	0	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	A	16	0	18	0	0
6	C	21	0	24	2	0
6	D	34	0	35	2	0
6	E	30	0	34	1	0
6	F	30	0	39	7	0
6	G	36	0	39	8	0
6	I	27	0	28	5	0
6	J	41	0	48	12	0
6	K	37	0	38	1	0
6	L	40	0	48	8	0
7	B	26	0	33	0	0
7	H	25	0	33	2	0
8	A	421	0	0	1	0
8	B	351	0	0	3	0
8	C	431	0	0	2	0
8	D	424	0	0	2	0
8	E	445	0	0	0	0
8	F	364	0	0	3	0
8	G	431	0	0	3	0
8	H	334	0	0	4	0
8	I	391	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	406	0	0	0	0
8	K	408	0	0	1	0
8	L	389	0	0	3	0
All	All	53295	0	47073	297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (297) 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)
6:G:623:1PE:C16	6:G:623:1PE:C26	1.76	1.64
6:F:618:1PE:C26	6:F:618:1PE:C16	1.74	1.60
6:L:620:1PE:C16	6:L:620:1PE:C26	1.75	1.55
6:G:623:1PE:C13	6:G:623:1PE:OH4	1.63	1.47
1:H:550:SER:OG	1:H:552:LYS:CD	1.80	1.29
1:H:550:SER:OG	1:H:552:LYS:HD2	1.03	1.19
1:I:531:ASN:H	6:I:623:1PE:H142	1.31	0.93
1:J:316:GLU:HG3	6:J:620:1PE:H141	1.52	0.92
1:H:550:SER:HG	1:H:552:LYS:HD2	1.05	0.87
1:C:223:THR:HG23	8:C:864:HOH:O	1.79	0.83
1:L:506:ASN:OD1	1:L:508:GLU:HG2	1.79	0.81
1:F:451:LYS:HE2	6:F:618:1PE:H151	1.62	0.79
1:K:338:MET:CE	1:K:468:ASP:HB3	2.12	0.79
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.65	0.79
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.66	0.78
1:E:338:MET:CE	1:E:468:ASP:HB3	2.15	0.75
1:B:392:MET:HE3	4:B:615:DGZ:H54	1.66	0.75
1:I:223:THR:HG23	8:I:900:HOH:O	1.86	0.74
1:F:137:LYS:CB	1:F:140:GLY:H	2.01	0.73
1:K:332:GLU:HG2	8:K:946:HOH:O	1.87	0.73
1:F:493:TYR:CE1	4:F:615:DGZ:H21	2.24	0.72
1:L:133:ASN:HA	1:L:167:VAL:HG11	1.70	0.71
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.77	0.67
1:F:493:TYR:HE1	4:F:615:DGZ:C21	2.07	0.67
1:F:493:TYR:HE1	4:F:615:DGZ:H21	1.58	0.67
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.61	0.66
1:F:138:GLU:N	1:F:139:ASN:HA	2.10	0.66
1:C:86:SER:N	8:C:752:HOH:O	2.28	0.65
1:D:533:TYR:O	1:D:536:THR:HG22	1.97	0.64
1:H:258:ASN:HB3	1:H:261:MET:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:550:SER:OG	1:H:552:LYS:HD3	1.89	0.64
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.80	0.63
4:K:615:DGZ:H32	4:K:615:DGZ:H25	1.79	0.63
1:F:320:LYS:NZ	6:F:617:1PE:H152	2.14	0.63
1:J:451:LYS:HG2	6:J:621:1PE:H241	1.81	0.63
1:J:437:ASN:HD22	1:L:436:LYS:NZ	1.96	0.62
1:F:320:LYS:HZ1	6:F:617:1PE:H152	1.64	0.62
1:B:233:ASN:ND2	1:B:519:THR:O	2.32	0.62
1:F:551:VAL:C	1:F:552:LYS:O	2.36	0.62
8:G:657:HOH:O	6:L:619:1PE:H242	2.00	0.61
1:J:533:TYR:O	1:J:536:THR:HG22	2.00	0.61
1:H:552:LYS:HG2	8:H:951:HOH:O	1.99	0.61
1:D:437:ASN:HD22	1:F:436:LYS:NZ	1.99	0.61
1:L:451:LYS:HG2	6:L:618:1PE:H232	1.82	0.60
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.83	0.60
1:L:548:SER:OG	1:L:550:SER:HB3	2.03	0.59
1:D:436:LYS:NZ	1:E:437:ASN:HD22	2.00	0.59
4:G:615:DGZ:H25	4:G:615:DGZ:H32	1.82	0.59
1:H:413:VAL:HG11	1:H:423:ILE:HD13	1.83	0.59
1:H:493:TYR:HE1	4:H:615:DGZ:H21	1.68	0.59
1:K:132:VAL:HG21	1:K:142:VAL:HG13	1.84	0.59
1:J:543:ASP:HB3	6:J:621:1PE:H242	1.84	0.58
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.86	0.58
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.86	0.58
1:A:493:TYR:HE1	4:A:615:DGZ:H21	1.68	0.58
1:B:413:VAL:HG11	1:B:423:ILE:HD13	1.85	0.57
4:L:615:DGZ:H32	8:L:787:HOH:O	2.04	0.57
4:C:615:DGZ:H25	4:C:615:DGZ:H32	1.86	0.57
1:C:411:TYR:CE1	6:C:622:1PE:H131	2.39	0.57
4:L:615:DGZ:HN3	4:L:615:DGZ:C27	2.18	0.57
1:G:332:GLU:HG3	8:G:844:HOH:O	2.05	0.56
1:C:326:LYS:HE3	1:C:328:LEU:HD11	1.87	0.56
1:J:413:VAL:HG11	1:J:423:ILE:HD13	1.87	0.56
1:D:248:THR:HG22	8:D:873:HOH:O	2.06	0.55
1:J:316:GLU:OE1	6:J:620:1PE:H251	2.06	0.55
1:A:493:TYR:HE1	4:A:615:DGZ:C21	2.19	0.55
6:F:618:1PE:C26	6:F:618:1PE:H162	2.18	0.55
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.89	0.55
1:G:392:MET:HE3	4:G:615:DGZ:H54	1.89	0.55
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.88	0.55
4:I:615:DGZ:H17	4:I:615:DGZ:H7A	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.89	0.54
1:A:493:TYR:CE1	4:A:615:DGZ:H21	2.41	0.54
1:D:436:LYS:HZ2	1:E:437:ASN:HD22	1.54	0.54
1:D:493:TYR:HE1	4:D:615:DGZ:C21	2.21	0.54
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.88	0.54
1:J:437:ASN:HD22	1:L:436:LYS:HZ1	1.55	0.54
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.90	0.54
1:C:392:MET:HE3	4:C:615:DGZ:H54	1.90	0.54
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.90	0.54
1:F:320:LYS:HE2	6:F:617:1PE:H142	1.89	0.54
1:L:248:THR:HG22	8:L:815:HOH:O	2.08	0.53
1:B:457:ASN:ND2	4:B:615:DGZ:H39	2.24	0.53
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.43	0.53
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.90	0.53
1:J:411:TYR:CE1	6:J:619:1PE:H152	2.44	0.53
1:B:258:ASN:HD22	1:B:260:ASN:H	1.55	0.53
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.91	0.52
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.91	0.52
2:F:612:CO3:O2	4:F:615:DGZ:H36A	2.10	0.52
1:H:258:ASN:HD22	1:H:260:ASN:H	1.56	0.52
1:K:320:LYS:HE2	6:K:617:1PE:H152	1.90	0.52
1:A:392:MET:HE3	4:A:615:DGZ:H54	1.90	0.52
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.91	0.52
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.92	0.52
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.91	0.52
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.92	0.52
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.91	0.52
1:L:326:LYS:HE3	1:L:328:LEU:HD11	1.91	0.52
1:D:326:LYS:HE3	1:D:328:LEU:HD11	1.91	0.52
1:B:392:MET:HE2	4:B:615:DGZ:H5	1.90	0.51
1:J:514:LEU:HD22	6:J:622:1PE:H242	1.92	0.51
1:J:518:LYS:NZ	6:J:622:1PE:H241	2.25	0.51
6:L:620:1PE:C26	6:L:620:1PE:H161	2.18	0.51
1:J:316:GLU:CD	6:J:620:1PE:H251	2.31	0.51
1:E:338:MET:HE2	1:E:468:ASP:HB3	1.93	0.51
1:B:551:VAL:HG12	1:B:552:LYS:O	2.11	0.51
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.92	0.51
1:I:392:MET:HE2	4:I:615:DGZ:H5	1.93	0.51
4:A:615:DGZ:H27	4:A:615:DGZ:H30A	1.93	0.51
1:J:338:MET:CE	1:J:468:ASP:HB3	2.41	0.51
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:551:VAL:O	1:H:552:LYS:O	2.28	0.50
4:G:615:DGZ:C27	1:L:493:TYR:HE2	2.24	0.50
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.93	0.50
1:H:493:TYR:CE1	4:H:615:DGZ:H21	2.47	0.50
6:G:623:1PE:H161	6:G:623:1PE:C26	2.19	0.50
1:B:392:MET:CE	4:B:615:DGZ:H54	2.39	0.50
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.94	0.50
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.43	0.50
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.93	0.49
1:D:413:VAL:HG11	1:D:423:ILE:HD13	1.92	0.49
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.94	0.49
1:G:552:LYS:N	8:G:639:HOH:O	2.44	0.49
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.93	0.49
1:H:493:TYR:HE1	4:H:615:DGZ:C21	2.25	0.49
1:L:133:ASN:HA	1:L:167:VAL:CG1	2.41	0.49
1:B:493:TYR:HE1	4:B:615:DGZ:C21	2.26	0.49
1:F:413:VAL:CG2	1:F:600:VAL:HG21	2.42	0.49
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.95	0.49
1:B:104:ASN:HB2	8:B:834:HOH:O	2.12	0.49
1:I:530:ILE:HA	6:I:623:1PE:H141	1.94	0.49
1:F:457:ASN:ND2	4:F:615:DGZ:H39	2.27	0.49
1:I:531:ASN:N	6:I:623:1PE:H142	2.14	0.49
1:H:392:MET:HE3	4:H:615:DGZ:H54	1.94	0.49
4:G:615:DGZ:H16	4:L:615:DGZ:H16	1.95	0.49
1:I:258:ASN:HD22	1:I:260:ASN:H	1.59	0.49
1:F:326:LYS:HE3	1:F:328:LEU:HD11	1.95	0.48
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.95	0.48
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.78	0.48
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.94	0.48
4:L:615:DGZ:C24	4:L:615:DGZ:H8A	2.43	0.48
1:E:493:TYR:HE1	4:E:615:DGZ:H21	1.77	0.48
1:K:117:ILE:HG12	1:K:270:TYR:HB3	1.94	0.48
1:G:316:GLU:HG3	6:G:623:1PE:H232	1.95	0.48
1:B:173:LYS:HB2	1:B:189:TYR:CE1	2.48	0.48
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.96	0.48
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.96	0.48
1:H:326:LYS:HE3	1:H:328:LEU:HD11	1.96	0.48
1:B:515:GLN:HG3	8:B:732:HOH:O	2.13	0.48
1:F:451:LYS:HG2	6:F:618:1PE:H141	1.96	0.47
1:E:493:TYR:CE1	4:E:615:DGZ:H21	2.48	0.47
4:I:615:DGZ:C27	1:J:493:TYR:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:LYS:HE3	1:G:328:LEU:HD11	1.96	0.47
1:E:230:VAL:HG13	1:E:234:LEU:HB3	1.96	0.47
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.79	0.47
1:F:548:SER:HB3	1:F:551:VAL:HA	1.95	0.47
1:E:493:TYR:HE1	4:E:615:DGZ:C21	2.27	0.47
1:L:167:VAL:O	1:L:167:VAL:HG12	2.13	0.47
4:H:615:DGZ:H27	4:H:615:DGZ:H30	1.96	0.47
1:C:493:TYR:HE1	4:C:615:DGZ:H21	1.79	0.47
1:B:326:LYS:HE3	1:B:328:LEU:HD11	1.97	0.47
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.96	0.47
1:D:493:TYR:HE1	4:D:615:DGZ:H21	1.80	0.47
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.97	0.47
1:I:261:MET:HA	5:I:618:SO4:O4	2.15	0.47
1:K:493:TYR:HE1	4:K:615:DGZ:H21	1.79	0.46
1:D:493:TYR:CE1	4:D:615:DGZ:H21	2.50	0.46
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.97	0.46
1:K:530:ILE:HD12	1:K:556:ILE:HD13	1.98	0.46
1:L:223:THR:HG23	8:L:808:HOH:O	2.15	0.46
1:D:451:LYS:NZ	6:D:620:1PE:H142	2.31	0.46
1:L:413:VAL:HG11	1:L:423:ILE:HD13	1.98	0.46
1:J:338:MET:HE2	1:J:468:ASP:HB3	1.97	0.46
1:J:320:LYS:HZ1	6:J:620:1PE:C26	2.28	0.46
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.97	0.46
1:A:361:SER:HB3	8:A:728:HOH:O	2.16	0.46
1:L:214:LEU:HD21	1:L:222:LEU:HD22	1.97	0.46
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.81	0.46
4:A:615:DGZ:H30A	4:A:615:DGZ:C27	2.45	0.46
4:J:615:DGZ:H7A	4:J:615:DGZ:C25	2.46	0.46
4:A:615:DGZ:HN3	4:A:615:DGZ:C27	2.27	0.45
1:H:548:SER:OG	1:H:552:LYS:HE2	2.16	0.45
1:F:248:THR:HG22	8:F:713:HOH:O	2.16	0.45
1:C:103:TYR:HB2	6:C:621:1PE:H251	1.98	0.45
6:L:620:1PE:H162	6:L:620:1PE:C26	2.18	0.45
1:B:552:LYS:O	1:B:553:ALA:C	2.54	0.45
1:K:321:LEU:HD11	1:K:411:TYR:HA	1.98	0.45
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.98	0.45
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.98	0.45
1:L:104:ASN:ND2	6:L:617:1PE:H241	2.31	0.45
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.98	0.45
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.98	0.45
1:F:248:THR:HG23	8:F:843:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:LYS:HZ1	6:G:623:1PE:H152	1.81	0.45
1:A:550:SER:HA	1:A:551:VAL:CB	2.47	0.45
1:B:551:VAL:C	1:B:552:LYS:O	2.55	0.45
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.99	0.45
1:B:233:ASN:HD21	1:B:519:THR:HA	1.82	0.45
1:J:518:LYS:HZ2	6:J:622:1PE:H241	1.82	0.45
1:B:493:TYR:HE1	4:B:615:DGZ:H21	1.82	0.44
1:B:258:ASN:ND2	1:B:260:ASN:H	2.15	0.44
1:D:411:TYR:HE1	6:D:618:1PE:H232	1.83	0.44
1:K:230:VAL:HG13	1:K:234:LEU:HB3	2.00	0.44
1:L:144:ILE:HD13	1:L:157:LEU:HD22	1.98	0.44
1:A:208:LEU:O	1:A:212:THR:HG23	2.17	0.44
4:I:615:DGZ:H32	4:I:615:DGZ:H25	2.00	0.44
6:G:623:1PE:C13	6:G:623:1PE:C24	2.85	0.44
1:G:493:TYR:HE2	4:L:615:DGZ:C27	2.31	0.44
1:F:413:VAL:HG22	1:F:600:VAL:HG21	2.00	0.44
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.99	0.44
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.99	0.44
2:J:612:CO3:O2	4:J:615:DGZ:H36A	2.17	0.44
1:B:493:TYR:CE1	4:B:615:DGZ:H21	2.53	0.44
1:F:392:MET:HE3	4:F:615:DGZ:H54	1.99	0.44
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.99	0.44
1:C:273:ASN:O	1:C:276:THR:HG22	2.18	0.44
1:K:127:LEU:HD11	1:K:129:ILE:HD11	1.99	0.44
1:F:493:TYR:CE1	4:F:615:DGZ:C21	2.89	0.43
1:J:413:VAL:CG2	1:J:600:VAL:HG21	2.48	0.43
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.48	0.43
1:L:550:SER:OG	1:L:551:VAL:N	2.50	0.43
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.98	0.43
1:E:127:LEU:HD11	1:E:129:ILE:HD11	2.00	0.43
1:D:218:LYS:HG2	1:D:261:MET:HA	2.00	0.43
1:K:214:LEU:HD11	1:K:222:LEU:HD22	2.00	0.43
1:D:248:THR:HG23	8:D:969:HOH:O	2.17	0.43
1:G:258:ASN:HB2	1:G:261:MET:H	1.83	0.43
1:C:275:ASP:HA	1:C:278:LYS:HD2	2.00	0.43
1:G:493:TYR:HE1	4:G:615:DGZ:H21	1.84	0.43
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.01	0.43
4:B:615:DGZ:H36	8:B:718:HOH:O	2.18	0.42
1:E:392:MET:HE3	4:E:615:DGZ:H54	2.01	0.42
7:H:619:2PE:H261	8:H:907:HOH:O	2.18	0.42
1:G:122:ASN:ND2	6:G:622:1PE:H151	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ILE:HG13	1:G:270:TYR:HB3	2.01	0.42
6:G:623:1PE:H162	6:G:623:1PE:C26	2.19	0.42
1:L:543:ASP:OD2	6:L:618:1PE:H131	2.18	0.42
1:D:127:LEU:HD11	1:D:129:ILE:HD11	2.01	0.42
1:L:104:ASN:HD22	6:L:617:1PE:H241	1.84	0.42
1:H:135:PRO:HA	1:H:194:SER:O	2.19	0.42
1:I:531:ASN:H	6:I:623:1PE:C14	2.17	0.42
4:H:615:DGZ:H16	4:K:615:DGZ:H16	2.01	0.42
4:K:615:DGZ:H32	4:K:615:DGZ:C25	2.47	0.42
1:C:208:LEU:O	1:C:212:THR:HG23	2.19	0.42
4:E:615:DGZ:H32A	4:E:615:DGZ:H30	1.78	0.42
1:F:127:LEU:HD11	1:F:129:ILE:HD11	2.01	0.42
1:E:198:LEU:HD22	1:E:202:ASP:HB3	2.01	0.42
1:J:103:TYR:CD1	6:J:620:1PE:H161	2.55	0.42
1:B:357:LEU:HB2	1:B:425:PHE:HB2	2.01	0.42
4:A:615:DGZ:C27	1:F:493:TYR:HE2	2.32	0.42
1:C:493:TYR:HE1	4:C:615:DGZ:C21	2.32	0.42
1:I:320:LYS:HE2	6:I:621:1PE:H231	2.02	0.41
1:F:357:LEU:HB2	1:F:425:PHE:HB2	2.02	0.41
1:B:150:ASP:OD1	1:B:179:ASN:HB2	2.21	0.41
1:A:441:PRO:HB2	1:B:394:ASP:HA	2.02	0.41
4:A:615:DGZ:H29A	4:A:615:DGZ:H31A	1.88	0.41
1:I:273:ASN:O	1:I:276:THR:HG22	2.20	0.41
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.02	0.41
1:H:103:TYR:O	7:H:619:2PE:H271	2.20	0.41
1:E:338:MET:HB3	1:E:338:MET:HE2	1.91	0.41
4:B:615:DGZ:H7A	4:B:615:DGZ:H17	2.01	0.41
1:L:357:LEU:HB2	1:L:425:PHE:HB2	2.01	0.41
4:A:615:DGZ:H16	4:F:615:DGZ:H16	2.03	0.41
1:J:210:LEU:HD23	1:J:242:LEU:HD13	2.01	0.41
1:J:321:LEU:HD11	1:J:411:TYR:HA	2.01	0.41
1:J:441:PRO:HB2	1:K:394:ASP:HA	2.03	0.41
1:J:543:ASP:CB	6:J:621:1PE:H242	2.50	0.41
1:I:357:LEU:HB2	1:I:425:PHE:HB2	2.03	0.41
1:H:258:ASN:ND2	1:H:260:ASN:H	2.17	0.41
4:C:615:DGZ:C27	1:D:493:TYR:HE2	2.34	0.41
1:H:492:LEU:HD22	1:K:552:LYS:HE3	2.03	0.41
1:G:249:ASP:HB2	5:G:619:SO4:O4	2.20	0.41
1:H:357:LEU:HB2	1:H:425:PHE:HB2	2.02	0.41
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.96	0.41
1:A:457:ASN:ND2	4:A:615:DGZ:H39	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:615:DGZ:H30A	8:H:890:HOH:O	2.21	0.41
1:I:258:ASN:ND2	1:I:260:ASN:H	2.18	0.41
1:C:357:LEU:HB2	1:C:425:PHE:HB2	2.03	0.41
1:F:365:VAL:HG22	8:F:851:HOH:O	2.20	0.41
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.21	0.40
1:H:441:PRO:HB2	1:I:394:ASP:HA	2.03	0.40
4:A:615:DGZ:H38	4:A:615:DGZ:H35	1.98	0.40
1:J:493:TYR:HE1	4:J:615:DGZ:C21	2.34	0.40
4:J:615:DGZ:C24	4:J:615:DGZ:H7A	2.51	0.40
4:H:615:DGZ:H32	8:H:890:HOH:O	2.21	0.40
1:B:233:ASN:ND2	1:B:519:THR:HA	2.36	0.40
1:E:316:GLU:HG3	6:E:619:1PE:H252	2.03	0.40
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.03	0.40
1:F:392:MET:HE2	4:F:615:DGZ:H5A	2.03	0.40
4:L:615:DGZ:H8A	4:L:615:DGZ:C25	2.51	0.40
1:J:392:MET:CE	4:J:615:DGZ:H54	2.51	0.40
1:G:106:PRO:HD2	1:G:247:MET:SD	2.62	0.40
1:A:421:VAL:CG2	1:A:423:ILE:HD11	2.52	0.40
1:D:214:LEU:HB3	1:D:246:TYR:CE1	2.56	0.40
1:C:173:LYS:HB2	1:C:189:TYR:CE1	2.56	0.40
1:F:114:VAL:HG12	1:F:274:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

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	517/528 (98%)	501 (97%)	15 (3%)	1 (0%)	52 48
1	B	513/528 (97%)	499 (97%)	12 (2%)	2 (0%)	39 33
1	C	512/528 (97%)	501 (98%)	11 (2%)	0	100 100
1	D	510/528 (97%)	502 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	503/528 (95%)	494 (98%)	9 (2%)	0	100 100
1	F	507/528 (96%)	494 (97%)	10 (2%)	3 (1%)	30 22
1	G	511/528 (97%)	501 (98%)	10 (2%)	0	100 100
1	H	516/528 (98%)	501 (97%)	13 (2%)	2 (0%)	39 33
1	I	516/528 (98%)	502 (97%)	13 (2%)	1 (0%)	52 48
1	J	510/528 (97%)	501 (98%)	9 (2%)	0	100 100
1	K	503/528 (95%)	495 (98%)	8 (2%)	0	100 100
1	L	507/528 (96%)	494 (97%)	10 (2%)	3 (1%)	30 22
All	All	6125/6336 (97%)	5985 (98%)	128 (2%)	12 (0%)	52 48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	552	LYS
1	H	552	LYS
1	I	551	VAL
1	L	550	SER
1	F	550	SER
1	F	552	LYS
1	H	138	GLU
1	L	551	VAL
1	B	138	GLU
1	F	551	VAL
1	L	552	LYS
1	A	550	SER

5.3.2 Protein sidechains (i)

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%)	410 (97%)	11 (3%)	54 54
1	B	410/455 (90%)	396 (97%)	14 (3%)	44 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	417/455 (92%)	404 (97%)	13 (3%)	47	46
1	D	415/455 (91%)	404 (97%)	11 (3%)	52	52
1	E	415/455 (91%)	403 (97%)	12 (3%)	50	49
1	F	400/455 (88%)	382 (96%)	18 (4%)	34	29
1	G	426/455 (94%)	416 (98%)	10 (2%)	58	60
1	H	412/455 (90%)	396 (96%)	16 (4%)	39	35
1	I	420/455 (92%)	405 (96%)	15 (4%)	42	39
1	J	414/455 (91%)	401 (97%)	13 (3%)	47	46
1	K	414/455 (91%)	404 (98%)	10 (2%)	57	58
1	L	397/455 (87%)	383 (96%)	14 (4%)	43	40
All	All	4961/5460 (91%)	4804 (97%)	157 (3%)	46	44

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	200	GLU
1	A	208	LEU
1	A	262	GLU
1	A	288	TYR
1	A	395	LEU
1	A	398	PHE
1	A	436	LYS
1	A	439	TYR
1	A	483	ASP
1	A	603	ASP
1	B	177	MET
1	B	208	LEU
1	B	210	LEU
1	B	233	ASN
1	B	258	ASN
1	B	272	ASN
1	B	288	TYR
1	B	322	ASN
1	B	395	LEU
1	B	398	PHE
1	B	436	LYS
1	B	439	TYR

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Mol	Chain	Res	Type
1	B	471	VAL
1	B	483	ASP
1	C	169	LEU
1	C	173	LYS
1	C	185	VAL
1	C	200	GLU
1	C	208	LEU
1	C	223	THR
1	C	272	ASN
1	C	288	TYR
1	C	331	LYS
1	C	398	PHE
1	C	439	TYR
1	C	483	ASP
1	C	603	ASP
1	D	132	VAL
1	D	200	GLU
1	D	204	LYS
1	D	208	LEU
1	D	216	ASP
1	D	288	TYR
1	D	395	LEU
1	D	398	PHE
1	D	436	LYS
1	D	439	TYR
1	D	600	VAL
1	E	143	LYS
1	E	163	GLU
1	E	169	LEU
1	E	208	LEU
1	E	219	LEU
1	E	239	LEU
1	E	288	TYR
1	E	395	LEU
1	E	398	PHE
1	E	436	LYS
1	E	439	TYR
1	E	483	ASP
1	F	116	ASP
1	F	134	ASN
1	F	145	SER
1	F	167	VAL

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Mol	Chain	Res	Type
1	F	169	LEU
1	F	198	LEU
1	F	200	GLU
1	F	208	LEU
1	F	223	THR
1	F	239	LEU
1	F	288	TYR
1	F	364	ASP
1	F	395	LEU
1	F	398	PHE
1	F	436	LYS
1	F	439	TYR
1	F	483	ASP
1	F	554	SER
1	G	117	ILE
1	G	200	GLU
1	G	208	LEU
1	G	261	MET
1	G	288	TYR
1	G	395	LEU
1	G	398	PHE
1	G	436	LYS
1	G	439	TYR
1	G	603	ASP
1	H	173	LYS
1	H	200	GLU
1	H	208	LEU
1	H	210	LEU
1	H	258	ASN
1	H	261	MET
1	H	272	ASN
1	H	288	TYR
1	H	395	LEU
1	H	398	PHE
1	H	436	LYS
1	H	439	TYR
1	H	483	ASP
1	H	549	SER
1	H	552	LYS
1	H	603	ASP
1	I	169	LEU
1	I	173	LYS

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Mol	Chain	Res	Type
1	I	200	GLU
1	I	208	LEU
1	I	223	THR
1	I	258	ASN
1	I	272	ASN
1	I	276	THR
1	I	288	TYR
1	I	331	LYS
1	I	395	LEU
1	I	398	PHE
1	I	439	TYR
1	I	483	ASP
1	I	603	ASP
1	J	154	SER
1	J	197	ASP
1	J	200	GLU
1	J	208	LEU
1	J	216	ASP
1	J	261	MET
1	J	288	TYR
1	J	395	LEU
1	J	398	PHE
1	J	436	LYS
1	J	439	TYR
1	J	483	ASP
1	J	567	GLN
1	K	169	LEU
1	K	208	LEU
1	K	216	ASP
1	K	239	LEU
1	K	288	TYR
1	K	395	LEU
1	K	398	PHE
1	K	436	LYS
1	K	439	TYR
1	K	483	ASP
1	L	134	ASN
1	L	137	LYS
1	L	169	LEU
1	L	200	GLU
1	L	208	LEU
1	L	239	LEU

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Mol	Chain	Res	Type
1	L	288	TYR
1	L	358	THR
1	L	395	LEU
1	L	398	PHE
1	L	436	LYS
1	L	439	TYR
1	L	483	ASP
1	L	603	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	449	ASN
1	B	233	ASN
1	B	258	ASN
1	B	319	GLN
1	B	322	ASN
1	B	521	ASN
1	C	161	ASN
1	D	437	ASN
1	E	181	ASN
1	E	273	ASN
1	E	437	ASN
1	F	104	ASN
1	F	134	ASN
1	F	567	GLN
1	G	515	GLN
1	H	258	ASN
1	H	319	GLN
1	I	161	ASN
1	I	258	ASN
1	J	437	ASN
1	K	161	ASN
1	L	104	ASN
1	L	134	ASN
1	L	217	ASN
1	L	602	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 112 ligands modelled in this entry, 24 are monoatomic - leaving 88 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CO3	A	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	A	615	3	78,78,78	1.02	1 (1%)	96,101,101	2.39	3 (3%)
5	SO4	A	616	-	4,4,4	0.21	0	6,6,6	0.24	0
5	SO4	A	617	-	4,4,4	0.90	0	6,6,6	0.17	0
6	1PE	A	618	-	8,8,15	2.06	2 (25%)	7,7,14	3.10	3 (42%)
6	1PE	A	619	-	6,6,15	1.63	1 (16%)	5,5,14	2.28	2 (40%)
2	CO3	B	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	B	615	3	78,78,78	1.00	1 (1%)	96,101,101	2.42	2 (2%)
7	2PE	B	616	-	25,25,27	0.95	0	24,24,26	0.57	0
2	CO3	C	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	C	615	3	78,78,78	1.00	1 (1%)	96,101,101	2.42	2 (2%)
5	SO4	C	616	-	4,4,4	0.53	0	6,6,6	0.50	0
5	SO4	C	617	-	4,4,4	0.21	0	6,6,6	0.10	0
5	SO4	C	618	-	4,4,4	0.41	0	6,6,6	0.20	0
5	SO4	C	619	-	4,4,4	1.50	0	6,6,6	0.28	0
5	SO4	C	620	-	4,4,4	0.56	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	1PE	C	621	-	11,11,15	2.26	4 (36%)	10,10,14	3.06	5 (50%)
6	1PE	C	622	-	8,8,15	2.44	3 (37%)	7,7,14	3.18	3 (42%)
2	CO3	D	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	D	615	3	78,78,78	1.01	1 (1%)	96,101,101	2.44	4 (4%)
5	SO4	D	616	-	4,4,4	0.46	0	6,6,6	0.10	0
5	SO4	D	617	-	4,4,4	0.87	0	6,6,6	0.28	0
6	1PE	D	618	-	9,9,15	2.24	3 (33%)	8,8,14	3.09	3 (37%)
6	1PE	D	619	-	7,7,15	2.18	3 (42%)	6,6,14	2.20	2 (33%)
6	1PE	D	620	-	10,10,15	2.14	3 (30%)	9,9,14	2.79	5 (55%)
6	1PE	D	621	-	4,4,15	2.73	4 (100%)	3,3,14	1.86	1 (33%)
2	CO3	E	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	E	615	3	78,78,78	1.00	1 (1%)	96,101,101	2.40	3 (3%)
5	SO4	E	616	-	4,4,4	0.32	0	6,6,6	0.13	0
5	SO4	E	617	-	4,4,4	0.44	0	6,6,6	0.12	0
5	SO4	E	618	-	4,4,4	1.12	0	6,6,6	0.42	0
6	1PE	E	619	-	11,11,15	2.43	4 (36%)	10,10,14	3.10	6 (60%)
6	1PE	E	620	-	9,9,15	2.20	4 (44%)	8,8,14	2.96	6 (75%)
6	1PE	E	621	-	7,7,15	2.20	3 (42%)	6,6,14	2.67	4 (66%)
2	CO3	F	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	F	615	3	78,78,78	1.03	1 (1%)	96,101,101	2.44	3 (3%)
6	1PE	F	616	-	9,9,15	2.53	4 (44%)	8,8,14	2.92	4 (50%)
6	1PE	F	617	-	9,9,15	2.59	4 (44%)	8,8,14	2.92	5 (62%)
6	1PE	F	618	-	9,9,15	3.05	5 (55%)	8,8,14	3.21	4 (50%)
2	CO3	G	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	G	615	3	78,78,78	0.99	1 (1%)	96,101,101	2.39	2 (2%)
5	SO4	G	616	-	4,4,4	0.19	0	6,6,6	0.20	0
5	SO4	G	617	-	4,4,4	1.38	0	6,6,6	0.40	0
5	SO4	G	618	-	4,4,4	0.37	0	6,6,6	0.14	0
5	SO4	G	619	-	4,4,4	1.30	0	6,6,6	0.18	0
6	1PE	G	620	-	8,8,15	2.15	3 (37%)	7,7,14	2.44	4 (57%)
6	1PE	G	621	-	5,5,15	1.57	1 (20%)	4,4,14	2.79	2 (50%)
6	1PE	G	622	-	5,5,15	1.57	1 (20%)	4,4,14	2.90	2 (50%)
6	1PE	G	623	-	14,14,15	3.18	7 (50%)	13,13,14	3.42	7 (53%)
2	CO3	H	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	H	615	3	78,78,78	1.02	1 (1%)	96,101,101	2.32	2 (2%)
5	SO4	H	616	-	4,4,4	0.27	0	6,6,6	0.36	0
5	SO4	H	617	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	H	618	-	4,4,4	1.26	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	2PE	H	619	-	24,24,27	0.75	0	23,23,26	0.68	0
2	CO3	I	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	I	615	3	78,78,78	1.01	1 (1%)	96,101,101	2.43	3 (3%)
5	SO4	I	616	-	4,4,4	0.50	0	6,6,6	0.10	0
5	SO4	I	617	-	4,4,4	1.00	0	6,6,6	0.36	0
5	SO4	I	618	-	4,4,4	1.01	0	6,6,6	0.27	0
5	SO4	I	619	-	4,4,4	0.21	0	6,6,6	0.10	0
5	SO4	I	620	-	4,4,4	1.24	0	6,6,6	0.29	0
6	1PE	I	621	-	11,11,15	2.38	4 (36%)	10,10,14	3.01	5 (50%)
6	1PE	I	622	-	9,9,15	2.28	4 (44%)	8,8,14	2.15	3 (37%)
6	1PE	I	623	-	4,4,15	1.63	1 (25%)	3,3,14	1.04	0
2	CO3	J	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	J	615	3	78,78,78	1.01	1 (1%)	96,101,101	2.40	4 (4%)
5	SO4	J	616	-	4,4,4	1.47	0	6,6,6	0.40	0
5	SO4	J	617	-	4,4,4	0.50	0	6,6,6	0.19	0
5	SO4	J	618	-	4,4,4	0.69	0	6,6,6	0.18	0
6	1PE	J	619	-	10,10,15	2.49	5 (50%)	9,9,14	2.06	5 (55%)
6	1PE	J	620	-	9,9,15	2.77	5 (55%)	8,8,14	3.08	4 (50%)
6	1PE	J	621	-	10,10,15	2.16	4 (40%)	9,9,14	2.71	3 (33%)
6	1PE	J	622	-	8,8,15	2.36	3 (37%)	7,7,14	2.80	3 (42%)
2	CO3	K	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	K	615	3	78,78,78	1.02	1 (1%)	96,101,101	2.43	3 (3%)
5	SO4	K	616	-	4,4,4	0.57	0	6,6,6	0.18	0
6	1PE	K	617	-	7,7,15	2.32	3 (42%)	6,6,14	2.54	3 (50%)
6	1PE	K	618	-	11,11,15	2.14	4 (36%)	10,10,14	3.05	4 (40%)
6	1PE	K	619	-	10,10,15	2.63	6 (60%)	9,9,14	2.50	5 (55%)
6	1PE	K	620	-	5,5,15	1.97	1 (20%)	4,4,14	1.78	2 (50%)
2	CO3	L	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	L	615	3	78,78,78	1.02	1 (1%)	96,101,101	2.41	3 (3%)
5	SO4	L	616	-	4,4,4	1.16	0	6,6,6	0.28	0
6	1PE	L	617	-	9,9,15	2.23	4 (44%)	8,8,14	1.83	3 (37%)
6	1PE	L	618	-	11,11,15	2.20	4 (36%)	10,10,14	3.30	6 (60%)
6	1PE	L	619	-	6,6,15	1.82	1 (16%)	5,5,14	2.14	2 (40%)
6	1PE	L	620	-	10,10,15	3.07	6 (60%)	9,9,14	2.69	6 (66%)

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
2	CO3	A	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	A	615	3	-	0/75/76/76	0/5/5/5
5	SO4	A	616	-	-	0/0/0/0	0/0/0/0
5	SO4	A	617	-	-	0/0/0/0	0/0/0/0
6	1PE	A	618	-	-	0/6/6/13	0/0/0/0
6	1PE	A	619	-	-	0/4/4/13	0/0/0/0
2	CO3	B	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	B	615	3	-	0/75/76/76	0/5/5/5
7	2PE	B	616	-	-	0/23/23/25	0/0/0/0
2	CO3	C	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	C	615	3	-	0/75/76/76	0/5/5/5
5	SO4	C	616	-	-	0/0/0/0	0/0/0/0
5	SO4	C	617	-	-	0/0/0/0	0/0/0/0
5	SO4	C	618	-	-	0/0/0/0	0/0/0/0
5	SO4	C	619	-	-	0/0/0/0	0/0/0/0
5	SO4	C	620	-	-	0/0/0/0	0/0/0/0
6	1PE	C	621	-	-	0/9/9/13	0/0/0/0
6	1PE	C	622	-	-	0/6/6/13	0/0/0/0
2	CO3	D	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	D	615	3	-	0/75/76/76	0/5/5/5
5	SO4	D	616	-	-	0/0/0/0	0/0/0/0
5	SO4	D	617	-	-	0/0/0/0	0/0/0/0
6	1PE	D	618	-	-	0/7/7/13	0/0/0/0
6	1PE	D	619	-	-	0/5/5/13	0/0/0/0
6	1PE	D	620	-	-	0/8/8/13	0/0/0/0
6	1PE	D	621	-	-	0/2/2/13	0/0/0/0
2	CO3	E	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	E	615	3	-	0/75/76/76	0/5/5/5
5	SO4	E	616	-	-	0/0/0/0	0/0/0/0
5	SO4	E	617	-	-	0/0/0/0	0/0/0/0
5	SO4	E	618	-	-	0/0/0/0	0/0/0/0
6	1PE	E	619	-	-	0/9/9/13	0/0/0/0
6	1PE	E	620	-	-	0/7/7/13	0/0/0/0
6	1PE	E	621	-	-	0/5/5/13	0/0/0/0
2	CO3	F	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	F	615	3	-	0/75/76/76	0/5/5/5
6	1PE	F	616	-	-	0/7/7/13	0/0/0/0
6	1PE	F	617	-	-	0/7/7/13	0/0/0/0
6	1PE	F	618	-	-	0/7/7/13	0/0/0/0
2	CO3	G	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	G	615	3	-	0/75/76/76	0/5/5/5
5	SO4	G	616	-	-	0/0/0/0	0/0/0/0
5	SO4	G	617	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	G	618	-	-	0/0/0/0	0/0/0/0
5	SO4	G	619	-	-	0/0/0/0	0/0/0/0
6	1PE	G	620	-	-	0/6/6/13	0/0/0/0
6	1PE	G	621	-	-	0/3/3/13	0/0/0/0
6	1PE	G	622	-	-	0/3/3/13	0/0/0/0
6	1PE	G	623	-	-	0/12/12/13	0/0/0/0
2	CO3	H	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	H	615	3	-	0/75/76/76	0/5/5/5
5	SO4	H	616	-	-	0/0/0/0	0/0/0/0
5	SO4	H	617	-	-	0/0/0/0	0/0/0/0
5	SO4	H	618	-	-	0/0/0/0	0/0/0/0
7	2PE	H	619	-	-	0/22/22/25	0/0/0/0
2	CO3	I	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	I	615	3	-	0/75/76/76	0/5/5/5
5	SO4	I	616	-	-	0/0/0/0	0/0/0/0
5	SO4	I	617	-	-	0/0/0/0	0/0/0/0
5	SO4	I	618	-	-	0/0/0/0	0/0/0/0
5	SO4	I	619	-	-	0/0/0/0	0/0/0/0
5	SO4	I	620	-	-	0/0/0/0	0/0/0/0
6	1PE	I	621	-	-	0/9/9/13	0/0/0/0
6	1PE	I	622	-	-	0/7/7/13	0/0/0/0
6	1PE	I	623	-	-	0/2/2/13	0/0/0/0
2	CO3	J	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	J	615	3	-	0/75/76/76	0/5/5/5
5	SO4	J	616	-	-	0/0/0/0	0/0/0/0
5	SO4	J	617	-	-	0/0/0/0	0/0/0/0
5	SO4	J	618	-	-	0/0/0/0	0/0/0/0
6	1PE	J	619	-	-	0/8/8/13	0/0/0/0
6	1PE	J	620	-	-	0/7/7/13	0/0/0/0
6	1PE	J	621	-	-	0/8/8/13	0/0/0/0
6	1PE	J	622	-	-	0/6/6/13	0/0/0/0
2	CO3	K	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	K	615	3	-	0/75/76/76	0/5/5/5
5	SO4	K	616	-	-	0/0/0/0	0/0/0/0
6	1PE	K	617	-	-	0/5/5/13	0/0/0/0
6	1PE	K	618	-	-	0/9/9/13	0/0/0/0
6	1PE	K	619	-	-	0/8/8/13	0/0/0/0
6	1PE	K	620	-	-	0/3/3/13	0/0/0/0
2	CO3	L	612	-	-	0/0/0/0	0/0/0/0
4	DGZ	L	615	3	-	0/75/76/76	0/5/5/5
5	SO4	L	616	-	-	0/0/0/0	0/0/0/0
6	1PE	L	617	-	-	0/7/7/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	L	618	-	-	0/9/9/13	0/0/0/0
6	1PE	L	619	-	-	0/4/4/13	0/0/0/0
6	1PE	L	620	-	-	0/8/8/13	0/0/0/0

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	620	1PE	OH5-C14	2.00	1.50	1.42
6	D	619	1PE	OH5-C14	2.01	1.50	1.42
6	K	619	1PE	OH4-C24	2.01	1.50	1.42
6	E	621	1PE	OH3-C23	2.08	1.53	1.42
6	I	623	1PE	OH4-C24	2.14	1.53	1.42
6	J	621	1PE	OH4-C13	2.17	1.62	1.42
6	F	618	1PE	C25-C15	2.18	1.60	1.48
6	I	622	1PE	OH3-C22	2.20	1.53	1.41
6	D	620	1PE	C23-C13	2.21	1.64	1.46
6	G	620	1PE	OH3-C23	2.22	1.54	1.40
6	D	621	1PE	OH6-C26	2.22	1.54	1.40
6	K	617	1PE	OH5-C25	2.22	1.51	1.42
6	J	622	1PE	OH3-C23	2.25	1.54	1.42
6	J	619	1PE	OH6-C15	2.26	1.51	1.42
6	E	620	1PE	OH6-C15	2.34	1.54	1.42
6	I	622	1PE	OH3-C23	2.40	1.55	1.40
6	K	619	1PE	OH3-C23	2.42	1.55	1.42
6	L	617	1PE	OH6-C15	2.42	1.52	1.42
6	K	618	1PE	OH6-C15	2.45	1.55	1.42
6	D	621	1PE	OH7-C16	2.47	1.55	1.42
6	J	620	1PE	OH5-C14	2.50	1.52	1.42
6	J	622	1PE	C13-C23	2.54	1.63	1.49
6	J	621	1PE	C23-C13	2.59	1.67	1.46
6	D	621	1PE	C26-C16	2.61	1.63	1.49
6	F	616	1PE	OH6-C15	2.64	1.53	1.42
6	E	620	1PE	C13-C23	2.68	1.64	1.49
6	K	619	1PE	OH6-C15	2.71	1.57	1.40
6	G	622	1PE	OH6-C15	2.72	1.56	1.42
6	D	619	1PE	OH6-C15	2.73	1.57	1.40
6	K	619	1PE	C13-C23	2.77	1.64	1.49
6	K	618	1PE	C23-C13	2.80	1.63	1.48
6	E	620	1PE	OH3-C23	2.81	1.57	1.42
6	C	621	1PE	OH3-C23	2.85	1.54	1.42
6	L	618	1PE	OH3-C23	2.85	1.54	1.42
6	D	618	1PE	C23-C13	2.86	1.63	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	618	1PE	C23-C13	2.86	1.63	1.48
6	L	618	1PE	C23-C13	2.86	1.63	1.48
6	A	619	1PE	OH6-C15	2.88	1.57	1.42
6	I	621	1PE	OH6-C15	2.89	1.57	1.42
6	D	618	1PE	OH3-C23	2.93	1.54	1.42
6	I	622	1PE	C23-C13	2.94	1.64	1.48
6	C	621	1PE	OH6-C15	2.94	1.57	1.42
6	L	617	1PE	OH7-C16	2.98	1.58	1.42
6	F	617	1PE	OH6-C15	2.99	1.54	1.42
6	K	617	1PE	OH6-C15	2.99	1.58	1.42
6	C	622	1PE	C23-C13	2.99	1.64	1.48
6	G	620	1PE	C23-C13	3.01	1.64	1.48
6	J	620	1PE	OH6-C15	3.02	1.54	1.42
6	I	621	1PE	C23-C13	3.03	1.64	1.48
6	E	621	1PE	C13-C23	3.05	1.66	1.49
6	K	618	1PE	OH3-C23	3.06	1.55	1.42
6	L	618	1PE	OH6-C15	3.09	1.58	1.42
6	G	621	1PE	OH6-C15	3.09	1.58	1.42
6	F	616	1PE	OH7-C16	3.12	1.58	1.42
6	E	619	1PE	C23-C13	3.13	1.65	1.48
6	L	619	1PE	OH6-C15	3.18	1.59	1.42
6	E	619	1PE	OH3-C23	3.19	1.55	1.42
6	E	619	1PE	OH6-C15	3.20	1.59	1.42
6	J	621	1PE	C16-C26	3.20	1.73	1.46
6	F	617	1PE	OH7-C16	3.21	1.59	1.42
6	D	620	1PE	C16-C26	3.23	1.73	1.46
6	J	620	1PE	OH7-C16	3.25	1.59	1.42
6	L	620	1PE	OH6-C15	3.28	1.56	1.42
6	C	622	1PE	OH3-C23	3.29	1.56	1.42
6	C	621	1PE	C23-C13	3.29	1.65	1.48
6	L	617	1PE	OH6-C26	3.32	1.56	1.42
6	I	621	1PE	OH3-C23	3.41	1.56	1.42
6	J	619	1PE	OH7-C16	3.42	1.60	1.42
6	J	619	1PE	C26-C16	3.43	1.68	1.49
6	L	620	1PE	OH7-C16	3.44	1.60	1.42
6	D	621	1PE	OH6-C15	3.48	1.60	1.41
6	L	618	1PE	OH4-C13	3.50	1.57	1.42
6	L	617	1PE	C26-C16	3.57	1.69	1.49
6	J	621	1PE	OH6-C15	3.58	1.57	1.42
6	K	617	1PE	OH4-C13	3.59	1.61	1.41
6	G	623	1PE	OH3-C23	3.60	1.57	1.42
6	G	623	1PE	OH7-C16	3.64	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	618	1PE	OH7-C16	3.69	1.61	1.42
6	K	620	1PE	OH4-C13	3.69	1.61	1.41
6	G	623	1PE	C23-C13	3.76	1.68	1.48
6	D	619	1PE	OH6-C26	3.80	1.62	1.41
6	L	620	1PE	OH4-C13	3.81	1.62	1.41
6	F	618	1PE	OH6-C15	3.83	1.58	1.42
6	J	619	1PE	OH4-C13	3.83	1.62	1.41
6	J	619	1PE	OH6-C26	3.85	1.58	1.42
6	D	620	1PE	OH6-C15	3.85	1.58	1.42
6	F	616	1PE	C26-C16	3.85	1.70	1.49
6	K	619	1PE	OH6-C26	3.88	1.62	1.41
6	K	618	1PE	OH4-C13	3.92	1.58	1.42
6	G	623	1PE	OH6-C15	3.94	1.58	1.42
6	F	617	1PE	C26-C16	4.02	1.71	1.49
6	J	620	1PE	OH6-C26	4.05	1.59	1.42
6	F	617	1PE	OH6-C26	4.06	1.59	1.42
6	G	620	1PE	OH4-C13	4.07	1.59	1.42
6	A	618	1PE	OH4-C13	4.09	1.59	1.42
6	F	616	1PE	OH6-C26	4.11	1.59	1.42
6	E	620	1PE	OH4-C13	4.12	1.59	1.42
6	C	621	1PE	OH4-C13	4.12	1.59	1.42
6	E	621	1PE	OH4-C13	4.12	1.59	1.42
6	J	620	1PE	C26-C16	4.19	1.72	1.49
6	E	619	1PE	OH4-C13	4.43	1.60	1.42
6	I	622	1PE	OH4-C13	4.48	1.61	1.42
6	I	621	1PE	OH4-C13	4.50	1.61	1.42
6	K	619	1PE	OH4-C13	4.54	1.61	1.42
6	F	618	1PE	C26-C16	4.61	1.74	1.49
6	C	622	1PE	OH4-C13	4.63	1.61	1.42
6	L	620	1PE	OH6-C26	4.63	1.61	1.42
6	D	618	1PE	OH4-C13	4.64	1.61	1.42
6	J	622	1PE	OH4-C13	4.71	1.62	1.42
6	L	620	1PE	C26-C16	4.72	1.75	1.49
6	F	618	1PE	OH6-C26	4.74	1.62	1.42
6	G	623	1PE	OH6-C26	4.86	1.62	1.42
6	G	623	1PE	C26-C16	4.89	1.76	1.49
6	G	623	1PE	OH4-C13	5.05	1.63	1.42
4	C	615	DGZ	C2-C1	6.25	1.32	1.17
4	I	615	DGZ	C2-C1	6.30	1.32	1.17
4	B	615	DGZ	C2-C1	6.35	1.32	1.17
4	F	615	DGZ	C2-C1	6.37	1.32	1.17
4	E	615	DGZ	C2-C1	6.37	1.32	1.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	615	DGZ	C2-C1	6.37	1.32	1.17
4	D	615	DGZ	C2-C1	6.38	1.32	1.17
4	L	615	DGZ	C2-C1	6.39	1.32	1.17
4	A	615	DGZ	C2-C1	6.41	1.32	1.17
4	H	615	DGZ	C2-C1	6.41	1.32	1.17
4	J	615	DGZ	C2-C1	6.44	1.32	1.17
4	K	615	DGZ	C2-C1	6.47	1.32	1.17

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	615	DGZ	C3-C2-C1	-22.46	119.55	177.17
4	F	615	DGZ	C3-C2-C1	-22.43	119.64	177.17
4	D	615	DGZ	C3-C2-C1	-22.34	119.86	177.17
4	I	615	DGZ	C3-C2-C1	-22.27	120.03	177.17
4	E	615	DGZ	C3-C2-C1	-22.24	120.11	177.17
4	B	615	DGZ	C3-C2-C1	-22.10	120.48	177.17
4	L	615	DGZ	C3-C2-C1	-22.08	120.53	177.17
4	A	615	DGZ	C3-C2-C1	-21.99	120.77	177.17
4	J	615	DGZ	C3-C2-C1	-21.98	120.78	177.17
4	K	615	DGZ	C3-C2-C1	-21.98	120.80	177.17
4	G	615	DGZ	C3-C2-C1	-21.95	120.87	177.17
4	H	615	DGZ	C3-C2-C1	-21.88	121.05	177.17
6	G	620	1PE	OH4-C24-C14	-3.44	95.08	110.36
6	A	618	1PE	OH4-C24-C14	-3.32	95.17	110.43
6	L	618	1PE	OH4-C24-C14	-3.26	95.88	110.36
6	E	620	1PE	OH4-C24-C14	-3.03	96.89	110.36
4	B	615	DGZ	O9-C48-C47	-2.92	103.67	110.47
6	E	619	1PE	OH4-C24-C14	-2.85	97.68	110.36
6	D	618	1PE	OH4-C24-C14	-2.71	98.31	110.36
6	C	622	1PE	OH4-C24-C14	-2.58	98.54	110.43
6	J	619	1PE	OH4-C24-C14	-2.48	90.33	111.29
6	E	621	1PE	OH4-C24-C14	-2.42	99.63	110.36
6	G	623	1PE	OH4-C24-C14	-2.36	99.88	110.36
6	K	619	1PE	OH4-C24-C14	-2.24	100.41	110.36
4	J	615	DGZ	O9-C48-C47	-2.23	105.28	110.47
6	E	620	1PE	OH4-C13-C23	-2.16	100.49	110.43
4	I	615	DGZ	C37-C36-C35	-2.16	107.13	113.41
6	F	617	1PE	OH4-C24-C14	-2.05	99.40	112.03
6	D	620	1PE	OH4-C24-C14	-2.02	101.37	110.36
4	A	615	DGZ	O9-C48-C47	-2.02	105.76	110.47
6	L	620	1PE	OH5-C14-C24	2.01	119.28	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	620	1PE	C26-OH6-C15	2.01	120.50	112.80
6	K	620	1PE	C13-OH4-C24	2.02	126.33	113.09
4	F	615	DGZ	C11-C57-N7	2.05	119.91	116.60
6	L	620	1PE	C13-OH4-C24	2.11	126.97	113.09
6	G	623	1PE	OH6-C26-C16	2.13	120.22	110.43
6	L	617	1PE	C25-OH5-C14	2.14	122.49	113.31
6	J	619	1PE	C13-OH4-C24	2.15	127.21	113.09
4	J	615	DGZ	C11-C57-N7	2.15	120.07	116.60
6	E	621	1PE	C25-OH5-C14	2.15	127.25	113.09
4	D	615	DGZ	C11-C57-N7	2.17	120.09	116.60
4	K	615	DGZ	C11-C57-N7	2.21	120.16	116.60
4	E	615	DGZ	C11-C57-N7	2.21	120.16	116.60
6	I	621	1PE	C25-OH5-C14	2.21	122.82	113.31
6	L	619	1PE	C25-OH5-C14	2.24	122.94	113.31
6	E	620	1PE	OH6-C15-C25	2.24	125.87	112.03
4	E	615	DGZ	O9-C48-C49	2.24	114.21	109.66
6	D	618	1PE	C24-OH4-C13	2.29	123.15	113.31
6	E	619	1PE	C22-OH3-C23	2.34	121.77	112.80
4	L	615	DGZ	C13-N3-C28	2.38	127.64	121.58
6	L	620	1PE	OH6-C26-C16	2.40	121.46	110.43
6	G	621	1PE	OH6-C15-C25	2.43	127.02	112.03
6	L	617	1PE	OH7-C16-C26	2.50	127.47	112.03
6	K	619	1PE	OH6-C15-C25	2.50	132.42	111.29
4	D	615	DGZ	C12-C13-N3	2.50	118.32	111.26
6	G	620	1PE	C25-OH5-C14	2.55	129.83	113.09
6	J	619	1PE	OH7-C16-C26	2.57	127.89	112.03
6	J	619	1PE	C26-OH6-C15	2.58	124.40	113.31
6	I	621	1PE	OH5-C14-C24	2.59	121.89	110.36
6	K	617	1PE	C13-OH4-C24	2.61	130.22	113.09
4	H	615	DGZ	O9-C48-C49	2.61	114.95	109.66
6	E	620	1PE	C25-OH5-C14	2.65	124.71	113.31
6	D	619	1PE	OH6-C15-C25	2.70	134.10	111.29
6	F	616	1PE	OH6-C26-C16	2.70	122.87	110.43
6	L	618	1PE	C25-OH5-C14	2.73	125.03	113.31
4	A	615	DGZ	O9-C48-C49	2.75	115.22	109.66
6	D	621	1PE	OH7-C16-C26	2.80	129.34	112.03
6	E	619	1PE	OH6-C15-C25	2.81	129.38	112.03
6	F	617	1PE	OH7-C16-C26	2.81	129.40	112.03
6	K	620	1PE	C25-OH5-C14	2.84	131.72	113.09
6	C	621	1PE	OH6-C15-C25	2.91	129.99	112.03
6	J	620	1PE	OH6-C26-C16	2.93	123.94	110.43
6	K	618	1PE	C25-OH5-C14	2.95	126.00	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	616	1PE	OH7-C16-C26	2.97	130.35	112.03
6	L	618	1PE	C22-OH3-C23	2.97	124.18	112.80
6	I	622	1PE	C24-OH4-C13	3.04	126.36	113.31
6	J	621	1PE	C13-OH4-C24	3.08	124.57	112.80
6	C	622	1PE	C24-OH4-C13	3.10	126.64	113.31
6	I	622	1PE	OH3-C23-C13	3.13	137.78	111.29
6	C	621	1PE	C22-OH3-C23	3.17	124.92	112.80
4	L	615	DGZ	O9-C48-C49	3.17	116.08	109.66
6	K	619	1PE	C25-OH5-C14	3.18	126.98	113.31
6	G	623	1PE	C25-OH5-C14	3.21	127.09	113.31
6	G	620	1PE	C24-OH4-C13	3.21	127.12	113.31
6	K	618	1PE	OH6-C15-C25	3.27	132.21	112.03
6	K	619	1PE	C24-OH4-C13	3.28	127.42	113.31
6	A	619	1PE	C25-OH5-C14	3.29	127.45	113.31
4	C	615	DGZ	O9-C48-C49	3.32	116.38	109.66
6	F	618	1PE	OH6-C26-C16	3.34	125.80	110.43
6	J	622	1PE	C24-OH4-C13	3.34	127.66	113.31
4	G	615	DGZ	O9-C48-C49	3.36	116.46	109.66
6	F	617	1PE	C25-OH5-C14	3.37	127.80	113.31
6	I	621	1PE	OH6-C15-C25	3.37	132.85	112.03
4	F	615	DGZ	O9-C48-C49	3.39	116.52	109.66
6	G	620	1PE	OH3-C23-C13	3.40	140.05	111.29
6	D	620	1PE	C25-OH5-C14	3.42	128.03	113.31
6	J	619	1PE	OH6-C15-C25	3.50	125.92	110.36
6	A	619	1PE	OH6-C15-C25	3.52	133.75	112.03
6	L	617	1PE	OH6-C15-C25	3.55	126.13	110.36
4	I	615	DGZ	O9-C48-C49	3.55	116.85	109.66
6	E	619	1PE	C25-OH5-C14	3.58	128.71	113.31
6	J	620	1PE	OH7-C16-C26	3.61	134.31	112.03
6	F	618	1PE	OH7-C16-C26	3.63	134.42	112.03
6	K	617	1PE	OH6-C15-C25	3.66	134.62	112.03
6	I	621	1PE	C24-OH4-C13	3.67	129.07	113.31
6	F	618	1PE	C25-OH5-C14	3.70	129.21	113.31
6	E	621	1PE	C24-OH4-C13	3.74	129.38	113.31
6	K	617	1PE	C25-OH5-C14	3.77	129.50	113.31
6	L	618	1PE	OH6-C15-C25	3.77	135.30	112.03
6	L	620	1PE	OH7-C16-C26	3.78	135.36	112.03
6	F	617	1PE	OH6-C26-C16	3.79	127.89	110.43
6	I	622	1PE	C25-OH5-C14	3.81	127.38	112.80
6	E	620	1PE	OH3-C23-C13	3.83	135.65	112.03
6	C	621	1PE	C24-OH4-C13	3.90	130.07	113.31
6	G	622	1PE	C14-OH5-C25	3.90	127.73	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	620	1PE	OH6-C15-C25	3.96	127.96	110.36
6	F	616	1PE	C25-OH5-C14	3.97	130.37	113.31
6	G	623	1PE	OH7-C16-C26	3.98	136.59	112.03
4	D	615	DGZ	O9-C48-C49	3.99	117.73	109.66
6	L	620	1PE	C25-OH5-C14	4.00	130.50	113.31
6	K	618	1PE	C24-OH4-C13	4.00	130.51	113.31
6	C	621	1PE	C25-OH5-C14	4.01	130.55	113.31
4	K	615	DGZ	O9-C48-C49	4.03	117.83	109.66
6	D	619	1PE	C25-OH5-C14	4.07	130.80	113.31
6	E	621	1PE	OH3-C23-C13	4.12	137.47	112.03
6	A	618	1PE	C24-OH4-C13	4.13	131.06	113.31
6	G	622	1PE	OH6-C15-C25	4.14	137.57	112.03
4	J	615	DGZ	O9-C48-C49	4.15	118.08	109.66
6	L	619	1PE	OH6-C15-C25	4.19	137.90	112.03
6	J	620	1PE	C25-OH5-C14	4.34	131.95	113.31
6	G	623	1PE	C24-OH4-C13	4.39	132.20	113.31
6	E	619	1PE	C24-OH4-C13	4.41	132.27	113.31
6	J	621	1PE	C25-OH5-C14	4.50	132.68	113.31
6	J	622	1PE	OH3-C23-C13	4.53	139.98	112.03
6	L	618	1PE	C24-OH4-C13	4.64	133.27	113.31
6	J	622	1PE	C25-OH5-C14	4.70	130.80	112.80
6	D	620	1PE	OH6-C15-C25	4.73	131.39	110.36
6	G	621	1PE	C14-OH5-C25	4.77	131.08	112.80
6	D	620	1PE	C13-OH4-C24	4.84	131.31	112.80
6	K	619	1PE	OH3-C23-C13	4.91	142.32	112.03
6	E	620	1PE	C24-OH4-C13	5.02	134.91	113.31
6	F	617	1PE	OH6-C15-C25	5.18	133.37	110.36
6	F	616	1PE	OH6-C15-C25	5.39	134.34	110.36
6	J	620	1PE	OH6-C15-C25	5.41	134.40	110.36
6	G	623	1PE	OH6-C15-C25	5.64	135.44	110.36
6	A	618	1PE	OH3-C23-C13	5.73	135.81	110.36
6	J	621	1PE	OH6-C15-C25	5.76	135.95	110.36
6	C	621	1PE	OH3-C23-C13	5.97	136.91	110.36
6	E	619	1PE	OH3-C23-C13	6.01	137.09	110.36
6	F	618	1PE	OH6-C15-C25	6.24	138.12	110.36
6	L	618	1PE	OH3-C23-C13	6.27	138.25	110.36
6	K	618	1PE	OH3-C23-C13	6.70	140.15	110.36
6	I	621	1PE	OH3-C23-C13	7.12	141.99	110.36
6	C	622	1PE	OH3-C23-C13	7.20	142.35	110.36
6	D	618	1PE	OH3-C23-C13	7.52	143.79	110.36
6	G	623	1PE	OH3-C23-C13	7.79	144.99	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

37 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	615	DGZ	12	0
4	B	615	DGZ	9	0
4	C	615	DGZ	5	0
6	C	621	1PE	1	0
6	C	622	1PE	1	0
4	D	615	DGZ	3	0
6	D	618	1PE	1	0
6	D	620	1PE	1	0
4	E	615	DGZ	5	0
6	E	619	1PE	1	0
2	F	612	CO3	1	0
4	F	615	DGZ	9	0
6	F	617	1PE	3	0
6	F	618	1PE	4	0
4	G	615	DGZ	5	0
5	G	619	SO4	1	0
6	G	622	1PE	1	0
6	G	623	1PE	7	0
4	H	615	DGZ	8	0
7	H	619	2PE	2	0
4	I	615	DGZ	4	0
5	I	618	SO4	1	0
6	I	621	1PE	1	0
6	I	623	1PE	4	0
2	J	612	CO3	1	0
4	J	615	DGZ	5	0
6	J	619	1PE	1	0
6	J	620	1PE	5	0
6	J	621	1PE	3	0
6	J	622	1PE	3	0
4	K	615	DGZ	4	0
6	K	617	1PE	1	0
4	L	615	DGZ	6	0
6	L	617	1PE	2	0
6	L	618	1PE	2	0
6	L	619	1PE	1	0
6	L	620	1PE	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	519/528 (98%)	-0.39	3 (0%) 90 90	5, 15, 35, 70	0
1	B	517/528 (97%)	-0.29	9 (1%) 73 73	5, 17, 46, 73	1 (0%)
1	C	516/528 (97%)	-0.39	4 (0%) 87 88	5, 15, 39, 76	0
1	D	514/528 (97%)	-0.43	6 (1%) 81 81	6, 14, 35, 80	0
1	E	509/528 (96%)	-0.51	0 100 100	7, 14, 30, 48	0
1	F	511/528 (96%)	-0.17	9 (1%) 71 72	6, 18, 40, 71	0
1	G	517/528 (97%)	-0.38	3 (0%) 90 90	6, 14, 36, 61	0
1	H	518/528 (98%)	-0.28	7 (1%) 78 78	6, 18, 46, 68	1 (0%)
1	I	518/528 (98%)	-0.39	4 (0%) 87 88	5, 16, 39, 81	0
1	J	514/528 (97%)	-0.40	5 (0%) 84 84	7, 15, 37, 82	0
1	K	509/528 (96%)	-0.50	0 100 100	7, 15, 32, 47	0
1	L	511/528 (96%)	-0.29	6 (1%) 81 81	6, 16, 37, 64	0
All	All	6173/6336 (97%)	-0.37	56 (0%) 85 86	5, 15, 39, 82	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	138	GLU	6.1
1	F	551	VAL	5.8
1	L	136	GLY	5.5
1	L	550	SER	4.7
1	A	551	VAL	4.7
1	J	260	ASN	4.6
1	H	551	VAL	4.4
1	H	136	GLY	4.4
1	B	550	SER	4.2
1	B	363	GLY	4.1
1	L	551	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	136	GLY	4.0
1	B	136	GLY	3.9
1	D	603	ASP	3.7
1	C	603	ASP	3.7
1	H	178	PHE	3.6
1	B	551	VAL	3.5
1	I	551	VAL	3.3
1	J	85	ALA	3.1
1	F	121	CYS	3.0
1	G	550	SER	3.0
1	B	181	ASN	2.9
1	D	219	LEU	2.8
1	F	136	GLY	2.8
1	D	136	GLY	2.8
1	I	549	SER	2.7
1	J	219	LEU	2.7
1	D	85	ALA	2.6
1	H	603	ASP	2.6
1	L	146	SER	2.5
1	B	603	ASP	2.5
1	F	361	SER	2.5
1	B	135	PRO	2.5
1	B	178	PHE	2.4
1	F	157	LEU	2.4
1	B	118	LYS	2.4
1	C	362	LYS	2.4
1	H	135	PRO	2.3
1	J	603	ASP	2.3
1	G	196	ALA	2.3
1	A	136	GLY	2.3
1	A	550	SER	2.2
1	F	272	ASN	2.2
1	C	549	SER	2.2
1	G	549	SER	2.2
1	F	114	VAL	2.2
1	F	550	SER	2.2
1	L	144	ILE	2.2
1	H	150	ASP	2.1
1	D	260	ASN	2.1
1	D	124	GLU	2.1
1	I	550	SER	2.1
1	L	161	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	603	ASP	2.0
1	H	181	ASN	2.0
1	C	552	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CO3	G	612	4/4	0.82	0.23	27.31	4,9,10,12	0
5	SO4	E	618	5/5	0.90	0.26	20.47	52,55,59,59	0
5	SO4	C	620	5/5	0.91	0.25	19.53	52,56,58,58	0
2	CO3	I	612	4/4	0.81	0.26	18.86	10,11,12,14	0
2	CO3	H	612	4/4	0.85	0.21	17.07	5,11,12,14	0
5	SO4	J	618	5/5	0.90	0.27	16.54	57,60,62,62	0
5	SO4	I	617	5/5	0.94	0.25	16.05	43,46,49,49	0
6	1PE	D	621	5/16	0.68	0.30	15.08	26,28,34,37	0
5	SO4	G	619	5/5	0.89	0.32	14.95	45,49,50,52	0
5	SO4	H	618	5/5	0.86	0.23	13.75	45,47,50,52	0
2	CO3	E	612	4/4	0.88	0.23	13.69	6,13,14,16	0
2	CO3	D	612	4/4	0.87	0.23	13.25	10,12,15,15	0
5	SO4	G	617	5/5	0.92	0.25	12.29	36,40,41,42	0
5	SO4	C	618	5/5	0.69	0.33	11.51	100,104,104,106	0
2	CO3	F	612	4/4	0.84	0.24	11.47	9,11,13,15	0
2	CO3	J	612	4/4	0.85	0.20	10.93	11,11,13,14	0
7	2PE	B	616	26/28	0.79	0.27	8.18	42,48,56,57	0
5	SO4	G	618	5/5	0.78	0.23	7.58	74,77,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	1PE	F	616	10/16	0.87	0.14	7.37	29,32,40,41	0
5	SO4	C	619	5/5	0.80	0.35	7.28	48,51,54,54	0
2	CO3	K	612	4/4	0.91	0.17	7.20	10,10,10,11	0
7	2PE	H	619	25/28	0.80	0.22	7.16	40,44,55,57	0
2	CO3	C	612	4/4	0.94	0.16	6.92	12,12,13,15	0
6	1PE	L	618	12/16	0.82	0.18	6.80	25,35,48,48	0
5	SO4	C	617	5/5	0.74	0.27	6.78	95,99,100,101	0
6	1PE	L	619	7/16	0.90	0.17	6.63	30,32,35,35	0
5	SO4	L	616	5/5	0.89	0.32	6.43	41,43,48,48	0
6	1PE	I	623	5/16	0.94	0.16	6.29	14,14,16,18	0
2	CO3	L	612	4/4	0.87	0.20	6.28	9,10,12,14	0
5	SO4	E	616	5/5	0.83	0.34	6.21	90,94,95,96	0
6	1PE	J	622	9/16	0.68	0.26	6.02	45,50,55,55	0
5	SO4	H	617	5/5	0.87	0.27	5.58	80,84,86,86	0
5	SO4	I	618	5/5	0.83	0.29	5.30	57,61,62,63	0
2	CO3	B	612	4/4	0.95	0.13	4.96	14,14,15,15	0
6	1PE	J	621	11/16	0.79	0.20	4.81	38,38,41,43	0
6	1PE	G	623	15/16	0.76	0.21	4.63	42,48,57,58	0
6	1PE	D	619	8/16	0.71	0.21	4.54	52,53,54,55	0
2	CO3	A	612	4/4	0.93	0.16	4.54	12,12,14,15	0
6	1PE	K	618	12/16	0.90	0.17	4.49	25,31,40,40	0
5	SO4	I	619	5/5	0.86	0.17	4.16	90,94,95,96	0
6	1PE	E	621	8/16	0.93	0.23	3.87	31,34,36,37	0
5	SO4	A	617	5/5	0.85	0.19	3.65	54,55,59,59	0
6	1PE	K	620	6/16	0.92	0.11	3.47	30,31,32,33	0
6	1PE	E	620	10/16	0.94	0.15	3.42	26,27,35,41	0
6	1PE	D	618	10/16	0.90	0.16	3.41	30,34,40,40	0
6	1PE	F	618	10/16	0.85	0.16	3.21	36,40,44,44	0
6	1PE	D	620	11/16	0.82	0.20	2.32	35,39,46,48	0
6	1PE	K	619	11/16	0.87	0.14	2.25	25,39,44,44	0
6	1PE	G	621	6/16	0.93	0.21	2.09	25,25,27,32	0
6	1PE	J	619	11/16	0.95	0.15	2.00	19,23,34,38	0
6	1PE	G	620	9/16	0.91	0.14	1.96	24,26,31,31	0
4	DGZ	I	615	74/74	0.93	0.16	1.71	5,42,189,216	0
6	1PE	A	618	9/16	0.92	0.12	1.47	23,24,26,29	0
4	DGZ	J	615	74/74	0.94	0.15	1.40	8,34,179,236	0
4	DGZ	C	615	74/74	0.94	0.15	1.32	10,38,182,231	0
4	DGZ	B	615	74/74	0.94	0.15	1.28	9,37,133,171	0
4	DGZ	E	615	74/74	0.94	0.15	1.19	10,41,146,207	0
6	1PE	C	622	9/16	0.88	0.15	1.11	27,29,35,40	0
4	DGZ	D	615	74/74	0.94	0.15	1.07	7,34,121,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	1PE	L	617	10/16	0.95	0.12	0.97	17,27,36,40	0
6	1PE	L	620	11/16	0.84	0.20	0.86	39,42,45,45	0
4	DGZ	A	615	74/74	0.93	0.16	0.80	5,38,181,208	0
4	DGZ	H	615	74/74	0.92	0.16	0.79	4,38,142,180	0
6	1PE	I	622	10/16	0.95	0.15	0.71	21,23,34,35	0
4	DGZ	F	615	74/74	0.92	0.16	0.58	8,35,127,202	0
4	DGZ	K	615	74/74	0.94	0.15	0.54	7,41,147,213	0
4	DGZ	G	615	74/74	0.94	0.15	0.23	6,36,151,232	0
4	DGZ	L	615	74/74	0.94	0.14	0.23	7,33,109,190	0
5	SO4	H	616	5/5	0.99	0.09	-0.19	12,12,14,14	0
5	SO4	D	617	5/5	0.99	0.09	-0.49	12,13,14,17	0
5	SO4	J	616	5/5	0.99	0.09	-0.67	14,14,17,17	0
6	1PE	G	622	6/16	0.93	0.10	-1.19	30,30,30,32	0
5	SO4	C	616	5/5	0.99	0.07	-1.31	9,9,10,12	0
3	ZN	J	614	1/1	1.00	0.07	-1.81	24,24,24,24	0
3	ZN	E	614	1/1	0.99	0.07	-2.11	28,28,28,28	0
3	ZN	K	614	1/1	0.99	0.06	-2.41	29,29,29,29	0
3	ZN	D	614	1/1	0.99	0.05	-2.41	29,29,29,29	0
3	ZN	A	613	1/1	1.00	0.07	-2.41	26,26,26,26	0
3	ZN	F	614	1/1	0.99	0.05	-2.57	27,27,27,27	0
3	ZN	A	614	1/1	1.00	0.06	-2.62	17,17,17,17	0
3	ZN	C	614	1/1	0.99	0.05	-2.85	25,25,25,25	0
3	ZN	I	614	1/1	0.99	0.06	-2.90	27,27,27,27	0
3	ZN	H	614	1/1	1.00	0.05	-2.96	29,29,29,29	0
3	ZN	L	613	1/1	1.00	0.05	-3.15	27,27,27,27	0
3	ZN	L	614	1/1	1.00	0.05	-3.35	17,17,17,17	0
3	ZN	J	613	1/1	1.00	0.07	-3.35	19,19,19,19	0
3	ZN	B	613	1/1	1.00	0.05	-3.49	26,26,26,26	0
3	ZN	G	614	1/1	1.00	0.05	-3.50	27,27,27,27	0
3	ZN	E	613	1/1	1.00	0.04	-3.72	18,18,18,18	0
3	ZN	F	613	1/1	1.00	0.05	-4.06	17,17,17,17	0
3	ZN	K	613	1/1	1.00	0.04	-4.61	18,18,18,18	0
3	ZN	H	613	1/1	1.00	0.04	-6.60	19,19,19,19	0
3	ZN	D	613	1/1	1.00	0.05	-7.02	16,16,16,16	0
3	ZN	I	613	1/1	1.00	0.05	-7.45	17,17,17,17	0
3	ZN	C	613	1/1	1.00	0.04	-9.11	17,17,17,17	0
3	ZN	G	613	1/1	1.00	0.05	-9.24	16,16,16,16	0
3	ZN	B	614	1/1	1.00	0.04	-9.37	16,16,16,16	0
5	SO4	G	616	5/5	0.92	0.31	-	75,79,81,81	0
5	SO4	E	617	5/5	0.90	0.35	-	73,78,79,79	0
6	1PE	I	621	12/16	0.89	0.21	-	35,37,40,43	0
5	SO4	A	616	5/5	0.94	0.32	-	62,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	1PE	C	621	12/16	0.87	0.18	-	42,44,47,48	0
5	SO4	J	617	5/5	0.92	0.40	-	77,81,82,83	0
6	1PE	J	620	10/16	0.89	0.19	-	27,35,41,41	0
6	1PE	A	619	7/16	0.85	0.23	-	43,44,48,51	0
5	SO4	I	616	5/5	0.92	0.41	-	75,80,80,80	0
6	1PE	F	617	10/16	0.88	0.22	-	46,50,52,52	0
6	1PE	E	619	12/16	0.83	0.20	-	40,42,46,47	0
5	SO4	I	620	5/5	0.92	0.28	-	39,41,44,47	0
6	1PE	K	617	8/16	0.90	0.14	-	32,37,42,43	0
5	SO4	D	616	5/5	0.90	0.39	-	73,78,78,80	0
5	SO4	K	616	5/5	0.85	0.36	-	72,76,78,79	0

6.5 Other polymers

There are no such residues in this entry.