Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2016 – 11:03 AM EDT

PDB ID	:	4ZX9
Title	:	X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10b
Authors	:	Drinkwater, N.; McGowan, S.
Deposited on	:	2015-05-20
Resolution	:	2.60 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 (i) symbol.

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

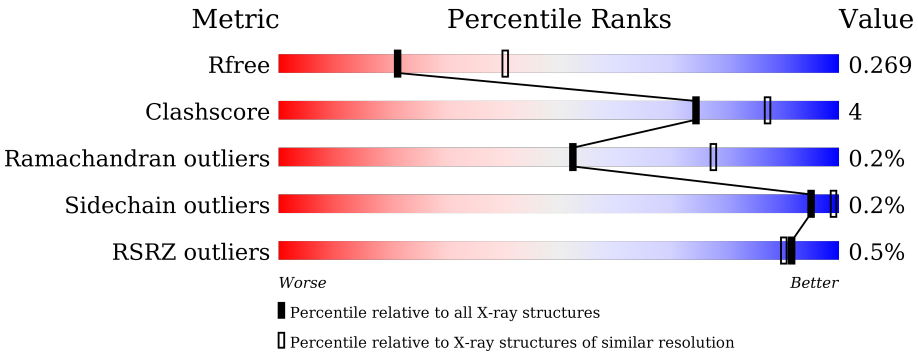
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	522	91% 8%
1	B	522	89% 10%
1	C	522	93% 7%
1	D	522	86% 12%
1	E	522	89% 8%
1	F	522	87% 11%

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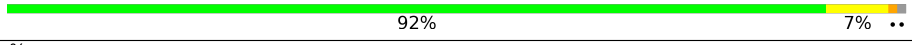
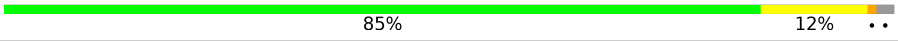
Mol	Chain	Length	Quality of chain
1	G	522	
1	H	522	
1	I	522	
1	J	522	
1	K	522	
1	L	522	

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	4TK	A	1001	-	-	-	X
2	4TK	D	1001	-	-	-	X
2	4TK	E	1001	-	-	-	X
2	4TK	G	1001	-	-	-	X
2	4TK	K	1001	-	-	-	X
2	4TK	L	1001	-	-	-	X
4	CO3	I	1004	-	-	-	X
5	GOL	A	1005	-	-	-	X
5	GOL	B	1005	-	-	-	X
5	GOL	G	1005	-	-	-	X
6	1PE	A	1007	-	-	-	X
6	1PE	B	1006	-	-	-	X
6	1PE	F	1005	-	-	-	X
6	1PE	G	1007	-	-	-	X
6	1PE	I	1008	-	-	-	X
6	1PE	K	1005	-	-	-	X
7	SO4	J	1008	-	-	-	X
8	DMS	D	1005	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 48710 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 Probable M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3966	2543	637	767	19			
1	B	516	Total	C	N	O	S	0	0	0
			3869	2483	630	737	19			
1	C	517	Total	C	N	O	S	0	0	0
			3926	2521	633	753	19			
1	D	513	Total	C	N	O	S	0	0	0
			3881	2500	628	733	20			
1	E	509	Total	C	N	O	S	0	0	0
			3873	2492	622	740	19			
1	F	511	Total	C	N	O	S	0	0	0
			3837	2467	618	733	19			
1	G	519	Total	C	N	O	S	0	0	0
			3961	2542	638	762	19			
1	H	517	Total	C	N	O	S	0	0	0
			3896	2504	633	740	19			
1	I	518	Total	C	N	O	S	0	0	0
			3953	2540	636	757	20			
1	J	512	Total	C	N	O	S	0	0	0
			3921	2524	632	745	20			
1	K	508	Total	C	N	O	S	0	0	0
			3882	2499	626	738	19			
1	L	511	Total	C	N	O	S	0	0	0
			3835	2468	619	729	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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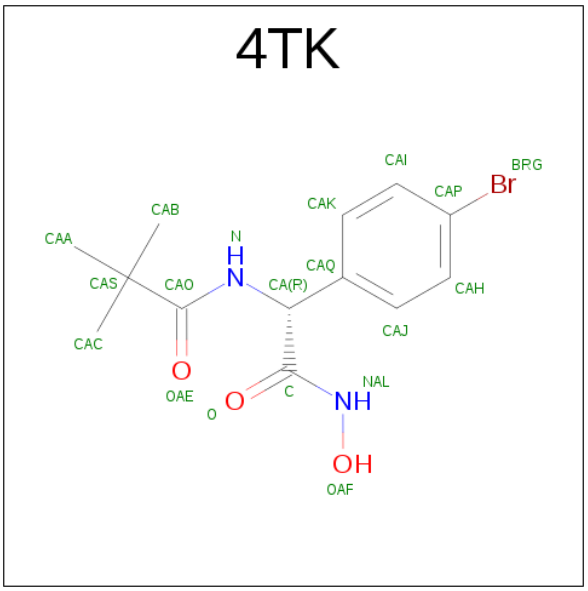
Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

- Molecule 2 is N-[(1R)-1-(4-bromophenyl)-2-(hydroxyamino)-2-oxoethyl]-2,2-dimethylpropanamide (three-letter code: 4TK) (formula: $C_{13}H_{17}BrN_2O_3$).

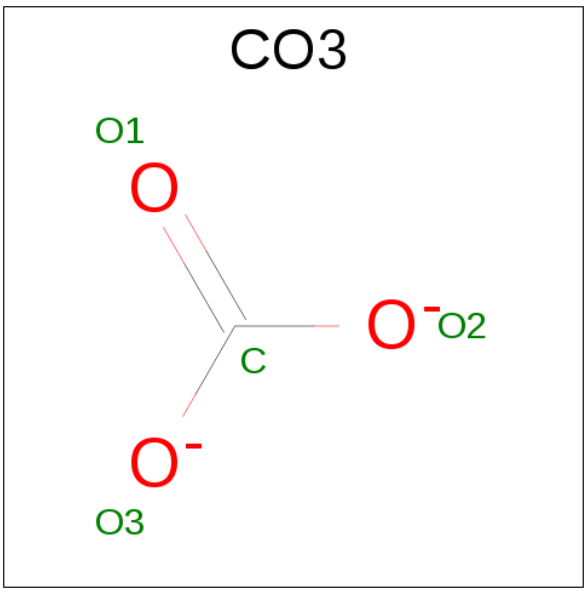


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	B	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	C	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	D	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	E	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	F	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	G	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	H	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	I	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	J	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	K	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	L	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		

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

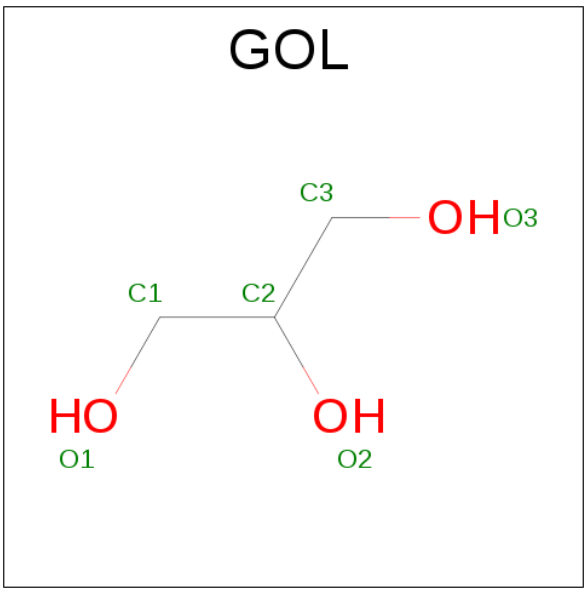
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	A	2	Total Zn 2 2	0	0
3	L	2	Total Zn 2 2	0	0
3	F	2	Total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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



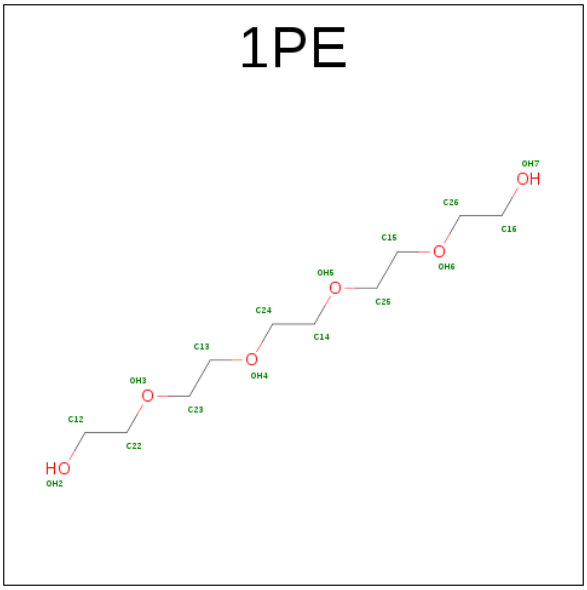
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	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 12 8 4	0	0
6	B	1	Total C O 10 7 3	0	0
6	C	1	Total C O 13 9 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 10 7 3	0	0

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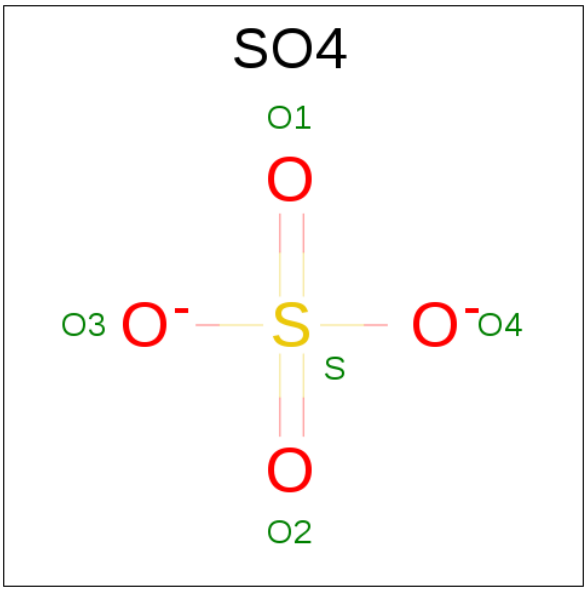
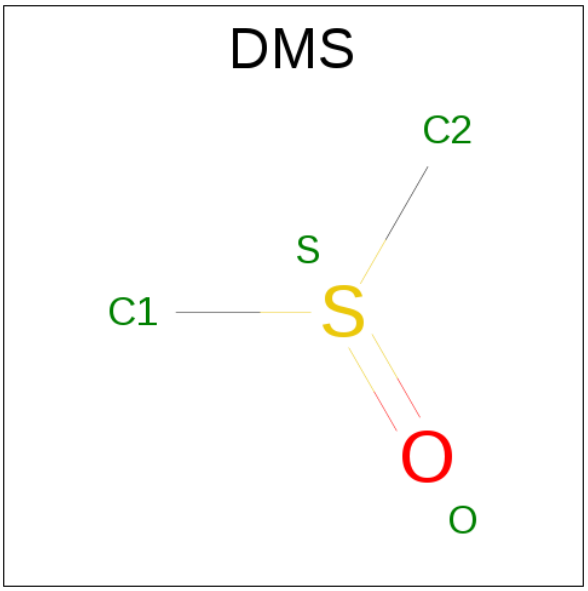
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			12	8	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	H	1	Total	C	O	0	0
			6	4	2		
6	H	1	Total	C	O	0	0
			10	7	3		
6	I	1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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O S 4 2 1 1	0	0
8	D	1	Total C O S 4 2 1 1	0	0
8	G	1	Total C O S 4 2 1 1	0	0
8	I	1	Total C O S 4 2 1 1	0	0
8	J	1	Total C O S 4 2 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	119	Total O 119 119	0	0
9	B	109	Total O 109 109	0	0
9	C	90	Total O 90 90	0	0
9	D	86	Total O 86 86	0	0
9	E	131	Total O 131 131	0	0
9	F	79	Total O 79 79	0	0
9	G	120	Total O 120 120	0	0

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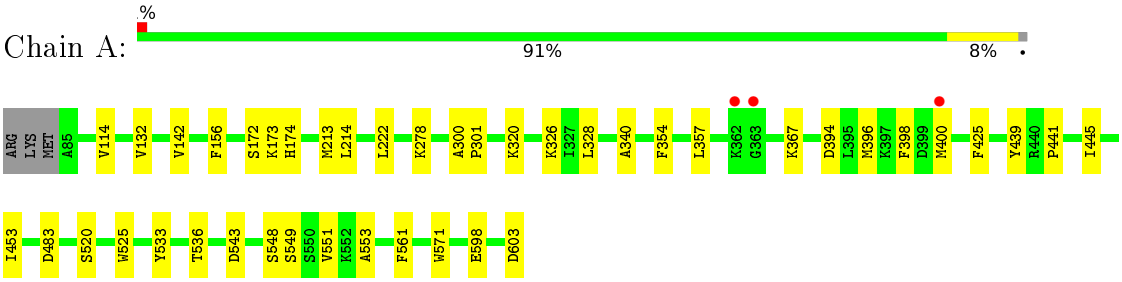
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	102	Total O 102 102	0	0
9	I	116	Total O 116 116	0	0
9	J	104	Total O 104 104	0	0
9	K	150	Total O 150 150	0	0
9	L	99	Total O 99 99	0	0

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.

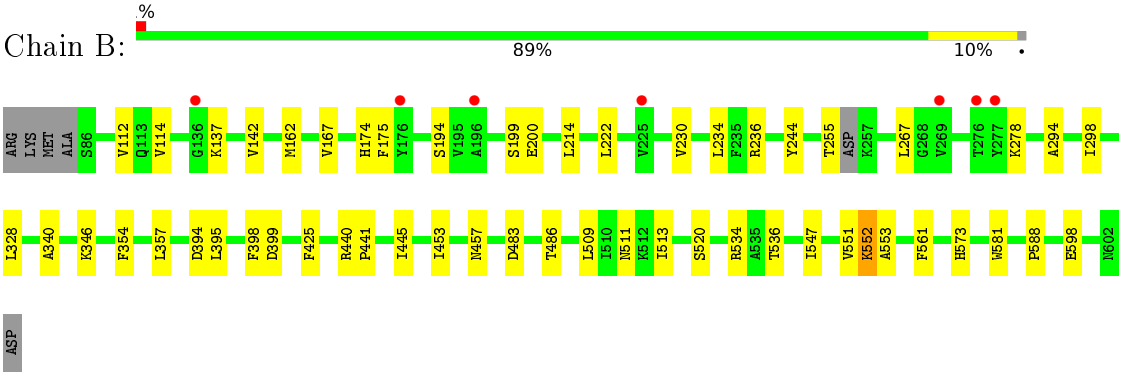
- Molecule 1: Probable M17 family aminopeptidase

Chain A:



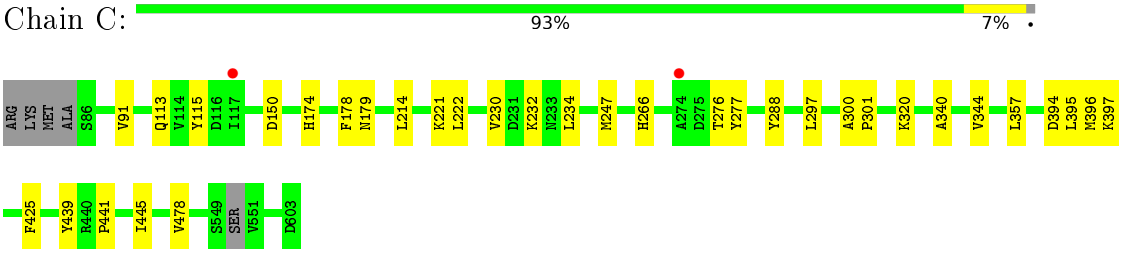
- Molecule 1: Probable M17 family aminopeptidase

Chain B:



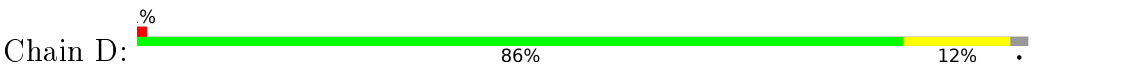
- Molecule 1: Probable M17 family aminopeptidase

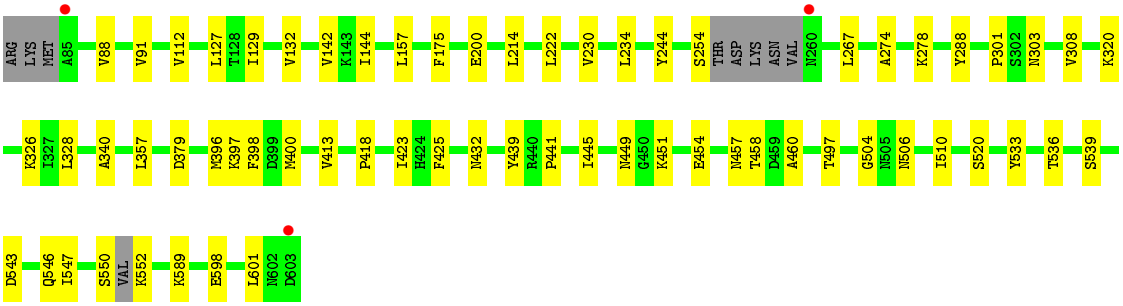
Chain C:



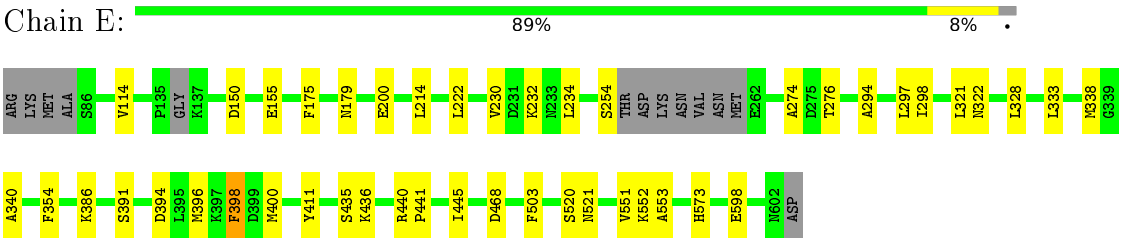
- Molecule 1: Probable M17 family aminopeptidase

Chain D:

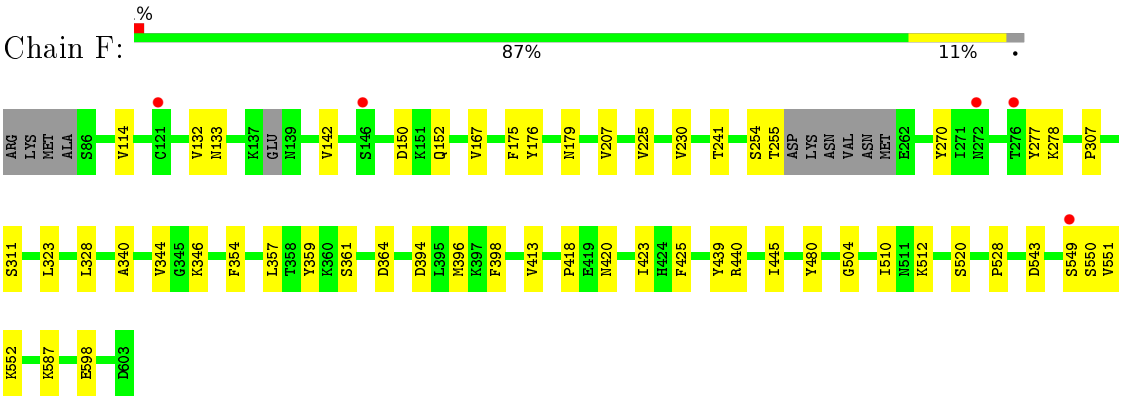




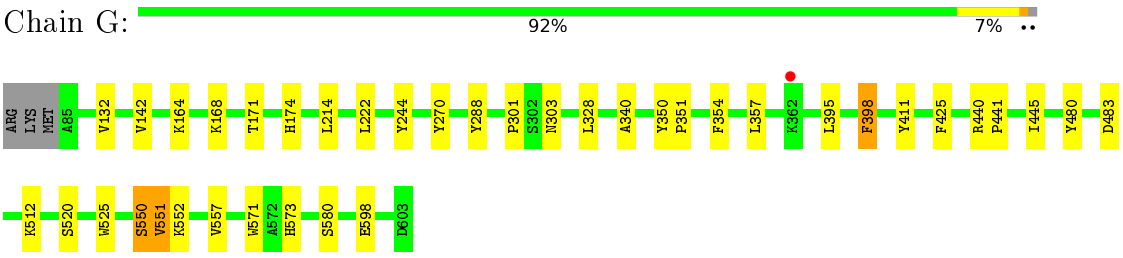
• Molecule 1: Probable M17 family aminopeptidase



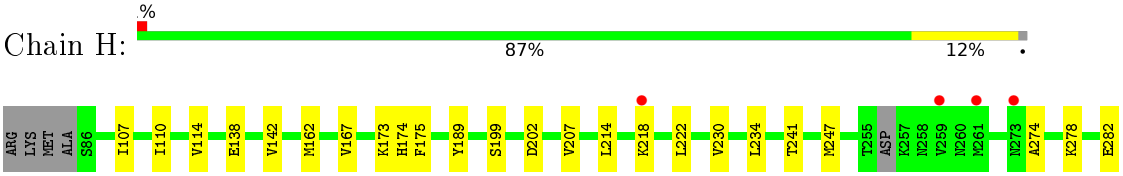
• Molecule 1: Probable M17 family aminopeptidase

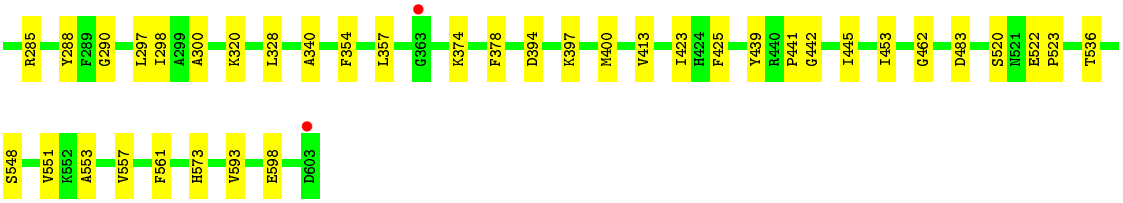


• Molecule 1: Probable M17 family aminopeptidase



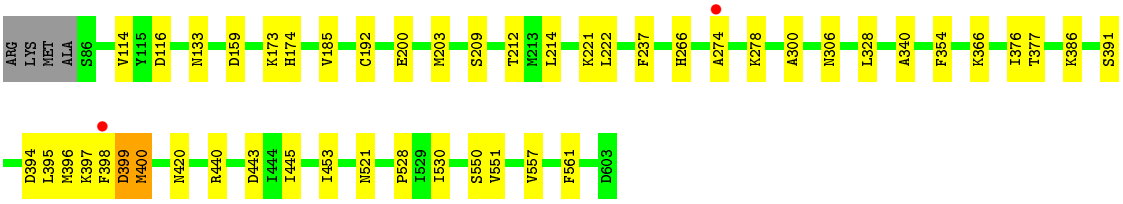
• Molecule 1: Probable M17 family aminopeptidase





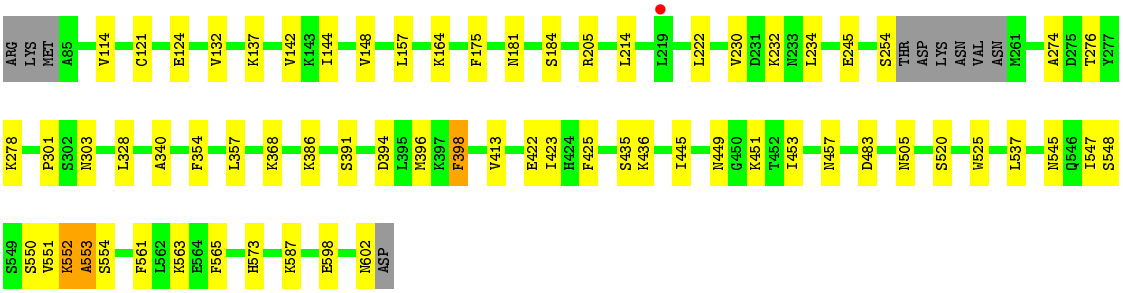
• Molecule 1: Probable M17 family aminopeptidase

Chain I:



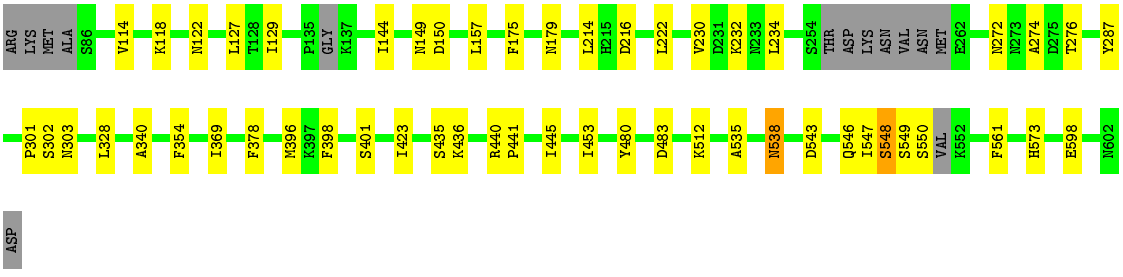
• Molecule 1: Probable M17 family aminopeptidase

Chain J:



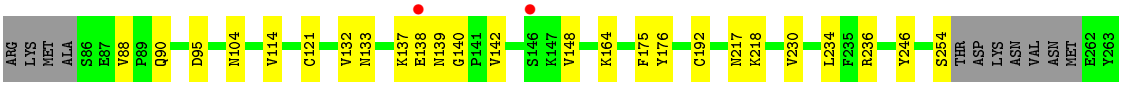
• Molecule 1: Probable M17 family aminopeptidase

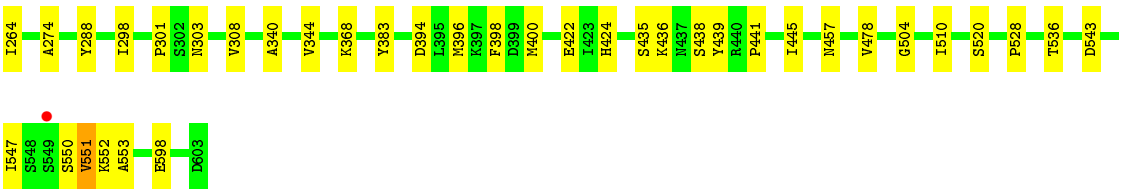
Chain K:



• Molecule 1: Probable M17 family aminopeptidase

Chain L:




I264
A274
Y288
I298
P301
S302
N303
V308
A340
V344
K368
Y383
D394
L395
M396
K397
F398
D399
N400
E422
I423
H424
S435
K436
N437
S438
Y439
R440
P441
T445
N457
V478
G504
L510
S520
P528
T536
D543
I547
S548
S549
S550
V551
K552
A553
E598
D603

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.85Å 176.97Å 229.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.74 – 2.60 48.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (46.74-2.60) 77.1 (48.48-2.60)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.267 0.227 , 0.269	Depositor DCC
R_{free} test set	9762 reflections (6.14%)	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	6 of 195719 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	48710	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 46.69 % 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 1.1039e-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: GOL, ZN, CO3, 1PE, 4TK, DMS, SO4

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	0.21	0/4044	0.38	0/5492
1	B	0.21	0/3946	0.37	0/5369
1	C	0.22	0/4003	0.37	0/5437
1	D	0.22	0/3957	0.38	0/5372
1	E	0.21	0/3949	0.37	0/5361
1	F	0.22	0/3913	0.39	0/5322
1	G	0.22	0/4039	0.38	0/5485
1	H	0.22	0/3973	0.38	0/5400
1	I	0.23	0/4031	0.39	0/5472
1	J	0.21	0/3998	0.37	0/5422
1	K	0.22	0/3957	0.39	0/5366
1	L	0.23	0/3912	0.39	0/5322
All	All	0.22	0/47722	0.38	0/64820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3966	0	3862	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3869	0	3717	37	0
1	C	3926	0	3809	24	0
1	D	3881	0	3788	41	0
1	E	3873	0	3773	28	0
1	F	3837	0	3685	36	0
1	G	3961	0	3862	28	0
1	H	3896	0	3768	41	0
1	I	3953	0	3857	30	0
1	J	3921	0	3860	40	0
1	K	3882	0	3802	35	0
1	L	3835	0	3696	39	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	1	0
2	D	19	0	0	1	0
2	E	19	0	0	0	0
2	F	19	0	0	1	0
2	G	19	0	0	0	0
2	H	19	0	0	0	0
2	I	19	0	0	0	0
2	J	19	0	0	0	0
2	K	19	0	0	0	0
2	L	19	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	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	1	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	G	6	0	8	0	0
5	I	6	0	8	1	0
5	J	6	0	8	0	0
6	A	21	0	22	2	0
6	B	10	0	10	0	0
6	C	22	0	24	2	0
6	D	20	0	20	1	0
6	E	24	0	28	0	0
6	F	10	0	13	0	0
6	G	21	0	20	2	0
6	H	16	0	16	2	0
6	I	23	0	26	0	0
6	J	11	0	13	0	0
6	K	12	0	14	0	0
6	L	10	0	13	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
7	G	10	0	0	1	0
7	H	5	0	0	0	0
7	I	10	0	0	0	0
7	J	10	0	0	1	0
7	L	5	0	0	1	0
8	C	4	0	6	0	0
8	D	4	0	6	1	0
8	G	4	0	6	1	0
8	I	4	0	6	0	0
8	J	4	0	6	0	0
9	A	119	0	0	1	0
9	B	109	0	0	6	0
9	C	90	0	0	3	0
9	D	86	0	0	0	0
9	E	131	0	0	1	0
9	F	79	0	0	3	0
9	G	120	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	102	0	0	2	0
9	I	116	0	0	3	0
9	J	104	0	0	1	0
9	K	150	0	0	1	0
9	L	99	0	0	1	0
All	All	48710	0	45768	376	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 4.

All (376) 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:538:ASN:H	1:K:538:ASN:HD22	1.11	0.95
1:G:398:PHE:HE1	1:G:580:SER:HB3	1.31	0.92
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.09	0.84
1:D:432:ASN:OD1	1:D:439:TYR:OH	1.96	0.82
1:K:538:ASN:N	1:K:538:ASN:HD22	1.77	0.82
1:G:551:VAL:HG21	1:G:557:VAL:HG21	1.63	0.80
1:B:553:ALA:O	9:B:1101:HOH:O	2.02	0.77
1:H:218:LYS:HE3	1:L:164:LYS:HA	1.69	0.75
1:L:550:SER:OG	1:L:551:VAL:N	2.20	0.73
1:C:320:LYS:HZ1	6:C:1006:1PE:H142	1.53	0.71
1:G:398:PHE:CE1	1:G:580:SER:HB3	2.21	0.70
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.56	0.70
1:I:366:LYS:HG3	1:I:420:ASN:HB3	1.74	0.69
1:C:232:LYS:NZ	1:C:276:THR:O	2.27	0.68
1:G:132:VAL:HG21	1:G:142:VAL:HG13	1.76	0.67
1:F:551:VAL:HA	1:F:552:LYS:HB2	1.77	0.67
1:B:114:VAL:O	1:B:278:LYS:NZ	2.28	0.66
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.76	0.66
1:J:551:VAL:O	1:J:553:ALA:N	2.29	0.66
1:L:536:THR:HG21	1:L:551:VAL:HG21	1.78	0.65
1:G:512:LYS:NZ	8:G:1006:DMS:O	2.29	0.65
1:H:300:ALA:O	9:H:1101:HOH:O	2.14	0.65
1:H:214:LEU:HD21	1:H:222:LEU:HD22	1.79	0.65
1:E:230:VAL:HG13	1:E:234:LEU:HB3	1.79	0.64
1:J:254:SER:OG	1:L:543:ASP:OD2	2.14	0.64
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.79	0.64
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.80	0.64
1:K:535:ALA:HA	1:K:538:ASN:HD21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:PRO:O	1:F:311:SER:OG	2.14	0.64
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.78	0.64
1:L:422:GLU:OE1	1:L:424:HIS:NE2	2.31	0.64
1:I:300:ALA:O	9:I:1101:HOH:O	2.15	0.64
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.80	0.64
1:H:110:ILE:O	1:H:285:ARG:NH2	2.30	0.64
1:K:232:LYS:NZ	1:K:276:THR:O	2.32	0.63
1:I:530:ILE:HA	5:I:1005:GOL:H31	1.79	0.63
1:A:551:VAL:HG12	1:A:553:ALA:H	1.64	0.62
1:E:232:LYS:NZ	1:E:276:THR:O	2.31	0.62
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.82	0.62
1:K:535:ALA:O	1:K:538:ASN:ND2	2.32	0.62
1:A:173:LYS:NZ	9:A:1105:HOH:O	2.33	0.62
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.81	0.62
1:D:379:ASP:OD1	1:D:432:ASN:ND2	2.22	0.62
1:E:551:VAL:O	1:E:553:ALA:N	2.33	0.62
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.82	0.62
1:I:395:LEU:O	1:I:397:LYS:N	2.31	0.61
1:D:379:ASP:HA	1:D:432:ASN:HB3	1.81	0.61
1:A:533:TYR:O	1:A:536:THR:HG22	2.01	0.61
1:G:164:LYS:NZ	7:J:1008:SO4:O2	2.33	0.61
1:E:440:ARG:NH2	9:E:1104:HOH:O	2.34	0.60
1:H:297:LEU:HB3	1:H:400:MET:HE1	1.82	0.60
1:K:538:ASN:N	1:K:538:ASN:ND2	2.45	0.60
1:I:551:VAL:HG21	1:I:557:VAL:HG21	1.83	0.60
1:G:483:ASP:OD1	1:G:573:HIS:ND1	2.31	0.60
1:D:88:VAL:HG12	1:D:308:VAL:HB	1.84	0.60
1:J:232:LYS:NZ	1:J:276:THR:O	2.34	0.60
1:H:114:VAL:O	1:H:278:LYS:NZ	2.34	0.60
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.83	0.60
1:I:306:ASN:ND2	9:I:1104:HOH:O	2.33	0.59
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.83	0.59
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.84	0.59
1:G:411:TYR:HE1	6:G:1007:1PE:H132	1.67	0.59
1:B:440:ARG:NH1	9:B:1104:HOH:O	2.34	0.59
1:K:483:ASP:OD1	1:K:573:HIS:ND1	2.32	0.59
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.85	0.59
1:A:548:SER:OG	1:A:549:SER:N	2.36	0.59
1:L:368:LYS:HG2	1:L:478:VAL:HA	1.85	0.59
1:G:550:SER:O	1:G:552:LYS:N	2.31	0.59
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.85	0.58
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.84	0.58
1:J:124:GLU:OE2	1:J:181:ASN:ND2	2.36	0.58
1:G:395:LEU:O	1:G:398:PHE:HB3	2.03	0.58
1:B:114:VAL:HB	1:B:278:LYS:HZ3	1.69	0.58
1:F:396:MET:SD	1:F:398:PHE:HE2	2.27	0.58
1:F:480:TYR:OH	1:F:512:LYS:NZ	2.34	0.57
1:H:282:GLU:OE1	1:H:285:ARG:NH1	2.37	0.57
1:H:199:SER:OG	1:H:202:ASP:OD2	2.19	0.57
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.87	0.57
1:C:395:LEU:O	1:C:397:LYS:N	2.37	0.57
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.87	0.56
1:G:440:ARG:NH1	9:G:1110:HOH:O	2.37	0.56
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.87	0.56
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.86	0.56
1:D:504:GLY:HA3	1:D:510:ILE:HD11	1.86	0.56
1:E:520:SER:HB3	1:E:598:GLU:HG3	1.87	0.56
1:I:377:THR:O	9:I:1102:HOH:O	2.18	0.56
1:H:551:VAL:HG12	1:H:553:ALA:H	1.69	0.56
1:F:114:VAL:O	1:F:278:LYS:NZ	2.39	0.55
7:G:1011:SO4:O4	1:J:164:LYS:NZ	2.34	0.55
1:F:440:ARG:NH2	9:F:1108:HOH:O	2.39	0.55
1:H:320:LYS:HZ3	6:H:1006:1PE:H142	1.72	0.55
1:J:205:ARG:NH1	9:J:1107:HOH:O	2.39	0.55
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.70	0.55
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.89	0.55
1:B:175:PHE:HD1	1:F:176:TYR:HB2	1.72	0.54
1:D:320:LYS:HZ1	6:D:1006:1PE:H142	1.70	0.54
1:D:439:TYR:CE1	1:D:458:THR:HB	2.42	0.54
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.88	0.54
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.90	0.54
1:C:221:LYS:HG3	1:C:266:HIS:HB2	1.89	0.54
1:J:245:GLU:OE1	1:J:587:LYS:NZ	2.30	0.54
1:F:361:SER:OG	1:F:418:PRO:O	2.20	0.54
1:F:150:ASP:OD2	1:F:179:ASN:HB2	2.06	0.54
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.89	0.54
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.88	0.54
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.88	0.53
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.89	0.53
1:G:244:TYR:HA	1:G:288:TYR:HE1	1.71	0.53
1:L:104:ASN:ND2	7:L:1006:SO4:O2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:ASP:OD1	1:I:159:ASP:N	2.41	0.53
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.91	0.53
1:J:368:LYS:HG2	1:J:422:GLU:HB3	1.91	0.53
1:I:221:LYS:HG3	1:I:266:HIS:HB2	1.90	0.53
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.89	0.53
1:C:344:VAL:HA	1:C:439:TYR:CE2	2.43	0.53
1:J:230:VAL:HG12	1:J:234:LEU:HD23	1.91	0.53
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.90	0.53
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.91	0.53
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.91	0.53
1:D:550:SER:O	1:D:552:LYS:N	2.42	0.52
1:I:398:PHE:C	1:I:400:MET:H	2.12	0.52
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.91	0.52
1:L:133:ASN:HB3	1:L:192:CYS:HB2	1.91	0.52
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.91	0.52
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.90	0.52
1:E:333:LEU:HD21	1:E:354:PHE:HB2	1.90	0.52
1:F:364:ASP:OD1	1:F:420:ASN:ND2	2.43	0.52
1:C:113:GLN:OE1	1:C:115:TYR:OH	2.23	0.52
1:C:230:VAL:O	1:C:277:TYR:OH	2.20	0.52
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.91	0.52
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.92	0.52
1:F:254:SER:OG	1:F:255:THR:N	2.41	0.52
1:A:398:PHE:C	1:A:400:MET:H	2.13	0.52
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.90	0.51
1:J:449:ASN:HD21	1:J:451:LYS:HD2	1.75	0.51
1:I:200:GLU:OE1	1:I:200:GLU:N	2.31	0.51
1:F:344:VAL:HA	1:F:439:TYR:CE2	2.45	0.51
1:B:511:ASN:ND2	9:B:1110:HOH:O	2.38	0.51
1:H:114:VAL:HG12	1:H:274:ALA:HB1	1.92	0.51
1:C:297:LEU:O	9:C:1101:HOH:O	2.19	0.51
1:E:214:LEU:HD21	1:E:222:LEU:HD22	1.93	0.51
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.92	0.51
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.93	0.51
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.91	0.50
2:C:1001:4TK:NAL	4:C:1004:CO3:O3	2.44	0.50
1:L:88:VAL:HG22	1:L:308:VAL:HB	1.92	0.50
1:A:326:LYS:HE3	1:A:328:LEU:HD11	1.94	0.50
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.92	0.50
1:C:247:MET:HG3	1:C:288:TYR:OH	2.10	0.50
1:J:483:ASP:OD1	1:J:573:HIS:ND1	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.93	0.50
1:L:344:VAL:HA	1:L:439:TYR:CE2	2.47	0.50
1:A:320:LYS:HZ1	6:A:1007:1PE:H152	1.76	0.49
1:F:150:ASP:OD1	1:F:152:GLN:N	2.46	0.49
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.94	0.49
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.95	0.49
1:H:483:ASP:OD1	1:H:573:HIS:ND1	2.35	0.49
1:B:236:ARG:NH1	9:B:1118:HOH:O	2.43	0.48
1:D:326:LYS:HE3	1:D:328:LEU:HD21	1.94	0.48
1:I:209:SER:O	1:I:212:THR:OG1	2.28	0.48
1:A:214:LEU:HD21	1:A:222:LEU:HD22	1.94	0.48
1:H:397:LYS:O	1:H:400:MET:HG2	2.12	0.48
1:D:91:VAL:HB	1:F:346:LYS:HE3	1.94	0.48
1:L:236:ARG:NH1	9:L:1101:HOH:O	2.39	0.48
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.35	0.48
1:B:453:ILE:HD13	1:B:561:PHE:HZ	1.79	0.48
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.96	0.48
1:D:200:GLU:OE1	1:D:200:GLU:N	2.46	0.48
1:J:396:MET:SD	1:J:398:PHE:HE2	2.37	0.48
1:G:480:TYR:OH	1:G:512:LYS:NZ	2.39	0.48
1:H:413:VAL:HG11	1:H:423:ILE:HD12	1.95	0.48
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.96	0.47
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.96	0.47
1:H:442:GLY:O	9:H:1102:HOH:O	2.20	0.47
1:J:121:CYS:HB2	1:J:148:VAL:HG12	1.96	0.47
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.95	0.47
1:D:397:LYS:O	1:D:400:MET:HG2	2.15	0.47
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.96	0.47
1:D:506:ASN:O	1:D:510:ILE:HG12	2.14	0.47
1:K:122:ASN:OD1	1:K:149:ASN:HB2	2.15	0.47
1:J:598:GLU:OE1	1:J:602:ASN:ND2	2.43	0.47
1:H:320:LYS:NZ	6:H:1006:1PE:H142	2.30	0.47
1:J:301:PRO:HB2	1:J:303:ASN:OD1	2.15	0.47
1:K:230:VAL:HG12	1:K:234:LEU:HD23	1.96	0.47
1:K:548:SER:HA	1:K:549:SER:CB	2.44	0.47
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.97	0.47
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.96	0.47
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.97	0.47
1:B:244:TYR:OH	1:B:588:PRO:O	2.31	0.47
2:D:1001:4TK:NAL	4:D:1004:CO3:O1	2.48	0.47
1:D:439:TYR:N	1:D:439:TYR:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:PHE:CD1	1:F:176:TYR:HB2	2.50	0.47
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.97	0.47
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.97	0.46
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.97	0.46
1:E:396:MET:SD	1:E:398:PHE:HE2	2.38	0.46
1:K:543:ASP:OD2	1:L:254:SER:OG	2.26	0.46
1:A:453:ILE:HD13	1:A:561:PHE:HZ	1.80	0.46
1:G:164:LYS:NZ	1:J:184:SER:OG	2.48	0.46
1:D:449:ASN:HD21	1:D:451:LYS:HD2	1.79	0.46
1:J:548:SER:OG	1:J:551:VAL:HG23	2.15	0.46
1:I:173:LYS:NZ	1:K:216:ASP:O	2.35	0.46
1:B:553:ALA:N	9:B:1120:HOH:O	2.47	0.46
1:E:230:VAL:HG22	1:E:234:LEU:HD23	1.96	0.46
1:F:225:VAL:HG22	1:F:270:TYR:HB2	1.98	0.46
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.97	0.46
1:I:440:ARG:NH1	1:I:443:ASP:OD2	2.49	0.46
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.98	0.46
1:B:395:LEU:O	1:B:398:PHE:HD2	1.98	0.46
1:E:150:ASP:OD2	1:E:179:ASN:HB2	2.15	0.46
1:H:374:LYS:HE3	1:H:462:GLY:HA3	1.96	0.46
1:L:550:SER:HG	1:L:551:VAL:H	1.62	0.46
1:D:396:MET:SD	1:D:398:PHE:HE2	2.37	0.46
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.98	0.46
1:H:453:ILE:HD13	1:H:561:PHE:HZ	1.81	0.46
1:J:457:ASN:HB2	1:J:547:ILE:HD13	1.97	0.46
1:D:457:ASN:HB2	1:D:547:ILE:HD13	1.97	0.46
1:F:230:VAL:O	1:F:277:TYR:OH	2.23	0.46
1:I:200:GLU:HA	1:I:203:MET:HB3	1.97	0.45
1:J:552:LYS:O	1:J:554:SER:N	2.48	0.45
1:F:413:VAL:HG11	1:F:423:ILE:HD13	1.99	0.45
1:C:300:ALA:O	9:C:1101:HOH:O	2.21	0.45
1:G:483:ASP:OD2	1:G:571:TRP:NE1	2.46	0.45
1:K:396:MET:SD	1:K:398:PHE:HE2	2.39	0.45
1:B:174:HIS:HB3	1:F:175:PHE:CD2	2.51	0.45
1:A:543:ASP:CG	1:B:255:THR:H	2.19	0.45
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.99	0.45
1:A:320:LYS:NZ	6:A:1007:1PE:H152	2.31	0.45
1:L:383:TYR:HE2	1:L:438:SER:HB2	1.80	0.45
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.99	0.45
6:C:1006:1PE:H142	6:C:1006:1PE:H132	1.69	0.45
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:GLU:HB2	1:I:237:PHE:CE2	2.52	0.45
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.99	0.45
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.98	0.45
1:I:114:VAL:HB	1:I:278:LYS:HG2	1.98	0.45
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.52	0.45
1:B:534:ARG:NE	9:B:1122:HOH:O	2.50	0.44
1:E:200:GLU:HG3	1:E:521:ASN:O	2.16	0.44
1:B:395:LEU:HD21	1:B:581:TRP:CD1	2.52	0.44
1:D:244:TYR:HA	1:D:288:TYR:HE1	1.82	0.44
1:K:440:ARG:NH2	9:K:1119:HOH:O	2.49	0.44
1:H:218:LYS:HB2	1:L:164:LYS:HA	1.99	0.44
1:L:217:ASN:OD1	1:L:218:LYS:N	2.49	0.44
1:E:503:PHE:HD1	1:E:573:HIS:HD1	1.65	0.44
1:H:247:MET:HG3	1:H:288:TYR:OH	2.18	0.44
1:J:274:ALA:O	1:J:278:LYS:HG3	2.18	0.44
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.51	0.44
1:D:413:VAL:HG11	1:D:423:ILE:HD12	2.00	0.44
1:I:133:ASN:HB3	1:I:192:CYS:HB2	1.99	0.44
1:I:386:LYS:HB3	1:I:391:SER:HB2	1.99	0.44
1:J:453:ILE:HD13	1:J:561:PHE:HZ	1.82	0.44
1:K:548:SER:CB	1:K:550:SER:H	2.30	0.44
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.99	0.44
1:H:207:VAL:HG11	1:H:241:THR:HG22	1.99	0.44
1:H:298:ILE:HA	1:H:400:MET:SD	2.58	0.44
1:B:399:ASP:OD1	1:B:486:THR:OG1	2.33	0.44
1:I:200:GLU:HG3	1:I:521:ASN:HB3	1.99	0.44
1:K:398:PHE:O	1:K:401:SER:OG	2.27	0.44
1:A:172:SER:HB2	1:A:213:MET:HE1	2.00	0.44
1:B:457:ASN:HB2	1:B:547:ILE:HD13	2.00	0.44
1:J:435:SER:OG	1:J:436:LYS:N	2.51	0.44
6:L:1005:1PE:H262	6:L:1005:1PE:H251	1.71	0.44
1:D:533:TYR:O	1:D:536:THR:HG22	2.18	0.43
1:F:133:ASN:HA	1:F:167:VAL:HG21	1.99	0.43
1:D:254:SER:OG	1:F:543:ASP:OD2	2.24	0.43
1:J:505:ASN:HB3	1:J:563:LYS:HE2	2.00	0.43
1:G:301:PRO:HB2	1:G:303:ASN:OD1	2.18	0.43
1:E:294:ALA:O	1:E:298:ILE:HG13	2.18	0.43
1:G:441:PRO:HD2	1:H:378:PHE:CZ	2.52	0.43
1:E:386:LYS:HE3	1:E:396:MET:SD	2.58	0.43
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.01	0.43
1:H:548:SER:HB2	1:H:557:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:TYR:HD2	1:A:439:TYR:H	1.65	0.43
1:D:439:TYR:HD2	1:D:439:TYR:H	1.67	0.43
1:A:132:VAL:HG21	1:A:142:VAL:HG13	2.00	0.43
1:B:199:SER:OG	1:B:200:GLU:N	2.51	0.43
1:J:453:ILE:HD11	1:J:565:PHE:HZ	1.83	0.43
1:K:546:GLN:HG2	1:K:547:ILE:HG23	2.01	0.43
1:C:301:PRO:HA	1:C:397:LYS:HD2	2.01	0.43
1:D:127:LEU:HD11	1:D:129:ILE:HD11	2.00	0.43
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.01	0.43
1:K:302:SER:OG	1:K:378:PHE:HB2	2.19	0.43
1:K:435:SER:OG	1:K:436:LYS:N	2.51	0.43
1:L:246:TYR:HE2	1:L:264:ILE:HG12	1.84	0.43
1:H:142:VAL:HG12	1:H:167:VAL:HG12	2.00	0.43
1:H:357:LEU:HB2	1:H:425:PHE:HB2	2.01	0.43
1:J:413:VAL:HG11	1:J:423:ILE:HD12	2.00	0.43
1:L:298:ILE:HG23	1:L:398:PHE:HA	2.00	0.43
1:L:137:LYS:CB	1:L:140:GLY:H	2.32	0.43
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.18	0.42
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.54	0.42
1:I:453:ILE:HD13	1:I:561:PHE:HZ	1.83	0.42
1:K:150:ASP:OD2	1:K:179:ASN:HB2	2.19	0.42
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.54	0.42
1:J:551:VAL:HG12	1:J:551:VAL:O	2.19	0.42
1:D:543:ASP:OD2	1:E:254:SER:OG	2.26	0.42
1:G:270:TYR:OH	6:G:1008:1PE:OH6	2.36	0.42
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.54	0.42
1:D:497:THR:O	1:D:589:LYS:NZ	2.52	0.42
1:K:214:LEU:HD21	1:K:222:LEU:HD22	2.01	0.42
1:H:174:HIS:HB3	1:L:175:PHE:CD2	2.54	0.42
1:A:156:PHE:CZ	8:D:1005:DMS:H11	2.55	0.42
1:B:551:VAL:HG12	1:B:552:LYS:O	2.19	0.42
1:C:230:VAL:HG23	1:C:234:LEU:HD23	2.02	0.42
1:C:478:VAL:N	9:C:1112:HOH:O	2.50	0.42
1:F:587:LYS:NZ	9:F:1109:HOH:O	2.39	0.42
1:K:127:LEU:HD11	1:K:129:ILE:HD11	2.01	0.42
1:D:418:PRO:HB3	1:D:601:LEU:HD23	2.02	0.42
1:E:435:SER:OG	1:E:436:LYS:N	2.53	0.42
1:E:338:MET:CE	1:E:468:ASP:HB3	2.50	0.42
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.02	0.42
1:G:168:LYS:HB3	1:G:171:THR:OG1	2.20	0.42
1:J:386:LYS:HB3	1:J:391:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:453:ILE:HD13	1:K:561:PHE:HZ	1.85	0.42
1:A:367:LYS:HG2	1:A:603:ASP:OD2	2.20	0.42
1:H:522:GLU:HA	1:H:523:PRO:HD2	1.94	0.42
1:J:537:LEU:HA	1:J:545:ASN:HB2	2.01	0.42
1:K:144:ILE:HG13	1:K:157:LEU:HD22	2.01	0.42
1:L:457:ASN:HB2	1:L:547:ILE:HD13	2.01	0.42
1:L:552:LYS:HB3	1:L:553:ALA:H	1.72	0.42
1:C:395:LEU:C	1:C:397:LYS:H	2.23	0.42
2:F:1001:4TK:OAF	4:F:1004:CO3:O3	2.38	0.42
1:I:116:ASP:HA	1:I:274:ALA:HB2	2.01	0.42
1:J:114:VAL:HG12	1:J:274:ALA:HB1	2.00	0.42
1:D:144:ILE:HG13	1:D:157:LEU:HD22	2.01	0.41
1:L:90:GLN:NE2	1:L:95:ASP:O	2.51	0.41
1:B:357:LEU:HB2	1:B:425:PHE:HB2	2.02	0.41
1:D:112:VAL:HG22	1:D:267:LEU:HB3	2.01	0.41
1:D:230:VAL:HG12	1:D:234:LEU:HD23	2.01	0.41
1:D:460:ALA:O	1:D:546:GLN:NE2	2.52	0.41
1:G:520:SER:HB3	1:G:598:GLU:HG3	2.03	0.41
1:F:396:MET:HA	1:F:398:PHE:CD2	2.56	0.41
1:K:118:LYS:NZ	1:K:272:ASN:OD1	2.54	0.41
1:K:480:TYR:OH	1:K:512:LYS:NZ	2.35	0.41
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.83	0.41
1:D:214:LEU:HD11	1:D:222:LEU:HD22	2.03	0.41
1:K:287:TYR:OH	1:K:598:GLU:OE2	2.30	0.41
1:A:483:ASP:OD2	1:A:571:TRP:NE1	2.53	0.41
1:B:509:LEU:O	1:B:513:ILE:HG12	2.20	0.41
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.55	0.41
1:L:121:CYS:HB2	1:L:148:VAL:HG12	2.02	0.41
1:L:138:GLU:N	1:L:139:ASN:HA	2.35	0.41
1:B:142:VAL:HG12	1:B:167:VAL:HG12	2.02	0.41
1:B:112:VAL:HG22	1:B:267:LEU:HB3	2.03	0.41
1:B:346:LYS:HE3	1:C:91:VAL:HB	2.02	0.41
1:E:386:LYS:HB3	1:E:391:SER:HB2	2.02	0.41
1:D:441:PRO:HB2	1:E:394:ASP:HA	2.02	0.41
1:E:297:LEU:HB3	1:E:400:MET:HE1	2.03	0.41
1:L:301:PRO:HB2	1:L:303:ASN:OD1	2.21	0.41
1:D:274:ALA:O	1:D:278:LYS:HG3	2.20	0.41
1:F:512:LYS:NZ	9:F:1112:HOH:O	2.43	0.41
1:I:376:ILE:HB	1:I:399:ASP:HB3	2.01	0.41
1:I:395:LEU:C	1:I:397:LYS:H	2.23	0.41
1:B:137:LYS:O	1:B:194:SER:OG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ALA:O	1:B:298:ILE:HG13	2.21	0.41
1:C:174:HIS:HB3	1:E:175:PHE:CD2	2.56	0.41
1:C:150:ASP:OD2	1:C:179:ASN:HB2	2.21	0.41
1:F:364:ASP:O	1:F:420:ASN:HA	2.20	0.41
1:K:301:PRO:HB2	1:K:303:ASN:OD1	2.20	0.41
1:D:454:GLU:OE1	1:D:539:SER:OG	2.35	0.41
1:H:290:GLY:C	1:H:593:VAL:HG11	2.41	0.41
1:L:230:VAL:HG12	1:L:234:LEU:HD23	2.02	0.41
1:A:114:VAL:HB	1:A:278:LYS:HG2	2.02	0.40
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.56	0.40
1:F:504:GLY:HA3	1:F:510:ILE:HD11	2.03	0.40
1:F:549:SER:HA	1:F:550:SER:HA	1.67	0.40
1:K:369:ILE:HB	1:K:423:ILE:HD13	2.02	0.40
1:C:394:ASP:N	1:C:394:ASP:OD1	2.50	0.40
1:G:350:TYR:HA	1:G:351:PRO:HD3	1.91	0.40
1:H:107:ILE:HG12	1:H:247:MET:HG2	2.03	0.40
1:L:435:SER:OG	1:L:436:LYS:N	2.55	0.40
1:A:525:TRP:CZ3	1:F:528:PRO:HB3	2.55	0.40
1:F:323:LEU:HD22	1:F:359:TYR:HB2	2.04	0.40
1:J:214:LEU:HD11	1:J:222:LEU:HD22	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	517/522 (99%)	502 (97%)	14 (3%)	1 (0%)	52	77
1	B	512/522 (98%)	496 (97%)	15 (3%)	1 (0%)	52	77
1	C	513/522 (98%)	501 (98%)	11 (2%)	1 (0%)	52	77
1	D	507/522 (97%)	494 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	503/522 (96%)	488 (97%)	14 (3%)	1 (0%)	52 77
1	F	505/522 (97%)	492 (97%)	13 (3%)	0	100 100
1	G	517/522 (99%)	501 (97%)	14 (3%)	2 (0%)	39 65
1	H	513/522 (98%)	493 (96%)	19 (4%)	1 (0%)	52 77
1	I	516/522 (99%)	502 (97%)	12 (2%)	2 (0%)	39 65
1	J	508/522 (97%)	491 (97%)	13 (3%)	4 (1%)	24 46
1	K	500/522 (96%)	485 (97%)	15 (3%)	0	100 100
1	L	507/522 (97%)	489 (96%)	16 (3%)	2 (0%)	39 65
All	All	6118/6264 (98%)	5934 (97%)	169 (3%)	15 (0%)	52 77

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	396	MET
1	E	552	LYS
1	G	551	VAL
1	I	396	MET
1	L	551	VAL
1	I	550	SER
1	J	552	LYS
1	J	553	ALA
1	A	396	MET
1	G	550	SER
1	J	137	LYS
1	J	550	SER
1	L	396	MET
1	B	552	LYS
1	H	138	GLU

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	422/450 (94%)	422 (100%)	0	100	100
1	B	401/450 (89%)	401 (100%)	0	100	100
1	C	413/450 (92%)	413 (100%)	0	100	100
1	D	406/450 (90%)	406 (100%)	0	100	100
1	E	409/450 (91%)	407 (100%)	2 (0%)	92	98
1	F	397/450 (88%)	397 (100%)	0	100	100
1	G	420/450 (93%)	419 (100%)	1 (0%)	95	99
1	H	405/450 (90%)	404 (100%)	1 (0%)	95	99
1	I	418/450 (93%)	415 (99%)	3 (1%)	88	96
1	J	417/450 (93%)	416 (100%)	1 (0%)	95	99
1	K	411/450 (91%)	409 (100%)	2 (0%)	92	98
1	L	397/450 (88%)	395 (100%)	2 (0%)	92	98
All	All	4916/5400 (91%)	4904 (100%)	12 (0%)	95	99

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	322	ASN
1	E	398	PHE
1	G	398	PHE
1	H	439	TYR
1	I	185	VAL
1	I	399	ASP
1	I	400	MET
1	J	398	PHE
1	K	538	ASN
1	K	548	SER
1	L	288	TYR
1	L	400	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	538	ASN
1	L	217	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 89 ligands modelled in this entry, 24 are monoatomic - leaving 65 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	4TK	A	1001	3	19,19,19	1.91	1 (5%)	27,27,27	0.83	0
4	CO3	A	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	A	1005	-	5,5,5	0.35	0	5,5,5	0.19	0
6	1PE	A	1006	-	8,8,15	0.54	0	7,7,14	0.41	0
6	1PE	A	1007	-	11,11,15	0.64	0	10,10,14	0.37	0
7	SO4	A	1008	-	4,4,4	0.25	0	6,6,6	0.07	0
2	4TK	B	1001	3	19,19,19	1.94	2 (10%)	27,27,27	0.84	0
4	CO3	B	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	B	1005	-	5,5,5	0.37	0	5,5,5	0.15	0
6	1PE	B	1006	-	9,9,15	0.55	0	8,8,14	0.32	0
7	SO4	B	1007	-	4,4,4	0.29	0	6,6,6	0.10	0
2	4TK	C	1001	3	19,19,19	1.96	2 (10%)	27,27,27	0.92	2 (7%)
4	CO3	C	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
8	DMS	C	1005	-	3,3,3	0.66	0	3,3,3	0.47	0
6	1PE	C	1006	-	12,12,15	0.64	0	11,11,14	0.33	0
6	1PE	C	1007	-	8,8,15	0.53	0	7,7,14	0.44	0
2	4TK	D	1001	3	19,19,19	2.02	2 (10%)	27,27,27	0.87	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CO3	D	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
8	DMS	D	1005	-	3,3,3	0.64	0	3,3,3	0.45	0
6	1PE	D	1006	-	9,9,15	0.55	0	8,8,14	0.40	0
6	1PE	D	1007	-	9,9,15	0.55	0	8,8,14	0.34	0
7	SO4	D	1008	-	4,4,4	0.26	0	6,6,6	0.05	0
2	4TK	E	1001	3	19,19,19	2.02	2 (10%)	27,27,27	0.86	1 (3%)
4	CO3	E	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	E	1005	-	11,11,15	0.60	0	10,10,14	0.44	0
6	1PE	E	1006	-	11,11,15	0.59	0	10,10,14	0.41	0
2	4TK	F	1001	3	19,19,19	2.05	2 (10%)	27,27,27	0.83	0
4	CO3	F	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	F	1005	-	9,9,15	0.91	0	8,8,14	0.48	0
2	4TK	G	1001	3	19,19,19	1.94	2 (10%)	27,27,27	0.88	0
4	CO3	G	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	G	1005	-	5,5,5	0.34	0	5,5,5	0.25	0
8	DMS	G	1006	-	3,3,3	0.65	0	3,3,3	0.47	0
6	1PE	G	1007	-	8,8,15	0.54	0	7,7,14	0.29	0
6	1PE	G	1008	-	5,5,15	0.66	0	4,4,14	0.64	0
6	1PE	G	1009	-	5,5,15	0.68	0	4,4,14	0.45	0
7	SO4	G	1010	-	4,4,4	0.24	0	6,6,6	0.08	0
7	SO4	G	1011	-	4,4,4	0.24	0	6,6,6	0.08	0
2	4TK	H	1001	3	19,19,19	1.84	1 (5%)	27,27,27	0.93	1 (3%)
4	CO3	H	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	H	1005	-	5,5,15	0.69	0	4,4,14	0.48	0
6	1PE	H	1006	-	9,9,15	0.55	0	8,8,14	0.40	0
7	SO4	H	1007	-	4,4,4	0.26	0	6,6,6	0.07	0
2	4TK	I	1001	3	19,19,19	1.97	2 (10%)	27,27,27	0.90	1 (3%)
4	CO3	I	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	I	1005	-	5,5,5	0.36	0	5,5,5	0.17	0
8	DMS	I	1006	-	3,3,3	0.66	0	3,3,3	0.47	0
6	1PE	I	1007	-	11,11,15	0.58	0	10,10,14	0.48	0
6	1PE	I	1008	-	10,10,15	0.57	0	9,9,14	0.39	0
7	SO4	I	1009	-	4,4,4	0.24	0	6,6,6	0.06	0
7	SO4	I	1010	-	4,4,4	0.23	0	6,6,6	0.08	0
2	4TK	J	1001	3	19,19,19	2.00	2 (10%)	27,27,27	0.84	1 (3%)
4	CO3	J	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	J	1005	-	5,5,5	0.34	0	5,5,5	0.22	0
8	DMS	J	1006	-	3,3,3	0.66	0	3,3,3	0.47	0
6	1PE	J	1007	-	10,10,15	0.86	0	9,9,14	0.39	0
7	SO4	J	1008	-	4,4,4	0.25	0	6,6,6	0.07	0
7	SO4	J	1009	-	4,4,4	0.28	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	4TK	K	1001	3	19,19,19	1.91	1 (5%)	27,27,27	0.93	2 (7%)
4	CO3	K	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	K	1005	-	11,11,15	0.60	0	10,10,14	0.38	0
2	4TK	L	1001	3	19,19,19	2.02	2 (10%)	27,27,27	0.88	1 (3%)
4	CO3	L	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	L	1005	-	9,9,15	0.91	0	8,8,14	0.43	0
7	SO4	L	1006	-	4,4,4	0.23	0	6,6,6	0.07	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
2	4TK	A	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	A	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
6	1PE	A	1006	-	-	0/6/6/13	0/0/0/0
6	1PE	A	1007	-	-	0/9/9/13	0/0/0/0
7	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
2	4TK	B	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	B	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1005	-	-	0/4/4/4	0/0/0/0
6	1PE	B	1006	-	-	0/7/7/13	0/0/0/0
7	SO4	B	1007	-	-	0/0/0/0	0/0/0/0
2	4TK	C	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	C	1004	-	-	0/0/0/0	0/0/0/0
8	DMS	C	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	C	1006	-	-	0/10/10/13	0/0/0/0
6	1PE	C	1007	-	-	0/6/6/13	0/0/0/0
2	4TK	D	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	D	1004	-	-	0/0/0/0	0/0/0/0
8	DMS	D	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	D	1006	-	-	0/7/7/13	0/0/0/0
6	1PE	D	1007	-	-	0/7/7/13	0/0/0/0
7	SO4	D	1008	-	-	0/0/0/0	0/0/0/0
2	4TK	E	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	E	1004	-	-	0/0/0/0	0/0/0/0
6	1PE	E	1005	-	-	0/9/9/13	0/0/0/0
6	1PE	E	1006	-	-	0/9/9/13	0/0/0/0
2	4TK	F	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	F	1004	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	F	1005	-	-	0/7/7/13	0/0/0/0
2	4TK	G	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	G	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	G	1005	-	-	0/4/4/4	0/0/0/0
8	DMS	G	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	G	1007	-	-	0/6/6/13	0/0/0/0
6	1PE	G	1008	-	-	0/3/3/13	0/0/0/0
6	1PE	G	1009	-	-	0/3/3/13	0/0/0/0
7	SO4	G	1010	-	-	0/0/0/0	0/0/0/0
7	SO4	G	1011	-	-	0/0/0/0	0/0/0/0
2	4TK	H	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	H	1004	-	-	0/0/0/0	0/0/0/0
6	1PE	H	1005	-	-	0/3/3/13	0/0/0/0
6	1PE	H	1006	-	-	0/7/7/13	0/0/0/0
7	SO4	H	1007	-	-	0/0/0/0	0/0/0/0
2	4TK	I	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	I	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	I	1005	-	-	0/4/4/4	0/0/0/0
8	DMS	I	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	I	1007	-	-	0/9/9/13	0/0/0/0
6	1PE	I	1008	-	-	0/8/8/13	0/0/0/0
7	SO4	I	1009	-	-	0/0/0/0	0/0/0/0
7	SO4	I	1010	-	-	0/0/0/0	0/0/0/0
2	4TK	J	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	J	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	J	1005	-	-	0/4/4/4	0/0/0/0
8	DMS	J	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	J	1007	-	-	0/8/8/13	0/0/0/0
7	SO4	J	1008	-	-	0/0/0/0	0/0/0/0
7	SO4	J	1009	-	-	0/0/0/0	0/0/0/0
2	4TK	K	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	K	1004	-	-	0/0/0/0	0/0/0/0
6	1PE	K	1005	-	-	0/9/9/13	0/0/0/0
2	4TK	L	1001	3	-	0/20/20/20	0/1/1/1
4	CO3	L	1004	-	-	0/0/0/0	0/0/0/0
6	1PE	L	1005	-	-	0/7/7/13	0/0/0/0
7	SO4	L	1006	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	4TK	CAQ-CA	-8.28	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	4TK	CAQ-CA	-8.06	1.39	1.52
2	C	1001	4TK	CAQ-CA	-8.01	1.39	1.52
2	I	1001	4TK	CAQ-CA	-7.99	1.39	1.52
2	L	1001	4TK	CAQ-CA	-7.98	1.39	1.52
2	J	1001	4TK	CAQ-CA	-7.98	1.39	1.52
2	K	1001	4TK	CAQ-CA	-7.96	1.39	1.52
2	B	1001	4TK	CAQ-CA	-7.91	1.39	1.52
2	A	1001	4TK	CAQ-CA	-7.90	1.39	1.52
2	D	1001	4TK	CAQ-CA	-7.88	1.39	1.52
2	H	1001	4TK	CAQ-CA	-7.62	1.40	1.52
2	G	1001	4TK	CAQ-CA	-7.58	1.40	1.52
2	B	1001	4TK	OAF-NAL	2.09	1.43	1.39
2	C	1001	4TK	OAF-NAL	2.12	1.43	1.39
2	E	1001	4TK	OAF-NAL	2.13	1.43	1.39
2	I	1001	4TK	OAF-NAL	2.30	1.44	1.39
2	L	1001	4TK	OAF-NAL	2.97	1.45	1.39
2	J	1001	4TK	OAF-NAL	3.03	1.45	1.39
2	G	1001	4TK	OAF-NAL	3.09	1.45	1.39
2	F	1001	4TK	OAF-NAL	3.18	1.45	1.39
2	D	1001	4TK	OAF-NAL	3.39	1.45	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	4TK	CAS-CAO-N	-2.53	114.46	117.87
2	L	1001	4TK	CAS-CAO-N	-2.26	114.82	117.87
2	J	1001	4TK	CAS-CAO-N	-2.24	114.86	117.87
2	K	1001	4TK	CAS-CAO-N	-2.16	114.96	117.87
2	C	1001	4TK	CAS-CAO-N	-2.14	114.98	117.87
2	H	1001	4TK	CAS-CAO-N	-2.13	115.00	117.87
2	I	1001	4TK	OAF-NAL-C	-2.08	116.90	119.92
2	C	1001	4TK	OAF-NAL-C	-2.06	116.93	119.92
2	E	1001	4TK	OAF-NAL-C	-2.04	116.96	119.92
2	K	1001	4TK	OAF-NAL-C	-2.04	116.97	119.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1007	1PE	2	0
2	C	1001	4TK	1	0
4	C	1004	CO3	1	0
6	C	1006	1PE	2	0
2	D	1001	4TK	1	0
4	D	1004	CO3	1	0
8	D	1005	DMS	1	0
6	D	1006	1PE	1	0
2	F	1001	4TK	1	0
4	F	1004	CO3	1	0
8	G	1006	DMS	1	0
6	G	1007	1PE	1	0
6	G	1008	1PE	1	0
7	G	1011	SO4	1	0
6	H	1006	1PE	2	0
5	I	1005	GOL	1	0
7	J	1008	SO4	1	0
6	L	1005	1PE	1	0
7	L	1006	SO4	1	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	519/522 (99%)	-0.30	3 (0%) 90 88	18, 30, 48, 62	1 (0%)
1	B	516/522 (98%)	-0.12	7 (1%) 78 74	19, 30, 61, 74	4 (0%)
1	C	517/522 (99%)	-0.29	2 (0%) 93 91	20, 28, 48, 60	3 (0%)
1	D	513/522 (98%)	-0.40	3 (0%) 90 88	20, 28, 44, 61	2 (0%)
1	E	509/522 (97%)	-0.38	0 100 100	17, 28, 41, 57	5 (0%)
1	F	511/522 (97%)	-0.09	5 (0%) 84 81	23, 37, 59, 71	4 (0%)
1	G	519/522 (99%)	-0.33	1 (0%) 95 95	18, 29, 48, 65	5 (0%)
1	H	517/522 (99%)	-0.13	6 (1%) 81 77	20, 31, 60, 70	1 (0%)
1	I	518/522 (99%)	-0.23	2 (0%) 93 91	20, 31, 53, 65	2 (0%)
1	J	512/522 (98%)	-0.38	1 (0%) 95 95	20, 29, 47, 62	3 (0%)
1	K	508/522 (97%)	-0.38	0 100 100	19, 29, 42, 60	3 (0%)
1	L	511/522 (97%)	-0.26	3 (0%) 90 88	22, 33, 56, 71	3 (0%)
All	All	6170/6264 (98%)	-0.28	33 (0%) 91 90	17, 30, 54, 74	36 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	ASN	3.7
1	H	603	ASP	3.4
1	F	549	SER	3.0
1	B	196	ALA	3.0
1	I	274	ALA	2.9
1	C	274	ALA	2.9
1	J	219	LEU	2.8
1	B	136	GLY	2.8
1	D	85	ALA	2.7
1	H	259	VAL	2.7
1	G	362	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	146	SER	2.6
1	B	276	THR	2.6
1	H	363	GLY	2.6
1	D	603	ASP	2.5
1	H	218	LYS	2.4
1	C	117	ILE	2.4
1	L	146	SER	2.4
1	L	138	GLU	2.4
1	F	276	THR	2.4
1	F	272	ASN	2.3
1	I	398	PHE	2.3
1	A	400	MET	2.3
1	B	176	TYR	2.3
1	H	273	ASN	2.3
1	A	362	LYS	2.3
1	L	549	SER	2.2
1	B	269	VAL	2.2
1	H	261	MET	2.2
1	B	277	TYR	2.1
1	F	121	CYS	2.0
1	A	363	GLY	2.0
1	B	225	VAL	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
6	1PE	F	1005	10/16	0.85	0.30	10.93	40,48,57,59	0
5	GOL	B	1005	6/6	0.90	0.28	7.33	36,39,43,43	0
5	GOL	G	1005	6/6	0.81	0.29	4.53	43,53,60,61	0
7	SO4	J	1008	5/5	0.97	0.33	4.27	41,44,47,54	0
6	1PE	B	1006	10/16	0.80	0.29	3.69	36,43,47,55	0
2	4TK	A	1001	19/19	0.92	0.23	3.63	18,23,28,50	19
5	GOL	A	1005	6/6	0.90	0.24	3.60	32,36,45,46	0
8	DMS	D	1005	4/4	0.94	0.25	3.48	31,34,52,52	0
4	CO3	I	1004	4/4	0.94	0.17	3.37	27,28,28,31	0
2	4TK	L	1001	19/19	0.92	0.22	3.30	17,22,28,38	19
2	4TK	D	1001	19/19	0.91	0.20	3.18	12,25,31,55	19
2	4TK	G	1001	19/19	0.91	0.23	3.11	18,23,31,38	19
6	1PE	I	1008	11/16	0.89	0.21	2.62	36,42,49,49	0
6	1PE	A	1007	12/16	0.79	0.22	2.59	36,43,52,52	0
2	4TK	K	1001	19/19	0.94	0.21	2.50	19,22,27,42	19
6	1PE	G	1007	9/16	0.88	0.18	2.46	30,35,40,40	0
6	1PE	K	1005	12/16	0.93	0.18	2.26	18,32,58,64	0
2	4TK	E	1001	19/19	0.92	0.22	2.25	18,22,28,39	19
6	1PE	G	1008	6/16	0.88	0.20	1.96	34,39,40,42	0
2	4TK	H	1001	19/19	0.93	0.18	1.94	17,23,27,51	19
6	1PE	H	1005	6/16	0.83	0.21	1.77	30,35,38,46	0
5	GOL	I	1005	6/6	0.88	0.21	1.75	28,32,34,39	0
2	4TK	I	1001	19/19	0.93	0.21	1.39	24,27,33,56	19
6	1PE	E	1006	12/16	0.94	0.17	1.27	25,32,59,63	0
4	CO3	C	1004	4/4	0.96	0.15	1.23	24,29,31,31	0
6	1PE	A	1006	9/16	0.94	0.19	1.19	26,31,35,41	0
7	SO4	G	1011	5/5	0.90	0.18	1.16	45,54,59,69	0
2	4TK	J	1001	19/19	0.93	0.18	1.15	15,20,25,55	19
6	1PE	D	1007	10/16	0.93	0.16	1.13	33,36,44,45	0
2	4TK	F	1001	19/19	0.93	0.21	1.08	22,26,33,47	19
2	4TK	B	1001	19/19	0.92	0.17	1.07	13,21,27,47	19
4	CO3	L	1004	4/4	0.97	0.16	1.00	24,24,27,28	0
2	4TK	C	1001	19/19	0.92	0.18	0.85	21,24,31,58	19
4	CO3	K	1004	4/4	0.94	0.17	0.80	27,28,31,33	0
6	1PE	L	1005	10/16	0.87	0.17	0.72	33,39,51,51	0
6	1PE	J	1007	11/16	0.93	0.16	0.56	28,34,39,43	0
6	1PE	C	1007	9/16	0.89	0.16	0.33	24,28,34,40	0
4	CO3	J	1004	4/4	0.96	0.12	0.27	23,23,24,26	0
4	CO3	H	1004	4/4	0.97	0.14	0.03	23,24,27,30	0
6	1PE	G	1009	6/16	0.88	0.13	-0.17	30,32,37,39	0
7	SO4	I	1010	5/5	0.86	0.17	-0.26	64,68,72,87	0
4	CO3	D	1004	4/4	0.96	0.13	-0.41	24,26,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	I	1002	1/1	0.99	0.13	-0.41	26,26,26,26	0
3	ZN	L	1003	1/1	0.99	0.13	-0.46	27,27,27,27	0
3	ZN	A	1003	1/1	0.98	0.13	-0.66	24,24,24,24	0
3	ZN	E	1002	1/1	0.99	0.12	-0.94	30,30,30,30	0
8	DMS	C	1005	4/4	0.95	0.12	-0.98	36,37,43,59	0
3	ZN	G	1003	1/1	1.00	0.13	-0.99	25,25,25,25	0
4	CO3	A	1004	4/4	0.97	0.12	-1.29	27,28,29,30	0
4	CO3	B	1004	4/4	0.98	0.10	-1.52	20,21,23,27	0
3	ZN	K	1003	1/1	0.97	0.11	-1.52	30,30,30,30	0
3	ZN	F	1003	1/1	0.98	0.13	-1.74	31,31,31,31	0
3	ZN	B	1003	1/1	0.99	0.10	-1.82	26,26,26,26	0
3	ZN	L	1002	1/1	0.99	0.11	-1.91	27,27,27,27	0
4	CO3	F	1004	4/4	0.96	0.11	-1.99	28,28,30,32	0
3	ZN	K	1002	1/1	0.97	0.12	-2.04	29,29,29,29	0
4	CO3	G	1004	4/4	0.96	0.12	-2.05	29,29,30,31	0
3	ZN	J	1002	1/1	0.99	0.09	-2.08	29,29,29,29	0
3	ZN	I	1003	1/1	0.98	0.09	-2.11	29,29,29,29	0
3	ZN	C	1002	1/1	0.98	0.11	-2.13	27,27,27,27	0
3	ZN	H	1002	1/1	0.97	0.10	-2.40	27,27,27,27	0
3	ZN	A	1002	1/1	1.00	0.10	-2.53	31,31,31,31	0
7	SO4	D	1008	5/5	0.99	0.08	-2.58	23,25,34,36	0
3	ZN	J	1003	1/1	0.99	0.07	-2.68	27,27,27,27	0
7	SO4	J	1009	5/5	0.99	0.08	-2.69	24,29,32,40	0
3	ZN	E	1003	1/1	0.99	0.09	-2.92	32,32,32,32	0
3	ZN	B	1002	1/1	0.99	0.07	-3.07	23,23,23,23	0
3	ZN	F	1002	1/1	0.98	0.10	-3.23	30,30,30,30	0
3	ZN	G	1002	1/1	0.98	0.09	-3.30	32,32,32,32	0
3	ZN	H	1003	1/1	0.99	0.10	-3.57	24,24,24,24	0
3	ZN	C	1003	1/1	0.98	0.09	-3.63	24,24,24,24	0
4	CO3	E	1004	4/4	0.98	0.07	-3.71	26,27,28,30	0
7	SO4	H	1007	5/5	0.97	0.08	-3.86	19,23,27,28	0
7	SO4	B	1007	5/5	0.99	0.07	-4.13	22,23,25,25	0
3	ZN	D	1003	1/1	0.98	0.08	-4.48	27,27,27,27	0
3	ZN	D	1002	1/1	0.99	0.08	-4.72	26,26,26,26	0
7	SO4	L	1006	5/5	0.97	0.16	-	38,51,55,60	0
8	DMS	J	1006	4/4	0.88	0.16	-	53,57,70,82	0
8	DMS	G	1006	4/4	0.73	0.29	-	53,61,64,98	0
6	1PE	I	1007	12/16	0.90	0.21	-	32,46,50,50	0
7	SO4	A	1008	5/5	0.95	0.11	-	52,53,56,66	0
6	1PE	H	1006	10/16	0.80	0.28	-	35,50,64,68	0
7	SO4	G	1010	5/5	0.95	0.14	-	47,56,60,62	0
7	SO4	I	1009	5/5	0.98	0.24	-	44,52,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	1PE	C	1006	13/16	0.88	0.33	-	32,48,56,62	0
6	1PE	D	1006	10/16	0.83	0.19	-	27,40,46,57	0
6	1PE	E	1005	12/16	0.87	0.17	-	26,36,39,44	0
5	GOL	J	1005	6/6	0.81	0.20	-	37,38,40,48	0
8	DMS	I	1006	4/4	0.87	0.35	-	41,46,62,81	0

6.5 Other polymers

There are no such residues in this entry.