



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 03:55 AM EDT

PDB ID : 4ZY1
Title : X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10r
Authors : Drinkwater, N.; McGowan, S.
Deposited on : unknown
Resolution : 2.50 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

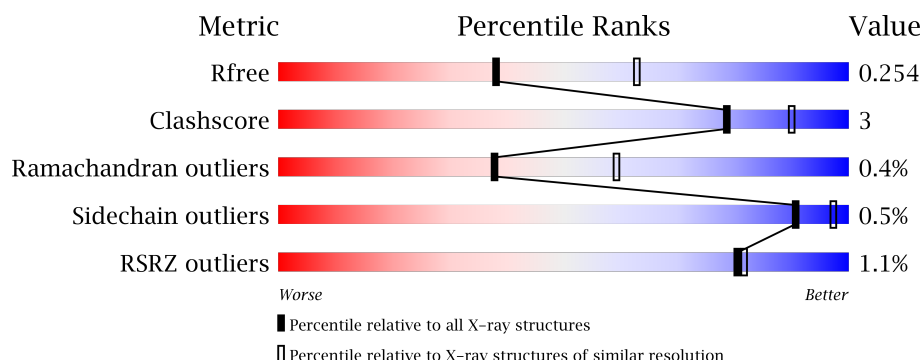
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	
1	B	522	
1	C	522	
1	D	522	
1	E	522	

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Mol	Chain	Length	Quality of chain
1	F	522	
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	4U5	D	1001	-	-	-	X
4	CO3	F	1004	-	-	-	X
4	CO3	G	1004	-	-	-	X
4	CO3	J	1004	-	-	-	X
4	CO3	K	1004	-	-	-	X
5	SO4	A	1007	-	-	X	-
5	SO4	D	1006	-	-	-	X
5	SO4	I	1006	-	-	-	X
5	SO4	J	1006	-	-	-	X
5	SO4	K	1006	-	-	-	X
5	SO4	K	1008	-	-	-	X
5	SO4	L	1006	-	-	-	X
6	1PE	A	1008	-	-	-	X
6	1PE	A	1009	-	-	-	X
6	1PE	D	1008	-	-	-	X
6	1PE	G	1007	-	-	-	X
6	1PE	I	1008	-	-	-	X
6	1PE	J	1008	-	-	-	X
6	1PE	L	1008	-	-	-	X
6	1PE	L	1009	-	-	-	X
7	GOL	G	1006	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49124 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	518	Total	C	N	O	S	0	0	0
			3970	2549	638	764	19			
1	B	516	Total	C	N	O	S	0	0	0
			3909	2513	634	743	19			
1	C	516	Total	C	N	O	S	0	0	0
			3946	2535	635	756	20			
1	D	514	Total	C	N	O	S	0	0	0
			3934	2532	635	747	20			
1	E	508	Total	C	N	O	S	0	0	0
			3890	2505	626	740	19			
1	F	511	Total	C	N	O	S	0	0	0
			3837	2468	620	730	19			
1	G	519	Total	C	N	O	S	0	0	0
			3971	2548	639	765	19			
1	H	517	Total	C	N	O	S	0	0	0
			3904	2507	634	744	19			
1	I	517	Total	C	N	O	S	0	0	0
			3944	2535	635	754	20			
1	J	514	Total	C	N	O	S	0	0	0
			3914	2517	633	744	20			
1	K	509	Total	C	N	O	S	0	0	0
			3890	2504	624	743	19			
1	L	510	Total	C	N	O	S	0	0	0
			3840	2468	618	735	19			

There are 36 discrepancies between the modelled and reference sequences:

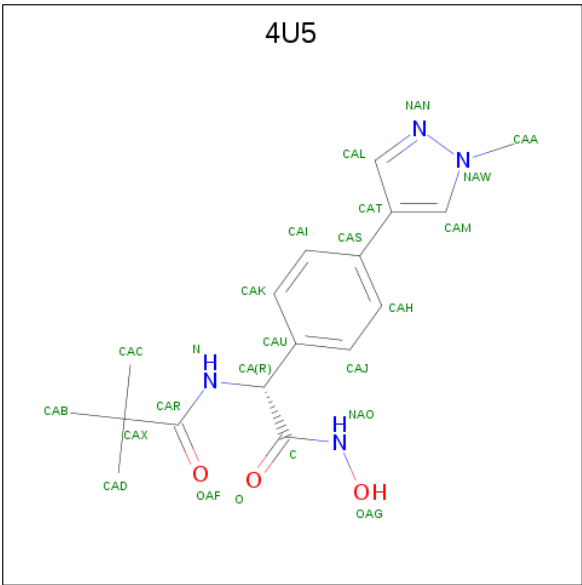
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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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)-2-(hydroxyamino)-1-[4-(1-methyl-1H-pyrazol-4-yl)phenyl]-2-oxoethyl}-2,2-dimethylpropanamide (three-letter code: 4U5) (formula: C₁₇H₂₂N₄O₃).

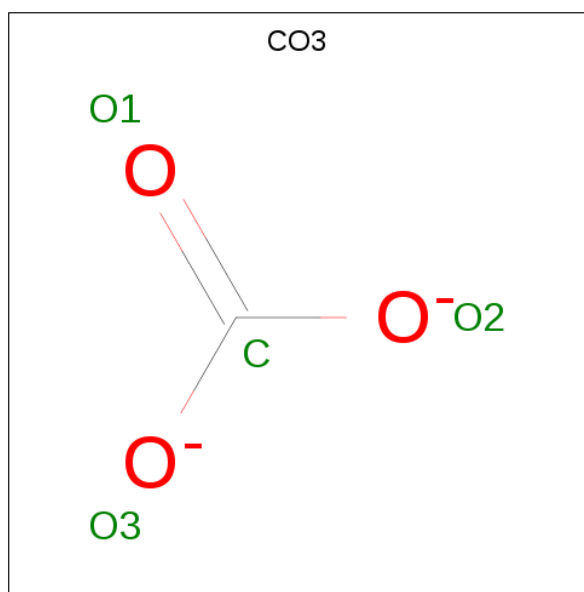


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	17	4	3		
2	B	1	Total	C	N	O	0	0
			24	17	4	3		
2	C	1	Total	C	N	O	0	0
			24	17	4	3		
2	D	1	Total	C	N	O	0	0
			24	17	4	3		
2	E	1	Total	C	N	O	0	0
			24	17	4	3		
2	F	1	Total	C	N	O	0	0
			24	17	4	3		
2	G	1	Total	C	N	O	0	0
			24	17	4	3		
2	H	1	Total	C	N	O	0	0
			24	17	4	3		
2	I	1	Total	C	N	O	0	0
			24	17	4	3		
2	J	1	Total	C	N	O	0	0
			24	17	4	3		
2	K	1	Total	C	N	O	0	0
			24	17	4	3		
2	L	1	Total	C	N	O	0	0
			24	17	4	3		

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

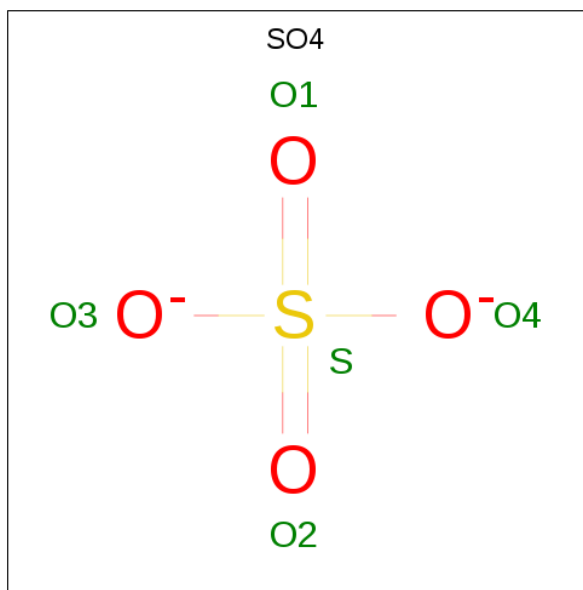
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	L	2	Total 2	Zn 2	0	0
3	F	2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

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



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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



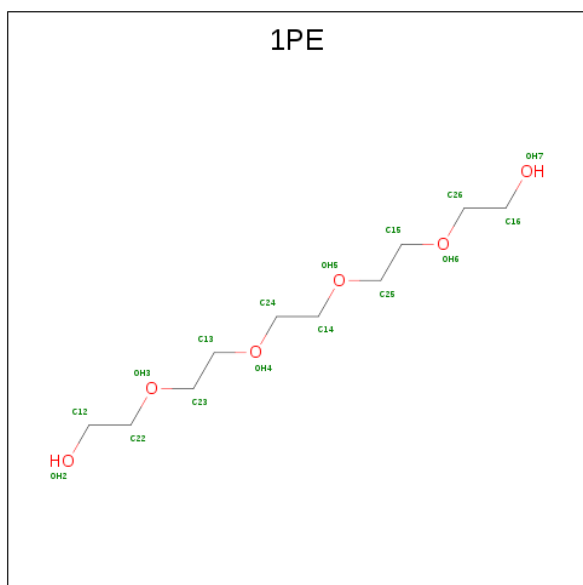
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0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

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

- 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	0	0
			9	6	3		
6	A	1	Total	C	O	0	0
			12	8	4		
6	B	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		
6	C	1	Total	C	O	0	0
			13	9	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	E	1	Total	C	O	0	0
			12	8	4		

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	110	Total	O	0	0
			110	110		
8	B	114	Total	O	0	0
			114	114		
8	C	121	Total	O	0	0
			121	121		
8	D	138	Total	O	0	0
			138	138		
8	E	129	Total	O	0	0
			129	129		
8	F	106	Total	O	0	0
			106	106		
8	G	116	Total	O	0	0
			116	116		
8	H	125	Total	O	0	0
			125	125		
8	I	138	Total	O	0	0
			138	138		
8	J	106	Total	O	0	0
			106	106		
8	K	140	Total	O	0	0
			140	140		

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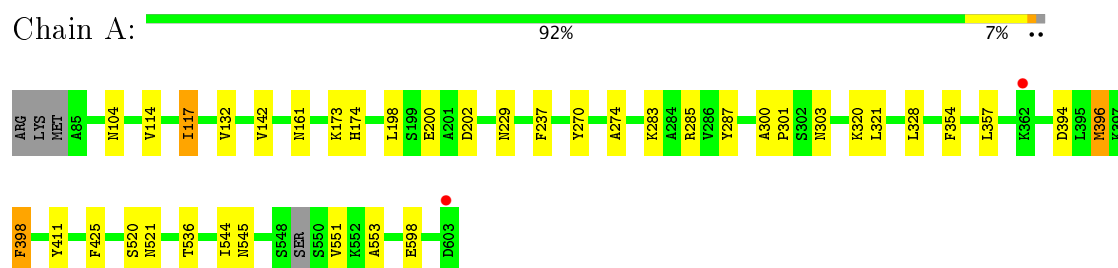
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	102	Total 102	O 102	0	0

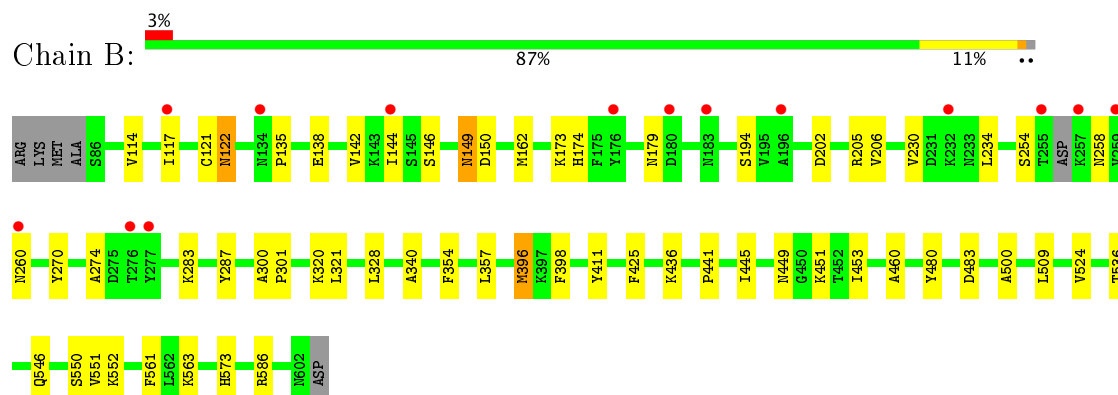
3 Residue-property plots [i](#)

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

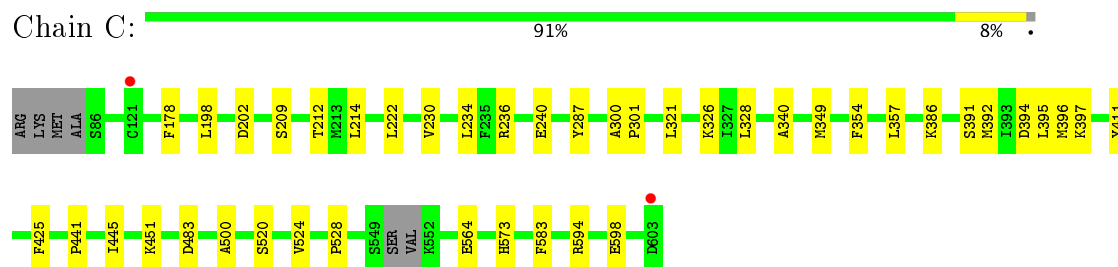
- Molecule 1: Probable M17 family aminopeptidase



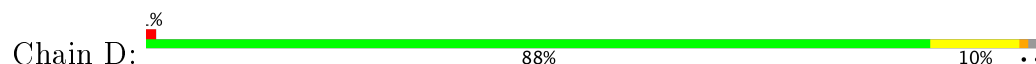
- Molecule 1: Probable M17 family aminopeptidase

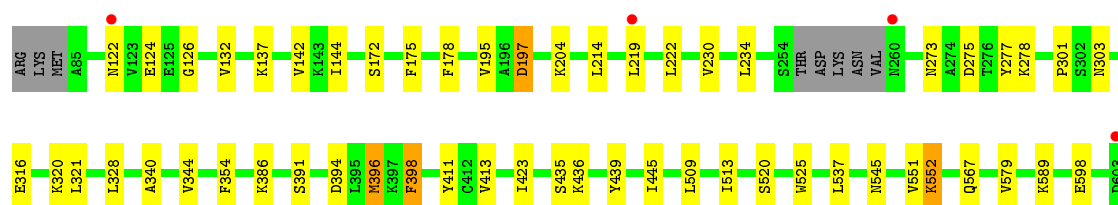


- Molecule 1: Probable M17 family aminopeptidase



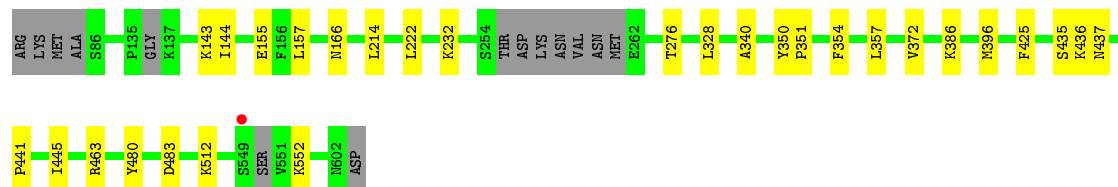
- Molecule 1: Probable M17 family aminopeptidase





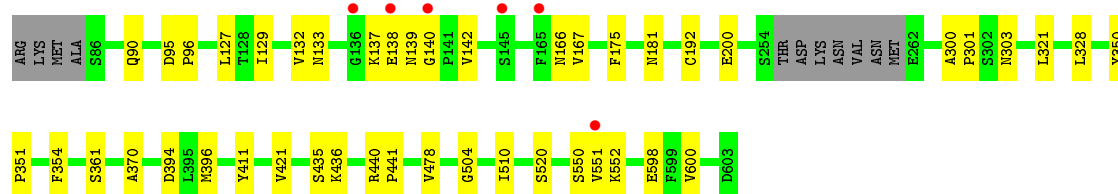
- Molecule 1: Probable M17 family aminopeptidase

Chain E: 92% 6%



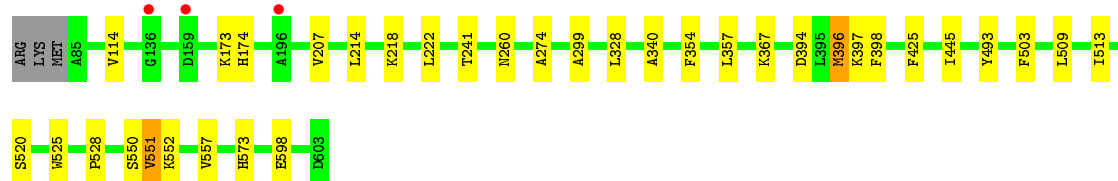
- Molecule 1: Probable M17 family aminopeptidase

Chain F: 89% 9%



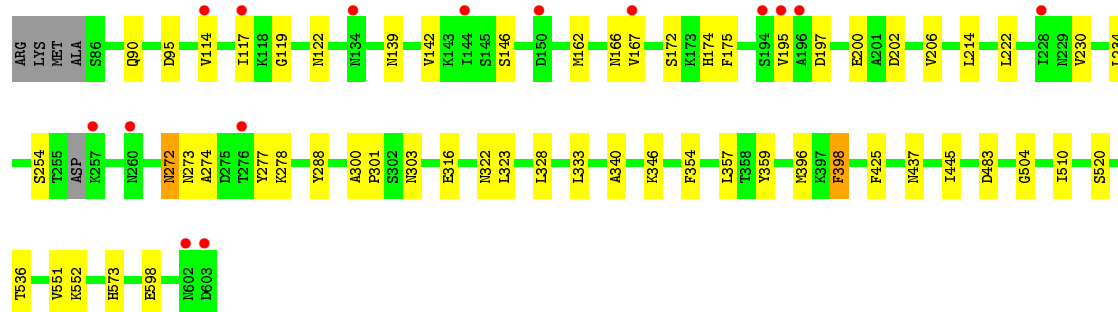
- Molecule 1: Probable M17 family aminopeptidase

Chain G: 93% 6%

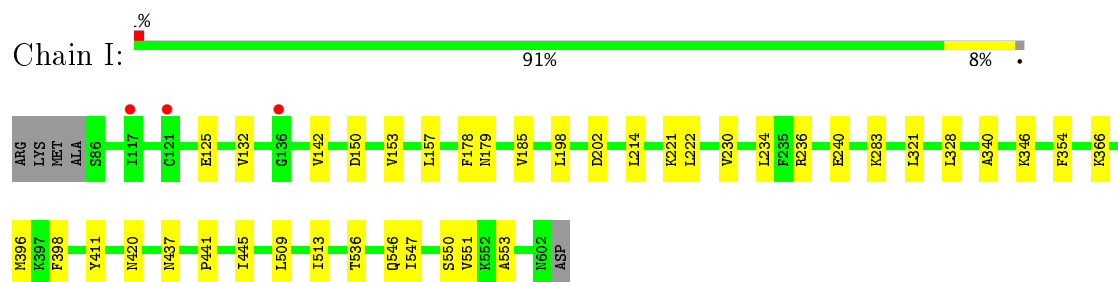


- Molecule 1: Probable M17 family aminopeptidase

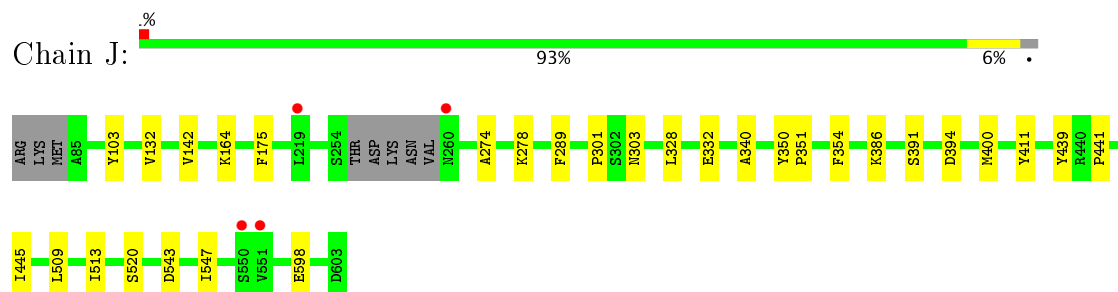
Chain H: 88% 11%



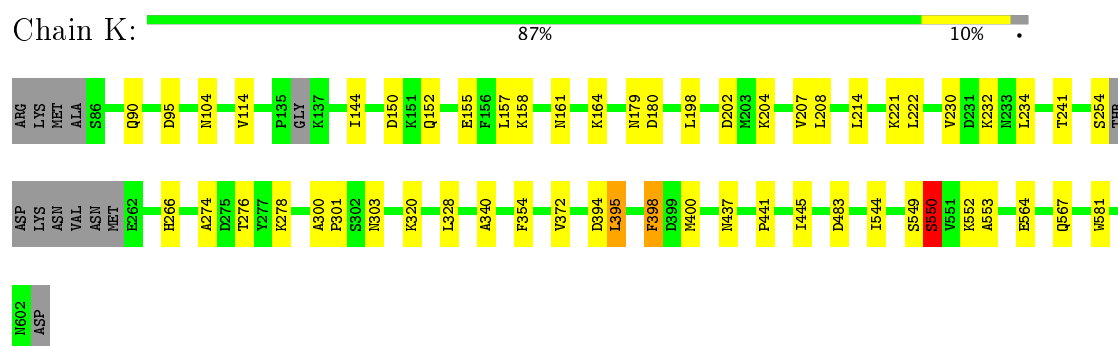
- Molecule 1: Probable M17 family aminopeptidase



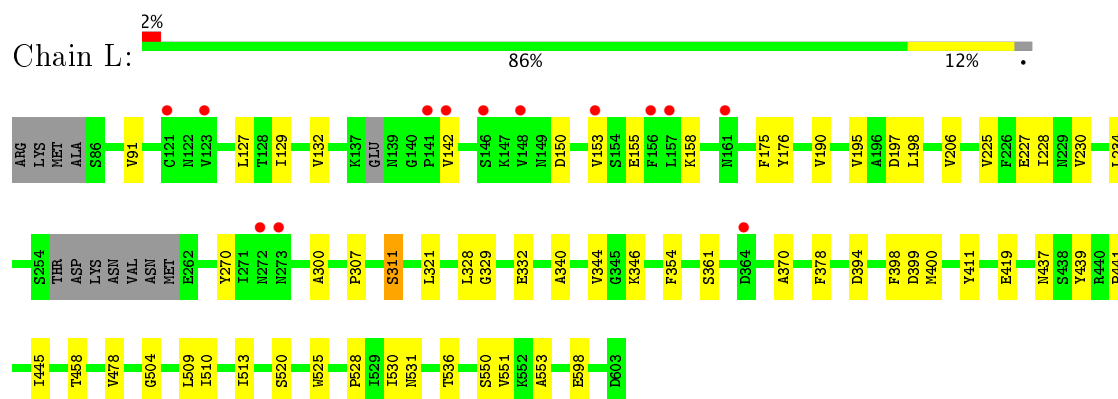
- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.10Å 177.32Å 229.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.50 48.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.90-2.50) 82.3 (48.90-2.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, R_{free}	0.203 , 0.257 0.205 , 0.254	Depositor DCC
R_{free} test set	11527 reflections (6.03%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49124	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 44.45 % 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 1.5228e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CO3, 4U5, SO4, 1PE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/4047	0.38	0/5491
1	B	0.23	0/3986	0.40	0/5414
1	C	0.22	0/4023	0.37	0/5458
1	D	0.22	0/4011	0.38	0/5439
1	E	0.21	0/3965	0.38	0/5376
1	F	0.23	0/3914	0.40	0/5323
1	G	0.22	0/4049	0.39	0/5497
1	H	0.24	0/3981	0.39	0/5411
1	I	0.22	0/4022	0.38	0/5459
1	J	0.22	0/3991	0.39	0/5416
1	K	0.22	0/3966	0.39	0/5381
1	L	0.23	0/3916	0.40	0/5327
All	All	0.22	0/47871	0.39	0/64992

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	3970	0	3881	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3909	0	3794	37	0
1	C	3946	0	3853	24	0
1	D	3934	0	3873	34	0
1	E	3890	0	3817	16	0
1	F	3837	0	3692	23	0
1	G	3971	0	3876	24	0
1	H	3904	0	3773	33	0
1	I	3944	0	3857	21	0
1	J	3914	0	3833	17	0
1	K	3890	0	3807	39	0
1	L	3840	0	3699	39	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	1	0
2	E	24	0	0	0	0
2	F	24	0	0	0	0
2	G	24	0	0	0	0
2	H	24	0	0	0	0
2	I	24	0	0	0	0
2	J	24	0	0	0	0
2	K	24	0	0	0	0
2	L	24	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	0	0
4	D	4	0	0	1	0
4	E	4	0	0	1	0
4	F	4	0	0	0	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	15	0	0	3	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	10	0	0	0	0
5	I	10	0	0	0	0
5	J	10	0	0	0	0
5	K	20	0	0	1	0
5	L	15	0	0	0	0
6	A	21	0	22	1	0
6	B	20	0	20	2	0
6	C	22	0	24	0	0
6	D	20	0	20	2	0
6	E	24	0	28	0	0
6	F	10	0	13	0	0
6	G	21	0	20	1	0
6	H	10	0	10	1	0
6	I	23	0	26	0	0
6	J	21	0	26	1	0
6	K	24	0	28	2	0
6	L	28	0	34	3	0
7	G	6	0	8	0	0
8	A	110	0	0	3	1
8	B	114	0	0	2	0
8	C	121	0	0	0	0
8	D	138	0	0	1	0
8	E	129	0	0	1	0
8	F	106	0	0	2	0
8	G	116	0	0	2	1
8	H	125	0	0	3	0
8	I	138	0	0	0	0
8	J	106	0	0	0	0
8	K	140	0	0	1	0
8	L	102	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49124	0	46034	307	1

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 (307) 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:328:LEU:HB2	1:K:354:PHE:HB3	1.62	0.80
1:G:551:VAL:HG21	1:G:557:VAL:HG21	1.65	0.79
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.70	0.73
1:L:531:ASN:H	6:L:1008:1PE:H251	1.55	0.72
1:H:117:ILE:HD11	1:H:146:SER:OG	1.90	0.71
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.73	0.69
1:L:329:GLY:N	1:L:332:GLU:OE1	2.25	0.69
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.74	0.67
1:H:139:ASN:HB3	1:H:166:ASN:HD22	1.60	0.67
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.77	0.66
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.79	0.65
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.78	0.65
1:A:200:GLU:HG3	1:A:521:ASN:HB3	1.79	0.64
1:H:322:ASN:ND2	8:H:1103:HOH:O	2.30	0.64
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.80	0.64
1:A:396:MET:SD	1:A:398:PHE:HE2	2.21	0.64
1:B:122:ASN:HD22	1:B:122:ASN:N	1.95	0.63
5:A:1007:SO4:O2	1:B:586:ARG:NH1	2.32	0.63
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.80	0.63
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.82	0.62
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.65	0.61
1:G:173:LYS:NZ	8:G:1103:HOH:O	2.32	0.61
1:L:155:GLU:O	1:L:158:LYS:HE3	2.00	0.61
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.82	0.60
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.84	0.60
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.83	0.60
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.83	0.60
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.83	0.60
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.82	0.60
1:I:546:GLN:HG2	1:I:547:ILE:HG23	1.84	0.59
1:A:104:ASN:ND2	5:A:1005:SO4:O1	2.35	0.58
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.84	0.58
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:LYS:NZ	8:B:1104:HOH:O	2.36	0.58
1:G:550:SER:O	1:G:552:LYS:N	2.36	0.58
1:J:543:ASP:OD2	1:K:254:SER:OG	2.21	0.58
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.85	0.58
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.86	0.58
1:I:125:GLU:HG3	1:I:221:LYS:HD3	1.86	0.57
1:L:150:ASP:HB3	1:L:153:VAL:HG22	1.87	0.57
1:L:307:PRO:O	1:L:311:SER:OG	2.23	0.57
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.85	0.56
1:E:480:TYR:OH	1:E:512:LYS:NZ	2.36	0.56
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.87	0.56
1:F:138:GLU:N	1:F:139:ASN:HA	2.21	0.56
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.86	0.56
1:E:232:LYS:NZ	1:E:276:THR:O	2.30	0.56
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.87	0.56
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.87	0.56
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.88	0.55
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.87	0.55
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.89	0.55
1:A:117:ILE:HD12	1:A:270:TYR:HB3	1.87	0.54
1:K:550:SER:O	1:K:550:SER:OG	2.19	0.54
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.71	0.54
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.89	0.54
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.88	0.54
1:B:500:ALA:HB3	1:B:524:VAL:HG22	1.89	0.54
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.90	0.54
1:F:440:ARG:NH1	8:F:1105:HOH:O	2.41	0.54
1:K:552:LYS:HA	1:K:553:ALA:HB3	1.89	0.53
2:D:1001:4U5:NAO	4:D:1004:CO3:O1	2.41	0.53
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.88	0.53
1:H:272:ASN:ND2	8:H:1106:HOH:O	2.35	0.53
1:F:137:LYS:CB	1:F:140:GLY:H	2.22	0.53
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.90	0.53
1:C:209:SER:O	1:C:212:THR:OG1	2.27	0.53
1:H:90:GLN:HB3	1:H:95:ASP:HB2	1.90	0.53
1:K:232:LYS:NZ	1:K:276:THR:O	2.40	0.53
1:K:549:SER:O	1:K:550:SER:HB3	2.08	0.53
1:B:396:MET:SD	1:B:398:PHE:HE2	2.32	0.53
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.91	0.52
1:D:413:VAL:HG11	1:D:423:ILE:HD12	1.89	0.52
1:K:214:LEU:HD21	1:K:222:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.91	0.52
1:B:436:LYS:HG3	1:C:349:MET:HB3	1.91	0.52
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.90	0.52
1:A:173:LYS:NZ	8:A:1110:HOH:O	2.43	0.52
1:I:551:VAL:HG12	1:I:553:ALA:H	1.74	0.52
1:H:230:VAL:O	1:H:277:TYR:OH	2.25	0.51
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.92	0.51
1:G:218:LYS:O	1:J:164:LYS:NZ	2.42	0.51
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.92	0.51
1:K:230:VAL:HG22	1:K:234:LEU:HD23	1.93	0.51
1:B:122:ASN:ND2	1:B:122:ASN:N	2.58	0.51
1:A:285:ARG:NH2	8:A:1106:HOH:O	2.38	0.51
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.92	0.51
1:B:121:CYS:HA	1:B:270:TYR:CE2	2.45	0.51
1:C:326:LYS:HE2	1:C:328:LEU:HD11	1.92	0.50
1:E:166:ASN:ND2	8:E:1108:HOH:O	2.41	0.50
1:K:158:LYS:HE2	1:K:161:ASN:HD21	1.75	0.50
1:A:545:ASN:ND2	5:A:1007:SO4:O4	2.45	0.50
1:B:122:ASN:ND2	1:B:149:ASN:HD22	2.10	0.50
1:G:509:LEU:O	1:G:513:ILE:HG12	2.12	0.50
1:K:207:VAL:HG11	1:K:241:THR:HG22	1.94	0.50
1:L:361:SER:OG	1:L:419:GLU:HA	2.12	0.50
1:D:396:MET:SD	1:D:398:PHE:HE2	2.35	0.49
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.93	0.49
1:I:132:VAL:HG21	1:I:142:VAL:HG13	1.94	0.49
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.95	0.49
1:G:396:MET:SD	1:G:398:PHE:HE2	2.35	0.49
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.93	0.49
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.95	0.49
1:K:204:LYS:NZ	8:K:1110:HOH:O	2.46	0.48
1:B:114:VAL:HG12	1:B:274:ALA:HB1	1.96	0.48
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.13	0.48
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.95	0.48
1:B:320:LYS:HB3	6:B:1006:1PE:H131	1.95	0.48
1:L:127:LEU:HD11	1:L:129:ILE:HD11	1.96	0.48
1:L:198:LEU:HD12	1:L:228:ILE:HD12	1.94	0.48
1:H:316:GLU:HG3	6:H:1007:1PE:H242	1.95	0.48
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.78	0.48
1:K:230:VAL:HG13	1:K:234:LEU:HB3	1.94	0.48
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.46	0.48
1:C:520:SER:HB3	1:C:598:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ASN:OD1	1:D:124:GLU:HG3	2.14	0.48
1:J:274:ALA:O	1:J:278:LYS:HG3	2.14	0.48
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.96	0.47
1:B:150:ASP:OD1	1:B:179:ASN:HB2	2.14	0.47
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.95	0.47
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.97	0.47
1:E:214:LEU:HD21	1:E:222:LEU:HD22	1.95	0.47
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.96	0.47
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.97	0.47
1:L:530:ILE:HG23	6:L:1008:1PE:H141	1.95	0.47
1:F:370:ALA:HB2	1:F:478:VAL:HG11	1.95	0.47
1:K:301:PRO:HB2	1:K:303:ASN:OD1	2.14	0.47
1:C:392:MET:HE1	1:C:583:PHE:HE2	1.79	0.47
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.49	0.47
1:E:435:SER:OG	1:E:436:LYS:N	2.47	0.47
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.97	0.47
1:D:275:ASP:HA	1:D:278:LYS:HD2	1.96	0.47
1:D:316:GLU:HG3	6:D:1007:1PE:H221	1.97	0.47
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.97	0.47
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.97	0.47
1:K:398:PHE:C	1:K:400:MET:H	2.18	0.47
1:L:536:THR:HG21	1:L:551:VAL:HG21	1.97	0.46
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.50	0.46
1:F:361:SER:HB2	1:F:421:VAL:H	1.80	0.46
1:B:449:ASN:HD21	1:B:451:LYS:HD2	1.81	0.46
1:H:504:GLY:HA3	1:H:510:ILE:HD11	1.98	0.46
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.96	0.46
1:A:320:LYS:HZ1	6:A:1009:1PE:H152	1.80	0.46
1:B:205:ARG:NH1	8:B:1106:HOH:O	2.42	0.46
1:F:435:SER:OG	1:F:436:LYS:N	2.49	0.46
1:G:503:PHE:O	1:G:573:HIS:N	2.42	0.46
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.97	0.46
1:H:272:ASN:H	1:H:272:ASN:HD22	1.63	0.46
1:D:230:VAL:HG12	1:D:234:LEU:HD23	1.98	0.45
1:F:90:GLN:NE2	1:F:95:ASP:O	2.46	0.45
1:H:122:ASN:ND2	8:H:1117:HOH:O	2.49	0.45
1:A:551:VAL:HG12	1:A:553:ALA:H	1.81	0.45
1:B:300:ALA:HA	1:B:301:PRO:HD3	1.85	0.45
1:C:386:LYS:HB3	1:C:391:SER:HB2	1.98	0.45
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.98	0.45
1:I:236:ARG:NE	1:I:240:GLU:OE2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.97	0.45
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.98	0.45
1:B:144:ILE:HD13	1:B:162:MET:HG3	1.98	0.45
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.98	0.45
1:I:536:THR:HG21	1:I:551:VAL:HG23	1.98	0.45
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.98	0.45
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.98	0.45
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.98	0.45
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.98	0.45
1:B:453:ILE:HD13	1:B:561:PHE:HZ	1.81	0.45
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.99	0.45
1:F:133:ASN:HA	1:F:167:VAL:HG21	1.98	0.45
1:D:567:GLN:OE1	1:D:567:GLN:N	2.49	0.45
1:H:396:MET:SD	1:H:398:PHE:HE2	2.40	0.45
1:I:236:ARG:HD2	1:I:283:LYS:HG2	1.99	0.45
1:B:174:HIS:HB3	1:F:175:PHE:CD1	2.52	0.45
6:G:1007:1PE:H232	6:G:1007:1PE:H242	1.63	0.45
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.86	0.45
1:K:204:LYS:HB2	1:K:204:LYS:HE3	1.76	0.45
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.99	0.44
1:C:483:ASP:OD2	1:C:573:HIS:ND1	2.42	0.44
1:H:114:VAL:HG12	1:H:274:ALA:HB1	1.99	0.44
1:H:274:ALA:O	1:H:278:LYS:HG3	2.17	0.44
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.98	0.44
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.98	0.44
1:D:320:LYS:NZ	6:D:1007:1PE:H142	2.33	0.44
1:E:372:VAL:O	1:E:483:ASP:HA	2.18	0.44
1:J:520:SER:HB3	1:J:598:GLU:HG3	2.00	0.44
1:K:437:ASN:HD22	1:L:91:VAL:HG22	1.82	0.44
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.18	0.44
1:A:536:THR:HG21	1:A:551:VAL:HG23	2.00	0.44
1:K:161:ASN:HA	1:K:164:LYS:HE3	1.99	0.44
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.00	0.43
1:B:135:PRO:HA	1:B:194:SER:O	2.18	0.43
1:H:333:LEU:HD21	1:H:354:PHE:HB2	2.00	0.43
1:K:208:LEU:HD23	1:K:208:LEU:HA	1.77	0.43
1:L:398:PHE:C	1:L:400:MET:H	2.21	0.43
1:L:225:VAL:HG22	1:L:270:TYR:HB2	2.00	0.43
1:A:161:ASN:ND2	1:D:178:PHE:HZ	2.17	0.43
1:A:544:ILE:HG12	1:A:545:ASN:H	1.84	0.43
1:C:395:LEU:O	1:C:397:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:SER:OG	1:D:436:LYS:N	2.51	0.43
1:E:386:LYS:HE3	1:E:396:MET:SD	2.58	0.43
1:I:198:LEU:HD22	1:I:202:ASP:HB3	2.00	0.43
1:K:221:LYS:HG3	1:K:266:HIS:HB2	1.99	0.43
1:G:493:TYR:HA	1:L:553:ALA:H	1.83	0.43
1:F:504:GLY:HA3	1:F:510:ILE:HD11	2.00	0.43
1:K:104:ASN:ND2	5:K:1007:SO4:O3	2.51	0.43
1:K:441:PRO:HD2	1:L:378:PHE:CZ	2.54	0.43
1:B:283:LYS:HE2	1:B:287:TYR:CZ	2.53	0.43
1:H:300:ALA:HA	1:H:301:PRO:HD3	1.89	0.43
1:D:273:ASN:O	1:D:277:TYR:HD2	2.01	0.43
1:E:463:ARG:NH2	4:E:1004:CO3:O2	2.44	0.43
1:D:436:LYS:NZ	1:E:437:ASN:OD1	2.39	0.43
1:E:441:PRO:HB2	1:F:394:ASP:HA	2.01	0.43
1:C:500:ALA:HB3	1:C:524:VAL:HG22	2.00	0.43
1:K:320:LYS:HB3	6:K:1010:1PE:H252	2.01	0.43
1:C:300:ALA:HA	1:C:301:PRO:HD3	1.84	0.43
1:D:537:LEU:HA	1:D:545:ASN:HB2	2.01	0.43
1:J:301:PRO:HB2	1:J:303:ASN:OD1	2.19	0.43
1:D:204:LYS:HE3	1:D:204:LYS:HB2	1.74	0.42
1:D:344:VAL:HA	1:D:439:TYR:CE2	2.54	0.42
1:L:346:LYS:HB3	1:L:437:ASN:O	2.19	0.42
1:D:195:VAL:HG12	1:D:197:ASP:H	1.83	0.42
1:G:520:SER:HB3	1:G:598:GLU:HG3	2.01	0.42
1:K:441:PRO:HB2	1:L:394:ASP:HA	2.01	0.42
1:L:439:TYR:OH	1:L:458:THR:O	2.36	0.42
1:B:258:ASN:OD1	1:B:260:ASN:N	2.50	0.42
1:D:386:LYS:HE3	1:D:396:MET:SD	2.60	0.42
1:I:396:MET:SD	1:I:398:PHE:HE2	2.42	0.42
1:L:509:LEU:O	1:L:513:ILE:HG12	2.19	0.42
1:A:229:ASN:ND2	8:A:1115:HOH:O	2.50	0.42
1:F:133:ASN:HB3	1:F:192:CYS:HB2	2.01	0.42
1:L:344:VAL:HA	1:L:439:TYR:CE2	2.55	0.42
1:B:117:ILE:HD11	1:B:146:SER:OG	2.20	0.42
1:C:287:TYR:CD2	1:C:594:ARG:HG2	2.54	0.42
1:D:126:GLY:HA2	1:D:219:LEU:HD13	2.02	0.42
1:D:551:VAL:HG12	1:D:552:LYS:O	2.19	0.42
1:B:460:ALA:O	1:B:546:GLN:NE2	2.52	0.42
1:F:350:TYR:HA	1:F:351:PRO:HD3	1.94	0.42
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.01	0.42
1:I:346:LYS:HB3	1:I:437:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASN:OD1	1:F:166:ASN:HB3	2.19	0.42
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.54	0.42
1:L:195:VAL:HG12	1:L:197:ASP:H	1.85	0.42
1:L:230:VAL:HG12	1:L:234:LEU:HD23	2.02	0.42
1:I:509:LEU:O	1:I:513:ILE:HG12	2.20	0.42
1:K:320:LYS:HE2	6:K:1009:1PE:H252	2.02	0.41
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.36	0.41
1:D:321:LEU:HD11	1:D:411:TYR:HA	2.02	0.41
1:G:260:ASN:N	1:G:260:ASN:OD1	2.52	0.41
1:L:370:ALA:HB2	1:L:478:VAL:HG11	2.02	0.41
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.02	0.41
1:B:480:TYR:CD1	1:B:509:LEU:HD13	2.55	0.41
1:I:366:LYS:CG	1:I:420:ASN:HB3	2.50	0.41
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.03	0.41
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.55	0.41
1:G:367:LYS:NZ	8:G:1115:HOH:O	2.53	0.41
1:H:301:PRO:HB2	1:H:303:ASN:OD1	2.20	0.41
1:I:153:VAL:O	1:I:157:LEU:HG	2.21	0.41
1:K:152:GLN:HG2	1:K:180:ASP:OD2	2.20	0.41
1:K:198:LEU:HD22	1:K:202:ASP:HB3	2.02	0.41
1:B:173:LYS:HD3	1:B:173:LYS:HA	1.93	0.41
1:F:127:LEU:HD11	1:F:129:ILE:HD11	2.02	0.41
1:H:323:LEU:HD22	1:H:359:TYR:HB2	2.02	0.41
1:L:411:TYR:HE1	6:L:1009:1PE:H261	1.85	0.41
1:A:283:LYS:HE2	1:A:287:TYR:CZ	2.56	0.41
1:E:357:LEU:HB2	1:E:425:PHE:HB2	2.03	0.41
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.85	0.41
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.55	0.41
1:G:551:VAL:HG23	1:G:552:LYS:H	1.86	0.41
1:K:372:VAL:O	1:K:483:ASP:HA	2.21	0.41
1:D:509:LEU:O	1:D:513:ILE:HG12	2.21	0.41
1:E:350:TYR:HA	1:E:351:PRO:HD3	1.93	0.41
1:H:483:ASP:OD1	1:H:573:HIS:ND1	2.35	0.41
1:J:411:TYR:HE1	6:J:1008:1PE:H252	1.85	0.41
1:J:509:LEU:O	1:J:513:ILE:HG12	2.20	0.41
1:I:150:ASP:OD1	1:I:179:ASN:HB2	2.21	0.41
1:J:103:TYR:HA	1:J:289:PHE:CZ	2.55	0.41
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.56	0.41
1:L:132:VAL:HG12	1:L:227:GLU:HB2	2.03	0.41
1:L:300:ALA:O	8:L:1101:HOH:O	2.22	0.41
1:G:551:VAL:HG23	1:G:552:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:LYS:HB3	1:D:391:SER:HB2	2.03	0.41
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.56	0.41
1:H:214:LEU:HD21	1:H:222:LEU:HD22	2.02	0.41
1:K:544:ILE:HD12	1:K:564:GLU:HG3	2.03	0.41
1:B:202:ASP:O	1:B:206:VAL:HG23	2.21	0.40
1:B:320:LYS:HE3	6:B:1007:1PE:H132	2.02	0.40
1:G:299:ALA:O	1:G:397:LYS:NZ	2.45	0.40
1:K:150:ASP:OD1	1:K:179:ASN:HB2	2.21	0.40
1:L:190:VAL:HG11	1:L:206:VAL:HG13	2.03	0.40
1:F:96:PRO:HG2	1:F:303:ASN:O	2.22	0.40
1:H:142:VAL:HG12	1:H:167:VAL:HG12	2.03	0.40
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.03	0.40
1:J:350:TYR:HA	1:J:351:PRO:HD3	1.92	0.40
1:J:547:ILE:HG13	1:J:547:ILE:H	1.78	0.40
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.87	0.40
1:K:90:GLN:NE2	1:K:95:ASP:O	2.54	0.40
1:H:346:LYS:HB3	1:H:437:ASN:O	2.21	0.40
1:J:386:LYS:HB3	1:J:391:SER:HB2	2.03	0.40
1:K:395:LEU:HD11	1:K:581:TRP:CD1	2.55	0.40
1:A:200:GLU:HG2	1:A:237:PHE:CZ	2.56	0.40
1:C:451:LYS:NZ	1:C:564:GLU:O	2.45	0.40
1:D:137:LYS:N	8:D:1105:HOH:O	2.45	0.40
1:D:579:VAL:O	1:D:589:LYS:HD2	2.22	0.40
1:F:181:ASN:ND2	8:F:1115:HOH:O	2.55	0.40
1:H:195:VAL:HG12	1:H:197:ASP:H	1.87	0.40
1:H:202:ASP:O	1:H:206:VAL:HG23	2.21	0.40
1:K:274:ALA:O	1:K:278:LYS:HG3	2.22	0.40
1:K:395:LEU:HD23	1:K:398:PHE:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1106:HOH:O	8:G:1104:HOH:O[2_685]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/522 (98%)	499 (97%)	14 (3%)	1 (0%)	51	73
1	B	512/522 (98%)	493 (96%)	13 (2%)	6 (1%)	15	27
1	C	512/522 (98%)	498 (97%)	13 (2%)	1 (0%)	51	73
1	D	510/522 (98%)	490 (96%)	18 (4%)	2 (0%)	38	59
1	E	500/522 (96%)	486 (97%)	13 (3%)	1 (0%)	51	73
1	F	507/522 (97%)	488 (96%)	15 (3%)	4 (1%)	22	39
1	G	517/522 (99%)	500 (97%)	15 (3%)	2 (0%)	38	59
1	H	513/522 (98%)	495 (96%)	14 (3%)	4 (1%)	22	39
1	I	515/522 (99%)	498 (97%)	16 (3%)	1 (0%)	51	73
1	J	510/522 (98%)	495 (97%)	15 (3%)	0	100	100
1	K	503/522 (96%)	486 (97%)	16 (3%)	1 (0%)	51	73
1	L	504/522 (97%)	480 (95%)	22 (4%)	2 (0%)	38	59
All	All	6117/6264 (98%)	5908 (97%)	184 (3%)	25 (0%)	38	59

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	550	SER
1	G	551	VAL
1	K	550	SER
1	B	550	SER
1	B	552	LYS
1	C	396	MET
1	H	273	ASN
1	I	550	SER
1	E	552	LYS
1	F	552	LYS
1	H	552	LYS
1	A	396	MET

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Mol	Chain	Res	Type
1	D	396	MET
1	D	552	LYS
1	H	119	GLY
1	H	254	SER
1	B	138	GLU
1	B	149	ASN
1	B	254	SER
1	B	396	MET
1	F	396	MET
1	F	551	VAL
1	L	550	SER
1	G	396	MET
1	L	399	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/450 (94%)	420 (100%)	2 (0%)	91	97
1	B	408/450 (91%)	407 (100%)	1 (0%)	94	98
1	C	418/450 (93%)	418 (100%)	0	100	100
1	D	418/450 (93%)	415 (99%)	3 (1%)	87	96
1	E	413/450 (92%)	412 (100%)	1 (0%)	94	98
1	F	396/450 (88%)	394 (100%)	2 (0%)	91	97
1	G	422/450 (94%)	422 (100%)	0	100	100
1	H	407/450 (90%)	402 (99%)	5 (1%)	75	91
1	I	418/450 (93%)	417 (100%)	1 (0%)	94	98
1	J	414/450 (92%)	411 (99%)	3 (1%)	87	96
1	K	413/450 (92%)	409 (99%)	4 (1%)	80	93
1	L	401/450 (89%)	400 (100%)	1 (0%)	94	98
All	All	4950/5400 (92%)	4927 (100%)	23 (0%)	91	97

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	398	PHE
1	B	122	ASN
1	D	172	SER
1	D	197	ASP
1	D	398	PHE
1	E	143	LYS
1	F	200	GLU
1	F	600	VAL
1	H	172	SER
1	H	200	GLU
1	H	272	ASN
1	H	288	TYR
1	H	398	PHE
1	I	185	VAL
1	J	332	GLU
1	J	400	MET
1	J	439	TYR
1	K	395	LEU
1	K	398	PHE
1	K	550	SER
1	K	567	GLN
1	L	311	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	ASN
1	F	104	ASN
1	H	166	ASN
1	H	272	ASN
1	K	161	ASN
1	K	437	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 97 ligands modelled in this entry, 24 are monoatomic - leaving 73 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	4U5	A	1001	3	23,25,25	2.15	3 (13%)	29,36,36	1.09	2 (6%)
4	CO3	A	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	A	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	A	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	A	1007	-	4,4,4	0.14	0	6,6,6	0.06	0
6	1PE	A	1008	-	8,8,15	0.53	0	7,7,14	0.41	0
6	1PE	A	1009	-	11,11,15	0.63	0	10,10,14	0.40	0
2	4U5	B	1001	3	23,25,25	2.15	3 (13%)	29,36,36	1.19	1 (3%)
4	CO3	B	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	B	1005	-	4,4,4	0.13	0	6,6,6	0.08	0
6	1PE	B	1006	-	9,9,15	0.53	0	8,8,14	0.38	0
6	1PE	B	1007	-	9,9,15	0.56	0	8,8,14	0.33	0
2	4U5	C	1001	3	23,25,25	2.19	4 (17%)	29,36,36	1.14	2 (6%)
4	CO3	C	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	C	1005	-	4,4,4	0.16	0	6,6,6	0.05	0
6	1PE	C	1006	-	12,12,15	0.64	0	11,11,14	0.41	0
6	1PE	C	1007	-	8,8,15	0.53	0	7,7,14	0.39	0
2	4U5	D	1001	3	23,25,25	2.22	4 (17%)	29,36,36	1.14	2 (6%)
4	CO3	D	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	D	1005	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1006	-	4,4,4	0.16	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	D	1007	-	9,9,15	0.55	0	8,8,14	0.36	0
6	1PE	D	1008	-	9,9,15	0.54	0	8,8,14	0.36	0
2	4U5	E	1001	3	23,25,25	2.18	3 (13%)	29,36,36	1.22	2 (6%)
4	CO3	E	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	E	1005	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	E	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
6	1PE	E	1007	-	11,11,15	0.59	0	10,10,14	0.44	0
6	1PE	E	1008	-	11,11,15	0.58	0	10,10,14	0.51	0
2	4U5	F	1001	3	23,25,25	2.21	4 (17%)	29,36,36	1.11	2 (6%)
4	CO3	F	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	F	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
6	1PE	F	1006	-	9,9,15	0.91	0	8,8,14	0.42	0
2	4U5	G	1001	3	23,25,25	2.19	4 (17%)	29,36,36	1.13	3 (10%)
4	CO3	G	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	G	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
7	GOL	G	1006	-	5,5,5	0.33	0	5,5,5	0.33	0
6	1PE	G	1007	-	8,8,15	0.53	0	7,7,14	0.30	0
6	1PE	G	1008	-	5,5,15	0.67	0	4,4,14	0.54	0
6	1PE	G	1009	-	5,5,15	0.67	0	4,4,14	0.45	0
2	4U5	H	1001	3	23,25,25	2.17	3 (13%)	29,36,36	1.22	2 (6%)
4	CO3	H	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	H	1005	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	H	1006	-	4,4,4	0.15	0	6,6,6	0.06	0
6	1PE	H	1007	-	9,9,15	0.54	0	8,8,14	0.42	0
2	4U5	I	1001	3	23,25,25	2.23	4 (17%)	29,36,36	1.09	2 (6%)
4	CO3	I	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	I	1005	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	I	1006	-	4,4,4	0.15	0	6,6,6	0.05	0
6	1PE	I	1007	-	11,11,15	0.58	0	10,10,14	0.43	0
6	1PE	I	1008	-	10,10,15	0.56	0	9,9,14	0.38	0
2	4U5	J	1001	3	23,25,25	2.18	4 (17%)	29,36,36	1.15	2 (6%)
4	CO3	J	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	J	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	J	1006	-	4,4,4	0.14	0	6,6,6	0.08	0
6	1PE	J	1007	-	10,10,15	0.88	0	9,9,14	0.34	0
6	1PE	J	1008	-	9,9,15	0.90	0	8,8,14	0.43	0
2	4U5	K	1001	3	23,25,25	2.19	4 (17%)	29,36,36	1.18	2 (6%)
4	CO3	K	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	K	1005	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	K	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1007	-	4,4,4	0.15	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	K	1008	-	4,4,4	0.15	0	6,6,6	0.05	0
6	1PE	K	1009	-	11,11,15	0.59	0	10,10,14	0.46	0
6	1PE	K	1010	-	11,11,15	0.59	0	10,10,14	0.38	0
2	4U5	L	1001	3	23,25,25	2.23	4 (17%)	29,36,36	1.08	2 (6%)
4	CO3	L	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	L	1005	-	4,4,4	0.16	0	6,6,6	0.06	0
5	SO4	L	1006	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	L	1007	-	4,4,4	0.15	0	6,6,6	0.08	0
6	1PE	L	1008	-	6,6,15	0.60	0	5,5,14	0.51	0
6	1PE	L	1009	-	9,9,15	0.91	0	8,8,14	0.42	0
6	1PE	L	1010	-	10,10,15	0.86	0	9,9,14	0.41	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	4U5	A	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	A	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
6	1PE	A	1008	-	-	0/6/6/13	0/0/0/0
6	1PE	A	1009	-	-	0/9/9/13	0/0/0/0
2	4U5	B	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	B	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	B	1006	-	-	0/7/7/13	0/0/0/0
6	1PE	B	1007	-	-	0/7/7/13	0/0/0/0
2	4U5	C	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	C	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	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	4U5	D	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	D	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	D	1007	-	-	0/7/7/13	0/0/0/0
6	1PE	D	1008	-	-	0/7/7/13	0/0/0/0
2	4U5	E	1001	3	-	0/24/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CO3	E	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	E	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	E	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	E	1007	-	-	0/9/9/13	0/0/0/0
6	1PE	E	1008	-	-	0/9/9/13	0/0/0/0
2	4U5	F	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	F	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	F	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	F	1006	-	-	0/7/7/13	0/0/0/0
2	4U5	G	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	G	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	G	1005	-	-	0/0/0/0	0/0/0/0
7	GOL	G	1006	-	-	0/4/4/4	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
2	4U5	H	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	H	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	H	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	H	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	H	1007	-	-	0/7/7/13	0/0/0/0
2	4U5	I	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	I	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	I	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	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
2	4U5	J	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	J	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	J	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	J	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	J	1007	-	-	0/8/8/13	0/0/0/0
6	1PE	J	1008	-	-	0/7/7/13	0/0/0/0
2	4U5	K	1001	3	-	0/24/24/24	0/2/2/2
4	CO3	K	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	K	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	K	1006	-	-	0/0/0/0	0/0/0/0
5	SO4	K	1007	-	-	0/0/0/0	0/0/0/0
5	SO4	K	1008	-	-	0/0/0/0	0/0/0/0
6	1PE	K	1009	-	-	0/9/9/13	0/0/0/0
6	1PE	K	1010	-	-	0/9/9/13	0/0/0/0
2	4U5	L	1001	3	-	0/24/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CO3	L	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	L	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	L	1006	-	-	0/0/0/0	0/0/0/0
5	SO4	L	1007	-	-	0/0/0/0	0/0/0/0
6	1PE	L	1008	-	-	0/4/4/13	0/0/0/0
6	1PE	L	1009	-	-	0/7/7/13	0/0/0/0
6	1PE	L	1010	-	-	0/8/8/13	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	4U5	CAU-CA	-7.55	1.40	1.52
2	D	1001	4U5	CAU-CA	-7.54	1.40	1.52
2	L	1001	4U5	CAU-CA	-7.53	1.40	1.52
2	K	1001	4U5	CAU-CA	-7.51	1.40	1.52
2	E	1001	4U5	CAU-CA	-7.51	1.40	1.52
2	I	1001	4U5	CAU-CA	-7.49	1.40	1.52
2	H	1001	4U5	CAU-CA	-7.48	1.40	1.52
2	J	1001	4U5	CAU-CA	-7.42	1.40	1.52
2	G	1001	4U5	CAU-CA	-7.40	1.40	1.52
2	C	1001	4U5	CAU-CA	-7.37	1.40	1.52
2	B	1001	4U5	CAU-CA	-7.31	1.40	1.52
2	A	1001	4U5	CAU-CA	-7.31	1.40	1.52
2	E	1001	4U5	CAS-CAT	-6.02	1.33	1.49
2	F	1001	4U5	CAS-CAT	-5.99	1.33	1.49
2	H	1001	4U5	CAS-CAT	-5.99	1.33	1.49
2	I	1001	4U5	CAS-CAT	-5.98	1.33	1.49
2	D	1001	4U5	CAS-CAT	-5.98	1.33	1.49
2	J	1001	4U5	CAS-CAT	-5.97	1.33	1.49
2	K	1001	4U5	CAS-CAT	-5.97	1.33	1.49
2	G	1001	4U5	CAS-CAT	-5.97	1.33	1.49
2	B	1001	4U5	CAS-CAT	-5.96	1.33	1.49
2	L	1001	4U5	CAS-CAT	-5.95	1.33	1.49
2	C	1001	4U5	CAS-CAT	-5.94	1.33	1.49
2	A	1001	4U5	CAS-CAT	-5.91	1.33	1.49
2	E	1001	4U5	CAM-CAT	-2.71	1.32	1.38
2	G	1001	4U5	CAM-CAT	-2.71	1.32	1.38
2	D	1001	4U5	CAM-CAT	-2.70	1.32	1.38
2	L	1001	4U5	CAM-CAT	-2.69	1.32	1.38
2	K	1001	4U5	CAM-CAT	-2.68	1.32	1.38
2	J	1001	4U5	CAM-CAT	-2.67	1.32	1.38
2	C	1001	4U5	CAM-CAT	-2.66	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1001	4U5	CAM-CAT	-2.66	1.32	1.38
2	F	1001	4U5	CAM-CAT	-2.66	1.32	1.38
2	B	1001	4U5	CAM-CAT	-2.66	1.32	1.38
2	A	1001	4U5	CAM-CAT	-2.64	1.32	1.38
2	H	1001	4U5	CAM-CAT	-2.62	1.33	1.38
2	K	1001	4U5	OAG-NAO	2.09	1.43	1.39
2	G	1001	4U5	OAG-NAO	2.27	1.43	1.39
2	J	1001	4U5	OAG-NAO	2.32	1.43	1.39
2	F	1001	4U5	OAG-NAO	2.47	1.44	1.39
2	C	1001	4U5	OAG-NAO	2.65	1.44	1.39
2	D	1001	4U5	OAG-NAO	2.74	1.44	1.39
2	L	1001	4U5	OAG-NAO	2.89	1.44	1.39
2	I	1001	4U5	OAG-NAO	2.95	1.45	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1001	4U5	CAX-CAR-N	-2.55	114.59	117.82
2	J	1001	4U5	CAX-CAR-N	-2.53	114.62	117.82
2	A	1001	4U5	CAX-CAR-N	-2.50	114.66	117.82
2	F	1001	4U5	CAX-CAR-N	-2.39	114.80	117.82
2	C	1001	4U5	CAX-CAR-N	-2.33	114.87	117.82
2	E	1001	4U5	CAX-CAR-N	-2.33	114.87	117.82
2	L	1001	4U5	CAX-CAR-N	-2.29	114.92	117.82
2	D	1001	4U5	CAX-CAR-N	-2.23	114.99	117.82
2	G	1001	4U5	CAX-CAR-N	-2.14	115.11	117.82
2	H	1001	4U5	CAX-CAR-N	-2.11	115.15	117.82
2	K	1001	4U5	CAX-CAR-N	-2.08	115.18	117.82
2	G	1001	4U5	CAU-CA-C	2.01	112.52	108.01
2	A	1001	4U5	CAA-NAW-NAN	3.40	124.48	120.59
2	I	1001	4U5	CAA-NAW-NAN	3.46	124.55	120.59
2	F	1001	4U5	CAA-NAW-NAN	3.55	124.64	120.59
2	L	1001	4U5	CAA-NAW-NAN	3.63	124.74	120.59
2	G	1001	4U5	CAA-NAW-NAN	3.79	124.92	120.59
2	C	1001	4U5	CAA-NAW-NAN	3.81	124.94	120.59
2	J	1001	4U5	CAA-NAW-NAN	3.83	124.96	120.59
2	B	1001	4U5	CAA-NAW-NAN	3.93	125.08	120.59
2	D	1001	4U5	CAA-NAW-NAN	3.96	125.12	120.59
2	H	1001	4U5	CAA-NAW-NAN	3.97	125.13	120.59
2	K	1001	4U5	CAA-NAW-NAN	4.05	125.22	120.59
2	E	1001	4U5	CAA-NAW-NAN	4.10	125.28	120.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	SO4	1	0
5	A	1007	SO4	2	0
6	A	1009	1PE	1	0
6	B	1006	1PE	1	0
6	B	1007	1PE	1	0
2	D	1001	4U5	1	0
4	D	1004	CO3	1	0
6	D	1007	1PE	2	0
4	E	1004	CO3	1	0
6	G	1007	1PE	1	0
6	H	1007	1PE	1	0
6	J	1008	1PE	1	0
5	K	1007	SO4	1	0
6	K	1009	1PE	1	0
6	K	1010	1PE	1	0
6	L	1008	1PE	2	0
6	L	1009	1PE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/522 (99%)	-0.30	2 (0%) 92 92	16, 32, 57, 96	1 (0%)
1	B	516/522 (98%)	-0.12	14 (2%) 55 58	20, 35, 71, 104	0
1	C	516/522 (98%)	-0.30	2 (0%) 92 92	18, 33, 65, 106	4 (0%)
1	D	514/522 (98%)	-0.41	4 (0%) 86 86	19, 31, 54, 88	5 (0%)
1	E	508/522 (97%)	-0.46	1 (0%) 94 95	19, 32, 47, 80	2 (0%)
1	F	511/522 (97%)	-0.26	6 (1%) 79 80	21, 35, 65, 97	3 (0%)
1	G	519/522 (99%)	-0.31	3 (0%) 89 89	19, 32, 61, 113	3 (0%)
1	H	517/522 (99%)	-0.12	15 (2%) 52 55	18, 35, 75, 98	3 (0%)
1	I	517/522 (99%)	-0.29	3 (0%) 89 89	19, 32, 61, 77	2 (0%)
1	J	514/522 (98%)	-0.43	4 (0%) 86 86	17, 31, 52, 86	6 (1%)
1	K	509/522 (97%)	-0.45	0 100 100	20, 31, 46, 88	3 (0%)
1	L	510/522 (97%)	-0.18	13 (2%) 58 60	22, 39, 70, 88	5 (0%)
All	All	6169/6264 (98%)	-0.30	67 (1%) 80 81	16, 33, 64, 113	37 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	ASN	4.8
1	F	551	VAL	4.5
1	B	255	THR	4.0
1	L	121	CYS	3.8
1	H	117	ILE	3.6
1	L	148	VAL	3.6
1	B	183	ASN	3.4
1	L	146	SER	3.3
1	J	260	ASN	3.2
1	G	136	GLY	3.2
1	I	117	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	121	CYS	3.0
1	F	138	GLU	3.0
1	L	157	LEU	2.9
1	F	145	SER	2.9
1	B	257	LYS	2.9
1	B	144	ILE	2.9
1	H	603	ASP	2.8
1	A	603	ASP	2.8
1	D	603	ASP	2.8
1	L	153	VAL	2.8
1	B	117	ILE	2.8
1	B	180	ASP	2.7
1	H	260	ASN	2.6
1	L	161	ASN	2.6
1	D	219	LEU	2.6
1	H	194	SER	2.6
1	J	550	SER	2.6
1	H	114	VAL	2.6
1	H	150	ASP	2.6
1	L	364	ASP	2.6
1	C	121	CYS	2.5
1	H	167	VAL	2.5
1	H	276	THR	2.5
1	L	123	VAL	2.5
1	B	196	ALA	2.5
1	L	156	PHE	2.5
1	H	196	ALA	2.5
1	H	195	VAL	2.5
1	G	196	ALA	2.4
1	E	549	SER	2.4
1	B	277	TYR	2.4
1	F	165	PHE	2.4
1	H	144	ILE	2.4
1	H	257	LYS	2.4
1	B	134	ASN	2.4
1	G	159	ASP	2.3
1	B	232	LYS	2.3
1	A	362	LYS	2.3
1	I	136	GLY	2.2
1	B	260	ASN	2.2
1	H	228	ILE	2.2
1	C	603	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	140	GLY	2.2
1	H	134	ASN	2.2
1	L	272	ASN	2.2
1	L	273	ASN	2.1
1	B	259	VAL	2.1
1	J	219	LEU	2.1
1	J	551	VAL	2.1
1	H	602	ASN	2.1
1	D	122	ASN	2.1
1	L	141	PRO	2.1
1	F	136	GLY	2.1
1	B	176	TYR	2.0
1	B	276	THR	2.0
1	L	142	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	1PE	L	1008	7/16	0.77	0.36	13.44	64,70,83,86	0
5	SO4	J	1006	5/5	0.85	0.30	7.95	103,106,107,107	0
6	1PE	G	1007	9/16	0.84	0.24	6.12	51,56,62,62	0
4	CO3	J	1004	4/4	0.97	0.16	5.43	32,32,33,36	0
5	SO4	D	1006	5/5	0.92	0.24	5.22	93,94,94,95	0
6	1PE	A	1008	9/16	0.91	0.20	4.71	42,45,49,51	0
7	GOL	G	1006	6/6	0.81	0.33	4.62	58,61,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	L	1006	5/5	0.89	0.27	4.25	104,104,105,107	0
4	CO3	G	1004	4/4	0.98	0.17	4.19	31,33,33,35	0
5	SO4	I	1006	5/5	0.94	0.23	4.17	92,92,93,93	0
6	1PE	L	1009	10/16	0.81	0.24	3.24	50,56,73,75	0
4	CO3	K	1004	4/4	0.96	0.18	3.18	32,34,34,34	0
6	1PE	J	1008	10/16	0.89	0.17	3.16	43,49,57,60	0
5	SO4	K	1008	5/5	0.90	0.18	3.13	93,96,97,97	0
6	1PE	I	1008	11/16	0.87	0.20	3.07	41,43,53,54	0
4	CO3	F	1004	4/4	0.98	0.17	3.00	21,24,26,27	0
5	SO4	K	1006	5/5	0.91	0.21	2.65	87,89,90,90	0
2	4U5	D	1001	24/24	0.94	0.18	2.29	25,37,44,47	0
6	1PE	D	1008	10/16	0.92	0.17	2.20	38,47,59,59	0
6	1PE	A	1009	12/16	0.82	0.19	2.08	52,56,62,62	0
6	1PE	B	1006	10/16	0.91	0.22	1.99	41,51,68,69	0
5	SO4	D	1005	5/5	0.92	0.19	1.77	91,93,93,94	0
6	1PE	G	1008	6/16	0.90	0.21	1.65	40,49,58,61	0
6	1PE	G	1009	6/16	0.90	0.18	1.64	45,48,49,53	0
2	4U5	E	1001	24/24	0.96	0.16	1.61	31,38,50,54	0
5	SO4	A	1006	5/5	0.93	0.18	1.39	71,75,78,79	0
5	SO4	L	1005	5/5	0.91	0.16	1.34	100,101,101,102	0
4	CO3	D	1004	4/4	0.96	0.13	1.30	33,37,38,40	0
4	CO3	L	1004	4/4	0.96	0.15	1.16	27,32,34,34	0
5	SO4	A	1007	5/5	0.89	0.20	1.11	81,82,83,87	0
4	CO3	E	1004	4/4	0.96	0.14	1.10	33,35,36,39	0
2	4U5	H	1001	24/24	0.94	0.15	1.08	25,37,42,45	0
6	1PE	C	1007	9/16	0.89	0.17	1.01	42,45,49,50	0
5	SO4	H	1006	5/5	0.91	0.17	1.00	89,91,93,93	0
4	CO3	C	1004	4/4	0.98	0.14	0.96	30,31,31,36	0
2	4U5	F	1001	24/24	0.96	0.14	0.69	30,36,45,52	0
2	4U5	J	1001	24/24	0.95	0.14	0.68	24,36,46,48	0
6	1PE	E	1008	12/16	0.91	0.14	0.54	24,39,58,58	0
2	4U5	B	1001	24/24	0.95	0.14	0.52	28,38,43,48	0
2	4U5	K	1001	24/24	0.95	0.14	0.52	25,34,38,44	0
3	ZN	D	1002	1/1	0.99	0.11	0.40	32,32,32,32	0
4	CO3	A	1004	4/4	0.98	0.13	0.33	32,35,37,37	0
6	1PE	K	1010	12/16	0.93	0.15	0.32	33,38,58,60	0
2	4U5	C	1001	24/24	0.96	0.13	0.20	22,30,35,39	0
4	CO3	B	1004	4/4	0.98	0.12	0.18	23,26,26,29	0
2	4U5	G	1001	24/24	0.96	0.14	0.01	25,36,39,41	0
2	4U5	I	1001	24/24	0.96	0.13	-0.01	22,34,40,45	0
4	CO3	H	1004	4/4	0.99	0.12	-0.10	24,26,27,27	0
5	SO4	E	1005	5/5	0.99	0.13	-0.18	30,30,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	4U5	A	1001	24/24	0.97	0.13	-0.26	26,33,42,46	0
5	SO4	I	1005	5/5	0.92	0.14	-0.31	103,104,105,105	0
3	ZN	E	1003	1/1	0.99	0.11	-0.32	30,30,30,30	0
2	4U5	L	1001	24/24	0.97	0.13	-0.32	29,38,45,48	0
3	ZN	G	1003	1/1	0.99	0.12	-0.35	27,27,27,27	0
6	1PE	F	1006	10/16	0.93	0.13	-0.38	42,44,57,59	0
5	SO4	G	1005	5/5	0.95	0.14	-0.39	79,83,84,85	0
5	SO4	K	1005	5/5	0.99	0.12	-0.41	31,32,33,33	0
3	ZN	A	1003	1/1	0.99	0.11	-0.55	26,26,26,26	0
3	ZN	E	1002	1/1	1.00	0.10	-0.77	32,32,32,32	0
3	ZN	K	1003	1/1	0.99	0.10	-0.88	31,31,31,31	0
3	ZN	L	1002	1/1	1.00	0.10	-1.28	30,30,30,30	0
3	ZN	J	1002	1/1	0.98	0.09	-1.34	31,31,31,31	0
3	ZN	K	1002	1/1	0.99	0.09	-1.52	30,30,30,30	0
3	ZN	I	1002	1/1	0.99	0.09	-1.56	30,30,30,30	0
3	ZN	I	1003	1/1	1.00	0.09	-1.61	25,25,25,25	0
5	SO4	H	1005	5/5	0.99	0.09	-1.68	24,27,29,30	0
4	CO3	I	1004	4/4	0.98	0.09	-1.78	29,35,36,37	0
5	SO4	B	1005	5/5	0.98	0.10	-1.82	24,25,30,33	0
3	ZN	F	1002	1/1	0.99	0.10	-1.87	27,27,27,27	0
3	ZN	A	1002	1/1	0.99	0.09	-2.15	31,31,31,31	0
3	ZN	L	1003	1/1	0.99	0.09	-2.23	33,33,33,33	0
3	ZN	D	1003	1/1	1.00	0.07	-2.41	25,25,25,25	0
3	ZN	C	1002	1/1	0.99	0.09	-2.60	23,23,23,23	0
3	ZN	G	1002	1/1	0.99	0.09	-2.60	32,32,32,32	0
3	ZN	F	1003	1/1	0.99	0.07	-2.85	30,30,30,30	0
3	ZN	J	1003	1/1	1.00	0.08	-2.87	25,25,25,25	0
3	ZN	C	1003	1/1	0.99	0.09	-3.09	28,28,28,28	0
3	ZN	H	1002	1/1	0.98	0.07	-3.37	30,30,30,30	0
3	ZN	B	1002	1/1	0.98	0.08	-3.65	30,30,30,30	0
3	ZN	H	1003	1/1	0.99	0.08	-4.30	23,23,23,23	0
3	ZN	B	1003	1/1	0.99	0.08	-5.33	22,22,22,22	0
6	1PE	L	1010	11/16	0.85	0.24	-	59,62,79,79	0
6	1PE	D	1007	10/16	0.87	0.17	-	36,49,56,58	0
6	1PE	J	1007	11/16	0.83	0.20	-	41,55,63,63	0
6	1PE	B	1007	10/16	0.88	0.23	-	55,70,76,76	0
6	1PE	C	1006	13/16	0.86	0.18	-	51,55,58,58	0
5	SO4	K	1007	5/5	0.97	0.16	-	68,70,72,73	0
6	1PE	H	1007	10/16	0.87	0.20	-	37,50,61,62	0
6	1PE	K	1009	12/16	0.89	0.13	-	47,49,52,52	0
5	SO4	A	1005	5/5	0.96	0.15	-	69,71,74,74	0
5	SO4	L	1007	5/5	0.95	0.14	-	72,72,73,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	C	1005	5/5	0.95	0.24	-	71,71,72,74	0
5	SO4	E	1006	5/5	0.96	0.15	-	69,70,72,74	0
5	SO4	F	1005	5/5	0.97	0.16	-	69,70,71,72	0
5	SO4	J	1005	5/5	0.95	0.23	-	84,84,85,87	0
6	1PE	E	1007	12/16	0.90	0.14	-	45,50,57,59	0
6	1PE	I	1007	12/16	0.91	0.20	-	37,53,55,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.