



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:16 PM GMT

PDB ID : 4R76  
Title : Structure of the m17 leucyl aminopeptidase from malaria complexed with a hydroxamic acid-based inhibitor  
Authors : Drinkwater, N.; McGowan, S.  
Deposited on : 2014-08-27  
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](mailto: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.

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

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

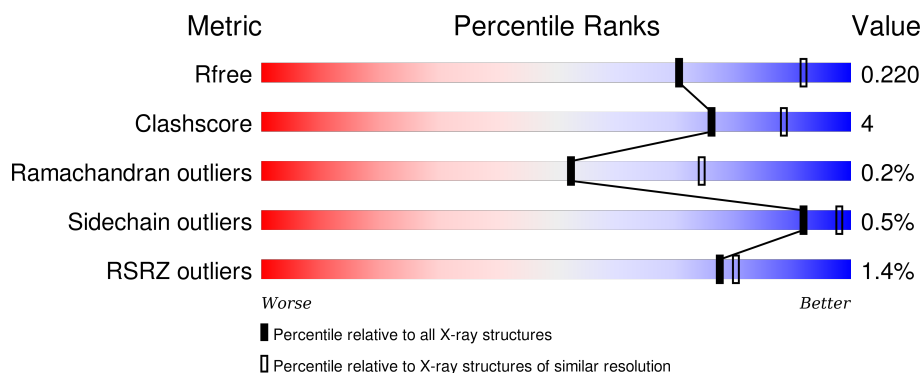
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 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	528	<div> <div>%</div> <div>88% 10% .</div> </div>
1	B	528	<div> <div>2%</div> <div>87% 10% .</div> </div>
1	C	528	<div> <div>%</div> <div>89% 9% .</div> </div>
1	D	528	<div> <div>%</div> <div>87% 10% . .</div> </div>
1	E	528	<div> <div>%</div> <div>86% 11% .</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1005	-	-	X	-
5	SO4	A	1006	-	-	-	X
6	1PE	B	1006	-	-	-	X
6	1PE	F	1006	-	-	-	X
6	1PE	F	1007	-	-	-	X
6	1PE	G	1005	-	-	-	X
6	1PE	G	1006	-	-	-	X
6	1PE	H	1006	-	-	-	X
6	1PE	K	1006	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 49162 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	1	0
			3953	2542	634	758	19			
1	B	511	Total	C	N	O	S	0	0	0
			3859	2484	625	731	19			
1	C	518	Total	C	N	O	S	0	1	0
			3961	2547	639	756	19			
1	D	514	Total	C	N	O	S	0	0	0
			3934	2533	633	748	20			
1	E	510	Total	C	N	O	S	0	0	0
			3902	2514	625	744	19			
1	F	509	Total	C	N	O	S	0	0	0
			3787	2440	611	717	19			
1	G	517	Total	C	N	O	S	0	0	0
			3973	2552	638	764	19			
1	H	515	Total	C	N	O	S	0	0	0
			3895	2504	630	742	19			
1	I	516	Total	C	N	O	S	0	0	0
			3918	2521	630	748	19			
1	J	511	Total	C	N	O	S	0	0	0
			3902	2513	629	741	19			
1	K	509	Total	C	N	O	S	0	0	0
			3894	2508	624	743	19			
1	L	510	Total	C	N	O	S	0	0	0
			3820	2455	614	732	19			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

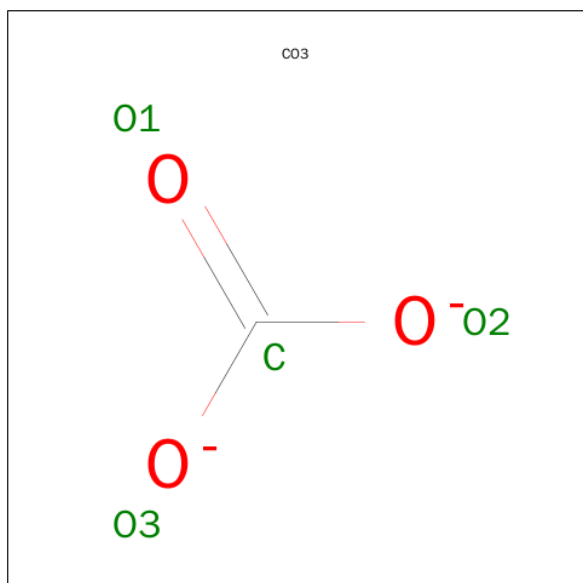
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Zn	0	0
			2	2		
2	J	2	Total	Zn	0	0
			2	2		

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



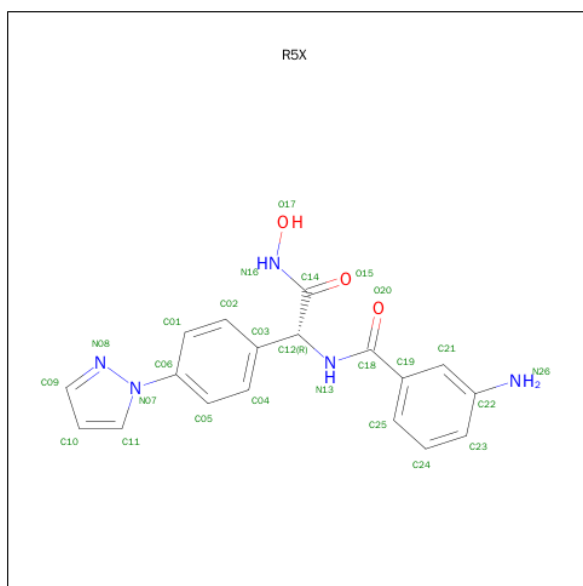
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0

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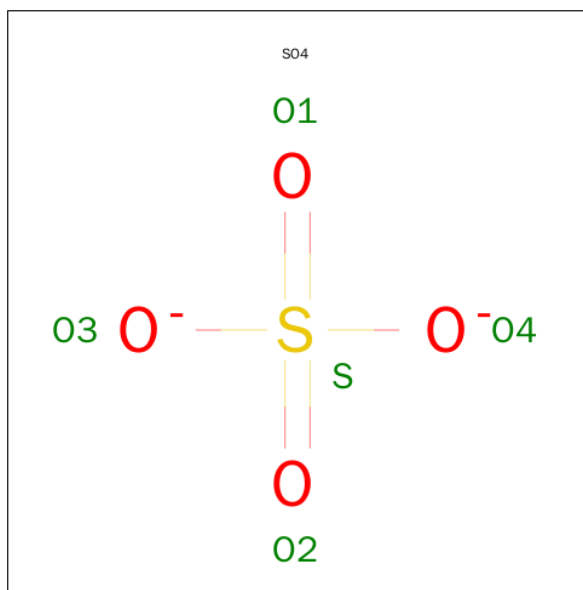
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total	C	O	0	0
			4	1	3		
3	J	1	Total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

- Molecule 4 is 3-AMINO-N-{(1R)-2-(HYDROXYAMINO)-2-OXO-1-[4-(1H-PYRAZOL-1-YL)PHENYL]ETHYL}BENZAMIDE (three-letter code: R5X) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>).



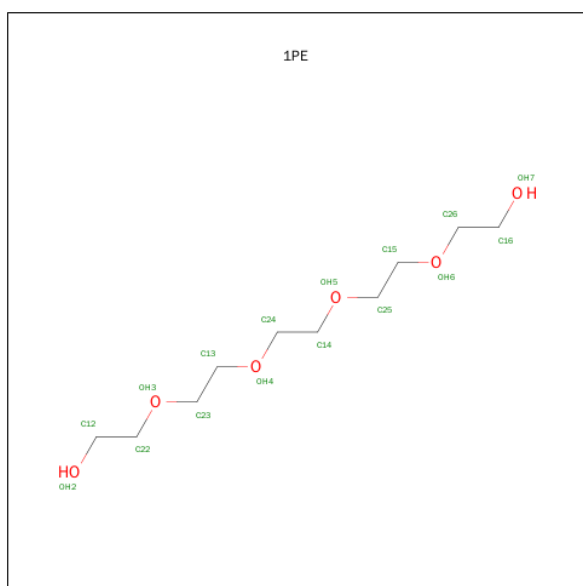
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	18	5	3		
4	B	1	Total	C	N	O	0	0
			26	18	5	3		
4	C	1	Total	C	N	O	0	0
			26	18	5	3		
4	D	1	Total	C	N	O	0	0
			26	18	5	3		
4	E	1	Total	C	N	O	0	0
			26	18	5	3		
4	F	1	Total	C	N	O	0	0
			26	18	5	3		
4	G	1	Total	C	N	O	0	0
			26	18	5	3		
4	H	1	Total	C	N	O	0	0
			26	18	5	3		
4	I	1	Total	C	N	O	0	0
			26	18	5	3		
4	J	1	Total	C	N	O	0	0
			26	18	5	3		
4	K	1	Total	C	N	O	0	0
			26	18	5	3		
4	L	1	Total	C	N	O	0	0
			26	18	5	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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	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	H	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 10 6 4	0	0
6	B	1	Total C O 9 6 3	0	0
6	E	1	Total C O 10 6 4	0	0
6	E	1	Total C O 10 7 3	0	0
6	F	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 9 6 3	0	0
6	F	1	Total C O 9 6 3	0	0
6	G	1	Total C O 13 8 5	0	0
6	G	1	Total C O 10 6 4	0	0
6	H	1	Total C O 10 7 3	0	0
6	I	1	Total C O 10 6 4	0	0
6	I	1	Total C O 11 8 3	0	0
6	J	1	Total C O 10 6 4	0	0
6	K	1	Total C O 13 8 5	0	0
6	L	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	170	Total O 170 170	0	0
7	B	125	Total O 125 125	0	0
7	C	155	Total O 155 155	0	0
7	D	174	Total O 174 174	0	0
7	E	151	Total O 151 151	0	0
7	F	119	Total O 119 119	0	0
7	G	150	Total O 150 150	0	0
7	H	133	Total O 133 133	0	0
7	I	143	Total O 143 143	0	0

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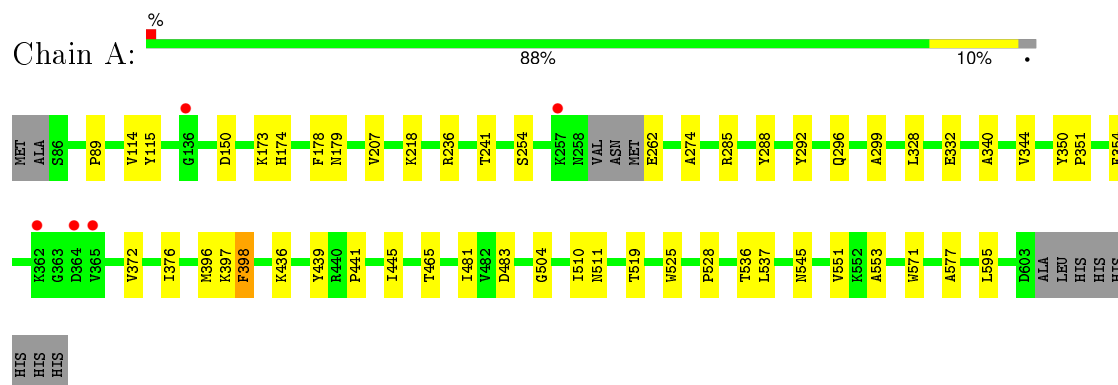
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	171	Total 171	O 171	0	0
7	K	163	Total 163	O 163	0	0
7	L	142	Total 142	O 142	0	0

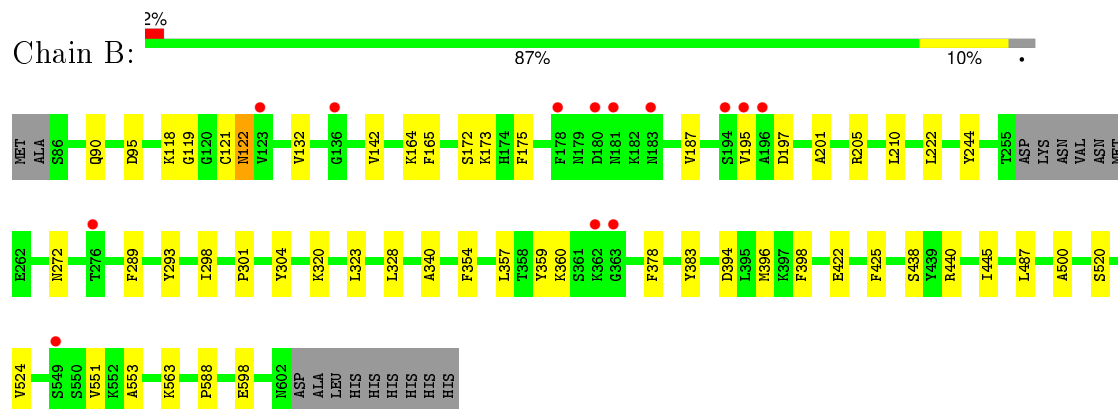
### 3 Residue-property plots

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

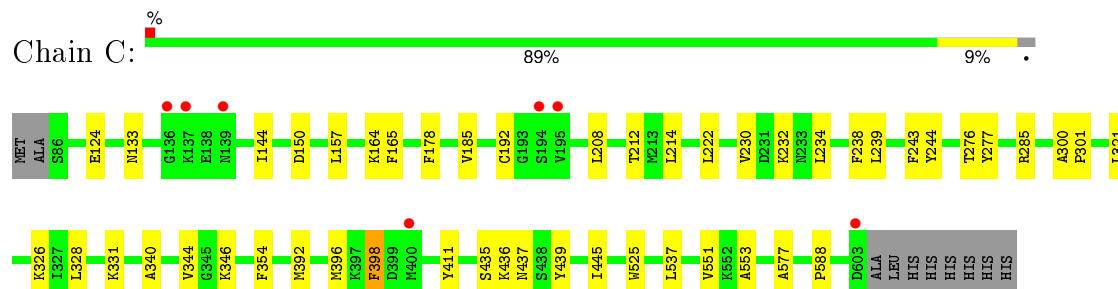
- Molecule 1: M17 family aminopeptidase



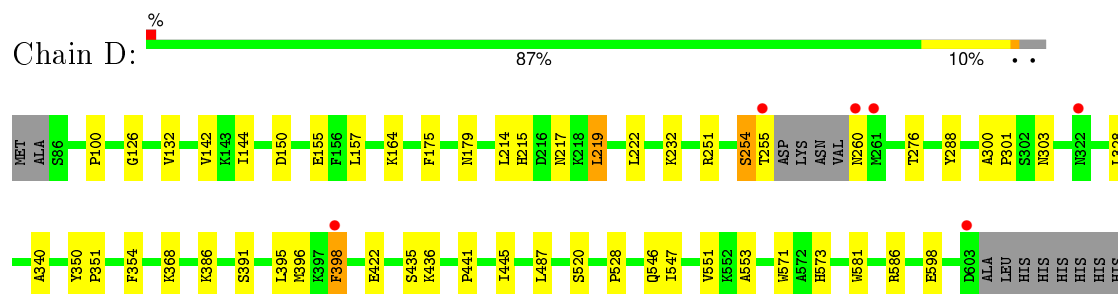
- Molecule 1: M17 family aminopeptidase



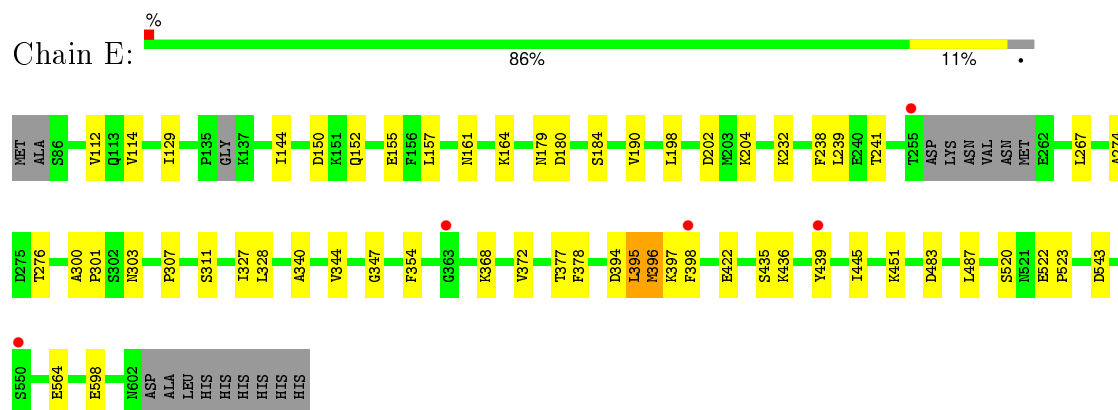
- Molecule 1: M17 family aminopeptidase



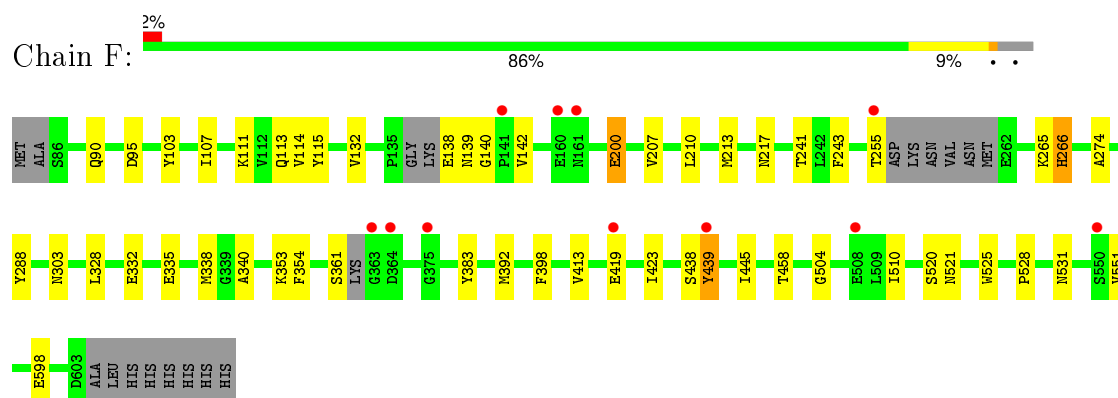
- Molecule 1: M17 family aminopeptidase



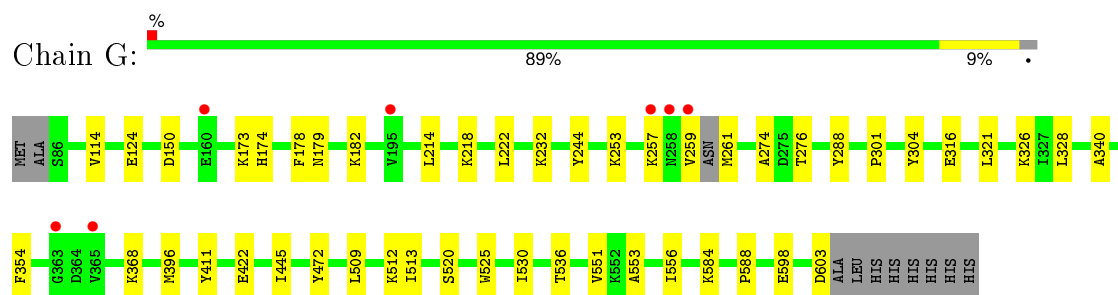
- Molecule 1: M17 family aminopeptidase



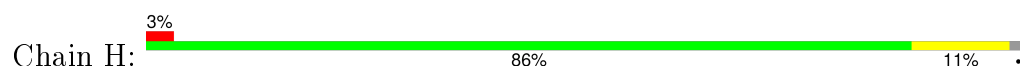
- Molecule 1: M17 family aminopeptidase

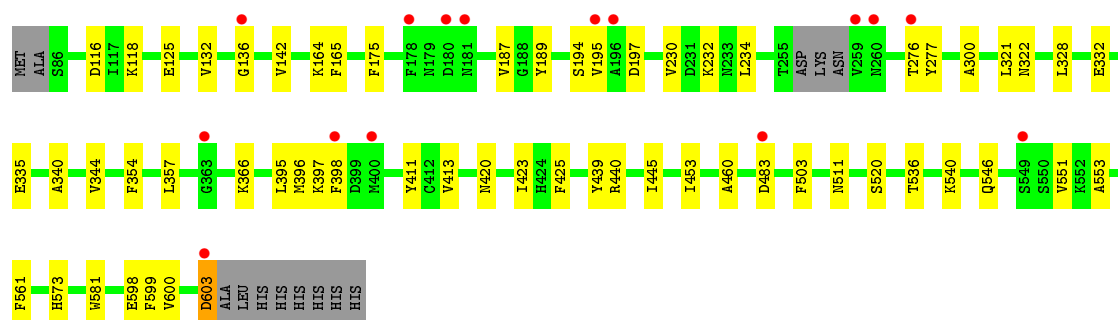


- Molecule 1: M17 family aminopeptidase

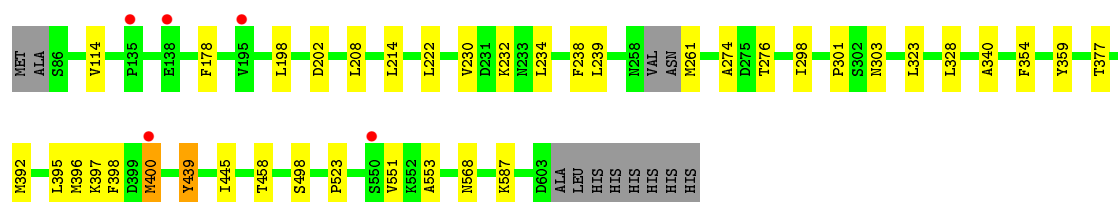
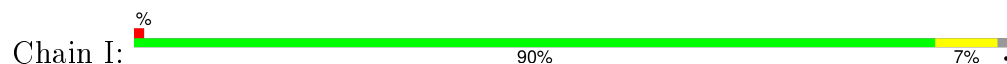


- Molecule 1: M17 family aminopeptidase

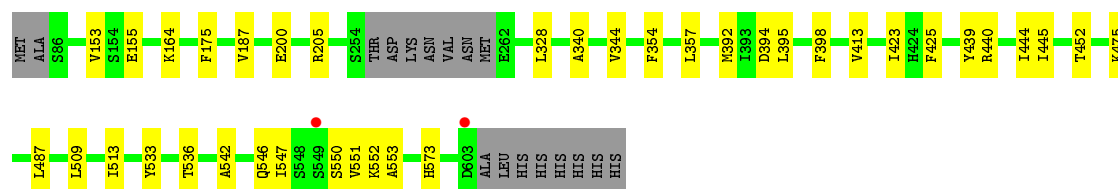




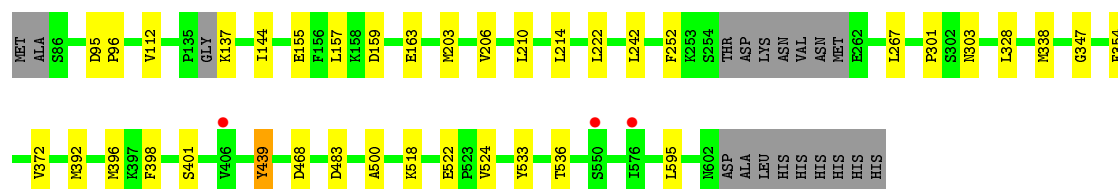
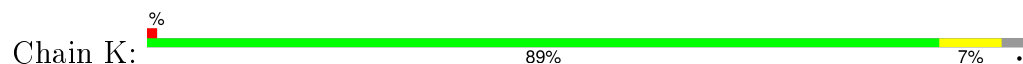
- Molecule 1: M17 family aminopeptidase



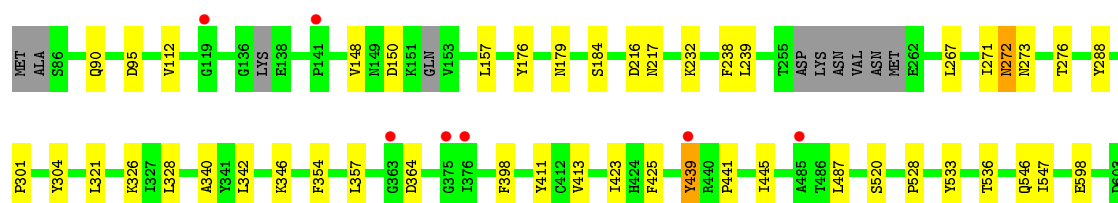
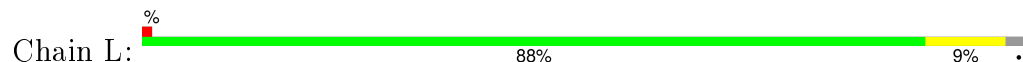
- Molecule 1: M17 family aminopeptidase



- Molecule 1: M17 family aminopeptidase



- Molecule 1: M17 family aminopeptidase



ALA
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.04Å 177.41Å 231.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.21 – 2.50 36.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.4 (36.21-2.50) 72.5 (36.21-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, $R_{free}$	0.207 , 0.248 0.209 , 0.220	Depositor DCC
$R_{free}$ test set	1839 reflections (1.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.1	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 193814 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	49162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 48.71 % 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 8.2745e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: R5X, SO4, CO3, ZN, 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	0/4033	0.39	0/5469
1	B	0.22	0/3936	0.40	0/5349
1	C	0.22	0/4042	0.39	0/5485
1	D	0.23	0/4011	0.40	0/5439
1	E	0.23	0/3978	0.41	1/5396 (0.0%)
1	F	0.24	0/3862	0.41	0/5257
1	G	0.22	0/4050	0.38	0/5491
1	H	0.23	0/3970	0.40	0/5394
1	I	0.23	0/3995	0.39	0/5422
1	J	0.22	0/3979	0.39	0/5398
1	K	0.22	0/3970	0.38	0/5386
1	L	0.22	0/3895	0.39	0/5299
All	All	0.22	0/47721	0.39	1/64785 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	395	LEU	CB-CG-CD2	-6.01	100.79	111.00

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	3953	0	3884	34	1
1	B	3859	0	3745	31	0
1	C	3961	0	3887	34	0
1	D	3934	0	3865	34	0
1	E	3902	0	3832	34	0
1	F	3787	0	3598	33	0
1	G	3973	0	3902	31	1
1	H	3895	0	3777	41	0
1	I	3918	0	3815	24	0
1	J	3902	0	3826	27	0
1	K	3894	0	3818	24	0
1	L	3820	0	3646	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	26	0	16	1	0
4	B	26	0	16	1	0
4	C	26	0	16	3	0
4	D	26	0	16	1	0
4	E	26	0	16	1	0
4	F	26	0	16	1	0
4	G	26	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	26	0	16	0	0
4	I	26	0	16	2	0
4	J	26	0	16	3	0
4	K	26	0	16	2	0
4	L	26	0	16	2	0
5	A	10	0	0	2	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
5	H	5	0	0	0	0
5	K	5	0	0	0	0
6	B	19	0	23	1	0
6	E	20	0	23	0	0
6	F	26	0	28	1	0
6	G	23	0	29	2	0
6	H	10	0	10	0	0
6	I	21	0	24	0	0
6	J	10	0	13	0	0
6	K	13	0	17	0	0
6	L	7	0	9	0	0
7	A	170	0	0	5	0
7	B	125	0	0	2	0
7	C	155	0	0	2	0
7	D	174	0	0	2	0
7	E	151	0	0	1	0
7	F	119	0	0	1	0
7	G	150	0	0	2	0
7	H	133	0	0	7	0
7	I	143	0	0	1	0
7	J	171	0	0	4	0
7	K	163	0	0	2	0
7	L	142	0	0	1	0
All	All	49162	0	45963	351	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 4.

All (351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:LEU:O	1:E:397:LYS:N	2.15	0.79
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:LYS:NZ	1:G:472:TYR:OH	2.20	0.73
1:L:176:TYR:OH	1:L:217:ASN:OD1	2.07	0.72
1:H:335:GLU:CG	1:H:335:GLU:OE2	2.38	0.72
1:C:164:LYS:NZ	1:E:184:SER:OG	2.23	0.71
1:H:335:GLU:CG	1:H:335:GLU:OE1	2.38	0.71
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.71	0.71
1:G:368:LYS:NZ	1:G:422:GLU:OE1	2.25	0.70
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.75	0.69
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.75	0.69
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.74	0.69
1:D:126:GLY:HA2	1:D:219:LEU:HG	1.76	0.68
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.76	0.68
1:L:232:LYS:NZ	7:L:1209:HOH:O	2.27	0.67
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.77	0.67
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.77	0.67
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.77	0.66
1:L:90:GLN:NE2	1:L:95:ASP:O	2.24	0.66
1:A:173:LYS:NZ	7:A:1104:HOH:O	2.29	0.66
1:H:366:LYS:HG3	1:H:420:ASN:HB3	1.76	0.65
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.76	0.65
1:G:173:LYS:NZ	7:G:1111:HOH:O	2.30	0.65
1:C:300:ALA:O	7:C:1101:HOH:O	2.14	0.65
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.78	0.64
1:I:551:VAL:HG12	1:I:553:ALA:H	1.63	0.64
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.63	0.64
1:H:136:GLY:N	7:H:1139:HOH:O	2.31	0.64
1:H:332:GLU:OE1	7:H:1137:HOH:O	2.15	0.63
1:H:322:ASN:OD1	7:H:1228:HOH:O	2.14	0.63
1:I:439:TYR:OH	1:I:458:THR:O	2.17	0.62
1:E:161:ASN:HA	1:E:164:LYS:HE2	1.81	0.62
1:B:122:ASN:HD22	1:B:122:ASN:N	1.97	0.62
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.82	0.62
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.81	0.62
1:G:253:LYS:HB2	1:G:257:LYS:HE3	1.83	0.61
1:A:577:ALA:HB1	4:A:1004:R5X:H9	1.83	0.61
1:H:232:LYS:NZ	1:H:276:THR:O	2.33	0.61
1:H:551:VAL:HG12	1:H:553:ALA:H	1.66	0.61
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.83	0.60
1:B:440:ARG:NH1	7:B:1106:HOH:O	2.31	0.60
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.83	0.60
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:PRO:O	1:D:251:ARG:NH1	2.29	0.60
1:H:460:ALA:O	1:H:546:GLN:NE2	2.34	0.60
1:B:551:VAL:HG12	1:B:553:ALA:H	1.66	0.60
1:E:232:LYS:NZ	1:E:276:THR:O	2.35	0.60
1:H:335:GLU:OE2	1:H:335:GLU:OE1	2.20	0.59
1:I:232:LYS:NZ	1:I:276:THR:O	2.34	0.59
1:E:112:VAL:HG22	1:E:267:LEU:HB3	1.84	0.59
1:G:232:LYS:NZ	1:G:276:THR:O	2.33	0.59
1:I:261:MET:N	7:I:1105:HOH:O	2.34	0.59
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.83	0.59
1:H:511:ASN:ND2	7:H:1124:HOH:O	2.35	0.58
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.68	0.58
1:L:112:VAL:HG22	1:L:267:LEU:HB3	1.86	0.58
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.86	0.58
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.86	0.57
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.87	0.57
1:B:132:VAL:HG21	1:B:142:VAL:HG13	1.87	0.57
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.84	0.57
1:J:395:LEU:O	1:J:398:PHE:HB3	2.05	0.56
1:G:259:VAL:O	1:G:261:MET:N	2.39	0.56
1:F:138:GLU:N	1:F:140:GLY:H	2.03	0.56
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.87	0.56
1:H:300:ALA:O	7:H:1102:HOH:O	2.17	0.56
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.87	0.56
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.87	0.56
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.87	0.56
1:B:320:LYS:NZ	6:B:1005:1PE:OH4	2.35	0.56
1:A:504:GLY:HA3	1:A:510:ILE:HD11	1.87	0.55
1:F:439:TYR:OH	1:F:458:THR:O	2.24	0.55
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.88	0.55
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.88	0.55
1:J:475:LYS:NZ	7:J:1232:HOH:O	2.39	0.55
1:H:600:VAL:O	1:H:603:ASP:HB3	2.06	0.55
1:A:551:VAL:HG12	1:A:553:ALA:H	1.70	0.55
1:G:326:LYS:HZ1	1:G:472:TYR:HH	1.52	0.55
1:C:232:LYS:NZ	1:C:276:THR:O	2.39	0.55
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.89	0.55
1:C:326:LYS:HE2	1:C:328:LEU:HD21	1.89	0.55
1:A:262:GLU:N	7:A:1219:HOH:O	2.40	0.55
1:D:232:LYS:NZ	1:D:276:THR:O	2.38	0.55
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:LYS:NZ	1:L:184:SER:OG	2.40	0.55
1:A:218:LYS:O	1:D:164:LYS:NZ	2.39	0.55
1:F:113:GLN:OE1	1:F:115:TYR:OH	2.24	0.55
1:D:217:ASN:HD21	1:D:219:LEU:HB2	1.72	0.54
1:H:483:ASP:OD2	1:H:573:HIS:ND1	2.26	0.54
1:I:238:PHE:HD2	1:I:239:LEU:HD12	1.73	0.54
1:G:551:VAL:HG12	1:G:553:ALA:H	1.72	0.54
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.73	0.54
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.89	0.54
1:L:413:VAL:HG11	1:L:423:ILE:HD12	1.89	0.54
1:F:90:GLN:NE2	1:F:95:ASP:O	2.38	0.53
1:C:230:VAL:O	1:C:277:TYR:OH	2.19	0.53
1:B:122:ASN:ND2	1:B:122:ASN:N	2.57	0.53
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.90	0.53
1:F:114:VAL:HG12	1:F:274:ALA:HB1	1.90	0.53
1:L:533:TYR:O	1:L:536:THR:HG22	2.09	0.53
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.90	0.53
1:D:551:VAL:HG12	1:D:553:ALA:H	1.74	0.52
1:B:175:PHE:N	1:B:187:VAL:O	2.39	0.52
1:E:451:LYS:NZ	1:E:564:GLU:O	2.37	0.52
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.92	0.52
1:B:500:ALA:HB3	1:B:524:VAL:HG22	1.92	0.52
1:C:392:MET:CE	4:C:1004:R5X:H8	2.40	0.52
1:K:533:TYR:O	1:K:536:THR:HG22	2.09	0.52
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.91	0.51
1:A:511:ASN:ND2	7:A:1238:HOH:O	2.40	0.51
1:C:243:PHE:CE2	1:C:285:ARG:HG2	2.45	0.51
1:B:244:TYR:OH	1:B:588:PRO:O	2.29	0.51
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.91	0.51
1:E:238:PHE:HD2	1:E:239:LEU:HD12	1.75	0.51
1:F:504:GLY:HA3	1:F:510:ILE:HD11	1.93	0.51
1:K:439:TYR:H	1:K:439:TYR:HD2	1.59	0.50
1:J:164:LYS:NZ	7:J:1206:HOH:O	2.40	0.50
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.93	0.50
1:H:540:LYS:NZ	1:I:587:LYS:HD3	2.27	0.50
1:A:536:THR:HG21	1:A:551:VAL:HG23	1.93	0.50
1:K:392:MET:CE	4:K:1004:R5X:H1	2.42	0.50
1:K:137:LYS:N	7:K:1186:HOH:O	2.45	0.50
1:L:546:GLN:HG2	1:L:547:ILE:HG23	1.93	0.49
1:I:114:VAL:HG12	1:I:274:ALA:HB1	1.94	0.49
1:C:243:PHE:HE2	1:C:285:ARG:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LYS:O	1:F:266:HIS:HB3	2.11	0.49
1:L:271:ILE:O	1:L:272:ASN:HB3	2.13	0.49
1:J:440:ARG:NH1	7:J:1127:HOH:O	2.42	0.49
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.94	0.49
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.94	0.49
1:E:543:ASP:CG	1:F:255:THR:H	2.16	0.49
1:C:244:TYR:OH	1:C:588:PRO:O	2.31	0.49
1:H:175:PHE:N	1:H:187:VAL:O	2.39	0.49
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.95	0.48
1:B:563:LYS:NZ	7:B:1216:HOH:O	2.38	0.48
1:I:392:MET:CE	4:I:1004:R5X:H1	2.43	0.48
1:C:238:PHE:HD2	1:C:239:LEU:HD12	1.78	0.48
1:L:238:PHE:HD2	1:L:239:LEU:HD12	1.77	0.48
1:A:396:MET:SD	1:A:398:PHE:HE2	2.36	0.48
1:A:376:ILE:HD11	1:A:465:THR:HG21	1.95	0.48
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.95	0.48
1:G:411:TYR:HE1	6:G:1005:1PE:H252	1.78	0.48
1:H:503:PHE:O	1:H:573:HIS:N	2.39	0.48
1:E:204:LYS:HG2	1:E:241:THR:HG21	1.94	0.48
1:J:550:SER:O	1:J:552:LYS:HD2	2.13	0.48
1:D:571:TRP:CZ2	1:D:573:HIS:HB2	2.49	0.48
1:B:210:LEU:HD21	1:B:222:LEU:HD21	1.95	0.48
1:J:551:VAL:HG12	1:J:553:ALA:H	1.79	0.48
1:H:230:VAL:O	1:H:277:TYR:OH	2.28	0.48
1:A:236:ARG:NH2	1:A:519:THR:O	2.42	0.47
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.79	0.47
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.96	0.47
1:F:265:LYS:C	1:F:266:HIS:CD2	2.87	0.47
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.94	0.47
1:K:392:MET:HE3	4:K:1004:R5X:H1	1.96	0.47
1:D:386:LYS:HB3	1:D:391:SER:HB2	1.97	0.47
1:B:323:LEU:HD22	1:B:359:TYR:HB2	1.96	0.47
1:J:444:ILE:HB	1:K:301:PRO:HG2	1.97	0.47
1:H:165:PHE:HB3	1:H:189:TYR:OH	2.15	0.47
1:J:413:VAL:HG11	1:J:423:ILE:HD12	1.96	0.47
1:C:551:VAL:HG12	1:C:553:ALA:H	1.80	0.47
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.50	0.47
1:A:254:SER:O	7:A:1267:HOH:O	2.20	0.47
1:K:210:LEU:HD23	1:K:242:LEU:HD13	1.96	0.47
1:H:194:SER:HB2	7:H:1139:HOH:O	2.15	0.47
1:B:121:CYS:C	1:B:122:ASN:HD22	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:536:THR:HG21	1:G:551:VAL:HG23	1.97	0.47
1:J:344:VAL:HA	1:J:439:TYR:CE2	2.49	0.47
1:I:395:LEU:O	1:I:397:LYS:N	2.47	0.47
1:J:392:MET:CE	4:J:1004:R5X:H1	2.44	0.47
1:E:372:VAL:O	1:E:483:ASP:HA	2.15	0.47
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.97	0.47
1:L:216:ASP:C	1:L:217:ASN:HD22	2.17	0.47
1:F:303:ASN:O	7:F:1121:HOH:O	2.20	0.46
1:F:439:TYR:HD2	1:F:439:TYR:H	1.64	0.46
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.97	0.46
1:H:599:PHE:O	1:H:603:ASP:HB2	2.15	0.46
1:C:577:ALA:HB1	4:C:1004:R5X:H9	1.98	0.46
1:G:316:GLU:HG3	6:G:1006:1PE:H142	1.98	0.46
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.98	0.46
1:H:413:VAL:HG11	1:H:423:ILE:HD12	1.98	0.46
1:D:260:ASN:N	7:D:1186:HOH:O	2.49	0.46
1:D:395:LEU:HD11	1:D:581:TRP:CG	2.51	0.46
1:A:299:ALA:O	1:A:397:LYS:NZ	2.37	0.46
1:C:133:ASN:HB3	1:C:192:CYS:HB2	1.97	0.46
1:D:254:SER:HA	1:D:255:THR:HA	1.56	0.46
1:I:498:SER:O	1:I:523:PRO:HG2	2.16	0.46
1:F:265:LYS:C	1:F:266:HIS:HD2	2.19	0.45
1:F:413:VAL:HG11	1:F:423:ILE:HD12	1.97	0.45
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.80	0.45
1:F:200:GLU:HG3	1:F:521:ASN:O	2.16	0.45
1:C:331:LYS:HA	1:C:331:LYS:HD2	1.74	0.45
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.98	0.45
1:G:509:LEU:O	1:G:513:ILE:HG12	2.16	0.45
1:C:144:ILE:HD12	1:C:157:LEU:HB3	1.99	0.45
1:J:153:VAL:HG13	1:J:187:VAL:HG21	1.98	0.45
1:K:112:VAL:HG22	1:K:267:LEU:HB3	1.99	0.45
1:E:307:PRO:HD3	1:E:377:THR:OG1	2.17	0.45
1:A:207:VAL:HG11	1:A:241:THR:HG22	1.98	0.45
1:G:326:LYS:HE2	1:G:326:LYS:HB3	1.85	0.45
1:E:311:SER:HB2	1:E:327:ILE:HD12	1.99	0.45
1:H:164:LYS:HE3	1:H:165:PHE:CE2	2.52	0.45
1:G:301:PRO:HG2	1:G:304:TYR:CD2	2.52	0.45
1:B:360:LYS:HG2	1:B:422:GLU:HG3	1.98	0.45
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.17	0.45
1:K:522:GLU:OE1	1:K:595:LEU:N	2.50	0.45
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.99	0.45
1:D:487:LEU:HD22	1:D:573:HIS:CE1	2.51	0.44
1:A:525:TRP:CZ3	1:F:528:PRO:HB3	2.52	0.44
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.98	0.44
1:H:132:VAL:HG21	1:H:142:VAL:HG13	1.98	0.44
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.53	0.44
1:E:439:TYR:HD2	1:E:439:TYR:H	1.64	0.44
1:G:512:LYS:NZ	1:G:603:ASP:OD1	2.40	0.44
1:J:392:MET:HE3	4:J:1004:R5X:H1	1.99	0.44
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.98	0.44
1:K:95:ASP:HA	1:K:96:PRO:HD3	1.89	0.44
1:F:332:GLU:O	1:F:335:GLU:HG2	2.18	0.44
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.17	0.44
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.99	0.44
1:L:148:VAL:HG21	1:L:157:LEU:HD12	1.99	0.44
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.99	0.44
1:J:487:LEU:O	4:J:1004:R5X:H10	2.18	0.44
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.99	0.44
1:A:537:LEU:HA	1:A:545:ASN:HB2	2.00	0.44
1:E:152:GLN:HG2	1:E:180:ASP:OD2	2.18	0.44
1:D:546:GLN:HG2	1:D:547:ILE:HG23	2.00	0.44
1:D:396:MET:SD	1:D:398:PHE:HE2	2.41	0.44
1:B:173:LYS:HE3	1:F:217:ASN:OD1	2.18	0.44
1:K:518:LYS:HD3	1:K:518:LYS:HA	1.75	0.44
1:L:90:GLN:HB3	1:L:95:ASP:HB2	1.99	0.43
1:C:124:GLU:O	1:C:185:VAL:HG12	2.18	0.43
1:L:326:LYS:HE3	1:L:328:LEU:HD11	2.00	0.43
1:G:218:LYS:HD2	1:J:164:LYS:HA	2.00	0.43
1:J:487:LEU:HD22	1:J:573:HIS:CE1	2.52	0.43
1:H:195:VAL:HG12	1:H:197:ASP:H	1.82	0.43
1:E:347:GLY:N	7:E:1195:HOH:O	2.43	0.43
1:C:164:LYS:HE3	1:C:165:PHE:CE1	2.53	0.43
1:C:344:VAL:HA	1:C:439:TYR:CE2	2.53	0.43
1:C:396:MET:SD	1:C:398:PHE:HE2	2.41	0.43
1:E:368:LYS:HG2	1:E:422:GLU:HB3	2.00	0.43
1:E:344:VAL:HA	1:E:439:TYR:CE2	2.53	0.43
1:K:347:GLY:N	7:K:1196:HOH:O	2.41	0.43
1:H:440:ARG:NH1	7:H:1135:HOH:O	2.39	0.43
1:H:357:LEU:HB2	1:H:425:PHE:HB2	2.01	0.43
1:I:568:ASN:O	1:I:568:ASN:OD1	2.37	0.43
1:L:357:LEU:HB2	1:L:425:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:546:GLN:HG2	1:J:547:ILE:HG23	2.01	0.43
1:A:344:VAL:HA	1:A:439:TYR:CE2	2.54	0.43
1:L:487:LEU:O	4:L:1004:R5X:H10	2.18	0.43
1:G:244:TYR:OH	1:G:588:PRO:O	2.36	0.43
1:K:372:VAL:O	1:K:483:ASP:HA	2.18	0.43
1:G:182:LYS:NZ	7:G:1217:HOH:O	2.50	0.43
1:L:232:LYS:HE2	1:L:276:THR:O	2.18	0.43
1:J:509:LEU:O	1:J:513:ILE:HG12	2.19	0.43
1:E:522:GLU:HA	1:E:523:PRO:HD3	1.86	0.43
1:H:116:ASP:OD2	1:H:118:LYS:HD2	2.19	0.43
1:D:386:LYS:HE3	1:D:396:MET:SD	2.59	0.42
1:B:90:GLN:NE2	1:B:95:ASP:O	2.51	0.42
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.01	0.42
1:H:453:ILE:HD13	1:H:561:PHE:HZ	1.84	0.42
1:F:383:TYR:HE2	1:F:438:SER:HB2	1.84	0.42
1:A:372:VAL:O	1:A:483:ASP:HA	2.19	0.42
1:C:525:TRP:CZ3	1:D:528:PRO:HB3	2.54	0.42
1:C:392:MET:HE3	4:C:1004:R5X:H8	2.01	0.42
1:E:129:ILE:HG21	1:E:190:VAL:HG23	2.01	0.42
1:F:361:SER:OG	1:F:419:GLU:HA	2.19	0.42
1:J:452:THR:HG22	1:J:542:ALA:HB1	2.01	0.42
1:C:208:LEU:O	1:C:212:THR:HG23	2.18	0.42
1:B:383:TYR:HE2	1:B:438:SER:HB2	1.84	0.42
1:A:332:GLU:N	1:A:332:GLU:OE1	2.51	0.42
1:K:203:MET:HE3	1:K:206:VAL:HB	2.01	0.42
1:H:395:LEU:O	1:H:397:LYS:N	2.53	0.42
1:F:210:LEU:HA	1:F:213:MET:HE2	2.00	0.42
1:I:208:LEU:HA	1:I:208:LEU:HD23	1.91	0.42
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.20	0.42
1:I:377:THR:HA	1:I:400:MET:HG2	2.02	0.42
1:L:150:ASP:OD1	1:L:179:ASN:HB2	2.20	0.42
1:F:338:MET:HE1	1:F:354:PHE:CE2	2.55	0.42
1:F:111:LYS:HA	1:F:111:LYS:HD2	1.74	0.42
1:A:441:PRO:HD2	1:B:378:PHE:CZ	2.55	0.42
1:G:530:ILE:HD12	1:G:556:ILE:HD13	2.01	0.42
1:D:586:ARG:NH1	7:D:1191:HOH:O	2.53	0.42
1:E:520:SER:HB3	1:E:598:GLU:HG3	2.02	0.42
1:D:340:ALA:HA	1:D:445:ILE:HD12	2.02	0.42
1:I:198:LEU:HD22	1:I:202:ASP:HB3	2.01	0.42
1:G:520:SER:HB3	1:G:598:GLU:HG3	2.02	0.42
1:L:342:LEU:O	1:L:346:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ALA:HA	1:C:301:PRO:HD3	1.86	0.41
1:I:392:MET:HE3	4:I:1004:R5X:H1	2.02	0.41
1:B:301:PRO:HG2	1:B:304:TYR:CD2	2.55	0.41
1:L:273:ASN:O	1:L:276:THR:HG22	2.20	0.41
1:J:205:ARG:NH1	7:J:1215:HOH:O	2.54	0.41
1:I:323:LEU:HD22	1:I:359:TYR:HB2	2.02	0.41
1:E:396:MET:HA	1:E:398:PHE:CE2	2.55	0.41
1:B:164:LYS:HE3	1:B:165:PHE:CZ	2.55	0.41
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.19	0.41
1:F:138:GLU:HA	1:F:139:ASN:HA	1.70	0.41
1:H:344:VAL:HA	1:H:439:TYR:CE2	2.55	0.41
1:C:150:ASP:N	7:C:1171:HOH:O	2.53	0.41
1:B:289:PHE:O	1:B:293:TYR:N	2.41	0.41
1:K:159:ASP:O	1:K:163:GLU:HB2	2.20	0.41
1:I:301:PRO:HB2	1:I:303:ASN:OD1	2.20	0.41
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.55	0.41
1:L:301:PRO:HG2	1:L:304:TYR:HD2	1.84	0.41
1:B:118:LYS:HE3	1:B:272:ASN:HD22	1.84	0.41
1:D:487:LEU:O	4:D:1004:R5X:H10	2.21	0.41
1:G:301:PRO:HG2	1:G:304:TYR:HD2	1.86	0.41
1:F:103:TYR:CD2	6:F:1005:1PE:H141	2.54	0.41
5:A:1005:SO4:O1	1:C:436:LYS:HE3	2.21	0.41
1:D:350:TYR:HA	1:D:351:PRO:HD3	1.90	0.41
1:A:89:PRO:HG2	1:A:350:TYR:CD2	2.56	0.41
1:K:301:PRO:HB2	1:K:303:ASN:OD1	2.20	0.41
1:H:398:PHE:CE1	1:H:581:TRP:HB2	2.55	0.41
1:D:435:SER:OG	1:D:436:LYS:N	2.53	0.41
1:C:537:LEU:HD23	1:C:537:LEU:HA	1.93	0.41
1:E:435:SER:OG	1:E:436:LYS:N	2.53	0.41
1:C:435:SER:OG	1:C:436:LYS:N	2.53	0.41
1:J:533:TYR:O	1:J:536:THR:HG22	2.20	0.41
1:G:584:LYS:HE2	1:G:584:LYS:HB3	1.86	0.41
4:L:1004:R5X:H15	4:L:1004:R5X:H11	1.56	0.41
1:E:300:ALA:HA	1:E:301:PRO:HD3	1.90	0.41
1:A:292:TYR:O	1:A:296:GLN:HG3	2.20	0.41
1:B:195:VAL:HG12	1:B:197:ASP:H	1.86	0.41
1:D:150:ASP:OD1	1:D:179:ASN:HB2	2.21	0.41
1:D:300:ALA:HA	1:D:301:PRO:HD3	1.90	0.41
1:A:285:ARG:NH2	7:A:1125:HOH:O	2.54	0.41
1:L:439:TYR:H	1:L:439:TYR:HD2	1.69	0.41
1:B:201:ALA:O	1:B:205:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ILE:HG21	1:F:243:PHE:HB3	2.03	0.41
1:I:298:ILE:HG23	1:I:398:PHE:HA	2.02	0.41
1:D:441:PRO:HD2	1:E:378:PHE:CZ	2.57	0.40
1:E:301:PRO:HB2	1:E:303:ASN:OD1	2.20	0.40
1:K:500:ALA:HB3	1:K:524:VAL:HG22	2.03	0.40
1:F:353:LYS:HD3	1:F:353:LYS:HA	1.87	0.40
1:A:436:LYS:NZ	5:A:1005:SO4:O1	2.54	0.40
1:K:398:PHE:O	1:K:401:SER:OG	2.32	0.40
1:C:346:LYS:HB3	1:C:437:ASN:O	2.20	0.40
1:B:487:LEU:O	4:B:1004:R5X:H10	2.21	0.40
1:H:540:LYS:HZ1	1:I:587:LYS:HD3	1.85	0.40
1:K:214:LEU:HD21	1:K:222:LEU:HD22	2.02	0.40
1:A:481:ILE:O	1:A:571:TRP:HA	2.22	0.40
1:B:298:ILE:HG23	1:B:398:PHE:HA	2.04	0.40
1:A:528:PRO:HB3	1:F:525:TRP:CE3	2.56	0.40
1:A:350:TYR:HA	1:A:351:PRO:HD2	1.94	0.40
1:H:536:THR:HG21	1:H:551:VAL:HG23	2.04	0.40
1:J:452:THR:HG21	1:K:252:PHE:O	2.21	0.40
1:E:487:LEU:O	4:E:1004:R5X:H10	2.22	0.40
1:F:392:MET:CE	4:F:1004:R5X:H1	2.52	0.40
1:D:368:LYS:NZ	1:D:422:GLU:OE1	2.54	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)
1:A:115:TYR:OH	1:G:124:GLU:OE1[2_564]	2.17	0.03

## 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	512/528 (97%)	493 (96%)	19 (4%)	0	100	100
1	B	507/528 (96%)	489 (96%)	16 (3%)	2 (0%)	39	61
1	C	517/528 (98%)	502 (97%)	15 (3%)	0	100	100
1	D	510/528 (97%)	493 (97%)	16 (3%)	1 (0%)	52	75
1	E	504/528 (96%)	491 (97%)	12 (2%)	1 (0%)	52	75
1	F	501/528 (95%)	486 (97%)	14 (3%)	1 (0%)	52	75
1	G	513/528 (97%)	498 (97%)	14 (3%)	1 (0%)	52	75
1	H	511/528 (97%)	490 (96%)	19 (4%)	2 (0%)	39	61
1	I	512/528 (97%)	495 (97%)	16 (3%)	1 (0%)	52	75
1	J	507/528 (96%)	493 (97%)	14 (3%)	0	100	100
1	K	503/528 (95%)	487 (97%)	15 (3%)	1 (0%)	52	75
1	L	502/528 (95%)	484 (96%)	16 (3%)	2 (0%)	39	61
All	All	6099/6336 (96%)	5901 (97%)	186 (3%)	12 (0%)	52	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	396	MET
1	F	551	VAL
1	H	396	MET
1	I	396	MET
1	B	119	GLY
1	K	396	MET
1	L	364	ASP
1	D	254	SER
1	G	396	MET
1	H	125	GLU
1	L	272	ASN
1	B	396	MET

### 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	422/455 (93%)	419 (99%)	3 (1%)	88	97
1	B	402/455 (88%)	400 (100%)	2 (0%)	92	98
1	C	421/455 (92%)	420 (100%)	1 (0%)	95	99
1	D	417/455 (92%)	413 (99%)	4 (1%)	82	95
1	E	415/455 (91%)	415 (100%)	0	100	100
1	F	382/455 (84%)	376 (98%)	6 (2%)	70	90
1	G	425/455 (93%)	424 (100%)	1 (0%)	95	99
1	H	406/455 (89%)	405 (100%)	1 (0%)	95	99
1	I	411/455 (90%)	409 (100%)	2 (0%)	92	98
1	J	412/455 (90%)	411 (100%)	1 (0%)	95	99
1	K	414/455 (91%)	413 (100%)	1 (0%)	95	99
1	L	393/455 (86%)	390 (99%)	3 (1%)	86	96
All	All	4920/5460 (90%)	4895 (100%)	25 (0%)	92	98

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	TYR
1	A	398	PHE
1	A	595	LEU
1	B	122	ASN
1	B	172	SER
1	C	398	PHE
1	D	215	HIS
1	D	219	LEU
1	D	288	TYR
1	D	398	PHE
1	F	200	GLU
1	F	266	HIS
1	F	288	TYR
1	F	398	PHE
1	F	439	TYR
1	F	531	ASN
1	G	288	TYR
1	H	603	ASP
1	I	400	MET
1	I	439	TYR
1	J	200	GLU
1	K	439	TYR

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Mol	Chain	Res	Type
1	L	288	TYR
1	L	398	PHE
1	L	439	TYR

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	B	174	HIS
1	B	272	ASN
1	F	266	HIS
1	H	322	ASN
1	I	134	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 24 are monoatomic - leaving 46 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
3	CO3	A	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	A	1004	2	26,28,28	2.15	4 (15%)	35,38,38	2.46	7 (20%)
5	SO4	A	1005	-	4,4,4	0.22	0	6,6,6	0.07	0
5	SO4	A	1006	-	4,4,4	0.21	0	6,6,6	0.07	0
3	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	B	1004	2	26,28,28	2.17	5 (19%)	35,38,38	2.37	7 (20%)
6	1PE	B	1005	-	9,9,15	0.46	0	8,8,14	0.25	0
6	1PE	B	1006	-	8,8,15	0.48	0	7,7,14	0.32	0
3	CO3	C	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	C	1004	2	26,28,28	2.19	4 (15%)	35,38,38	2.40	7 (20%)
3	CO3	D	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	D	1004	2	26,28,28	2.18	5 (19%)	35,38,38	2.14	4 (11%)
3	CO3	E	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	E	1004	2	26,28,28	2.24	5 (19%)	35,38,38	2.15	5 (14%)
5	SO4	E	1005	-	4,4,4	0.25	0	6,6,6	0.14	0
6	1PE	E	1006	-	9,9,15	0.44	0	8,8,14	0.29	0
6	1PE	E	1007	-	9,9,15	0.48	0	8,8,14	0.30	0
5	SO4	E	1008	-	4,4,4	0.25	0	6,6,6	0.20	0
3	CO3	F	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	F	1004	2	26,28,28	2.21	5 (19%)	35,38,38	2.21	7 (20%)
6	1PE	F	1005	-	7,7,15	0.53	0	6,6,14	0.26	0
6	1PE	F	1006	-	8,8,15	0.48	0	7,7,14	0.28	0
6	1PE	F	1007	-	8,8,15	0.47	0	7,7,14	0.37	0
5	SO4	F	1008	-	4,4,4	0.21	0	6,6,6	0.09	0
3	CO3	G	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	G	1004	2	26,28,28	2.21	5 (19%)	35,38,38	2.39	6 (17%)
6	1PE	G	1005	-	12,12,15	0.43	0	11,11,14	0.43	0
6	1PE	G	1006	-	9,9,15	0.43	0	8,8,14	0.31	0
3	CO3	H	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	H	1004	2	26,28,28	2.22	6 (23%)	35,38,38	2.21	7 (20%)
5	SO4	H	1005	-	4,4,4	0.22	0	6,6,6	0.06	0
6	1PE	H	1006	-	9,9,15	0.47	0	8,8,14	0.40	0
3	CO3	I	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	I	1004	2	26,28,28	2.37	6 (23%)	35,38,38	2.09	3 (8%)
6	1PE	I	1005	-	9,9,15	0.44	0	8,8,14	0.29	0
6	1PE	I	1006	-	10,10,15	0.49	0	9,9,14	0.34	0
3	CO3	J	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	J	1004	2	26,28,28	2.25	6 (23%)	35,38,38	2.12	4 (11%)
6	1PE	J	1005	-	9,9,15	0.43	0	8,8,14	0.33	0
3	CO3	K	1002	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	R5X	K	1004	2	26,28,28	2.27	5 (19%)	35,38,38	2.13	5 (14%)
5	SO4	K	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
6	1PE	K	1006	-	12,12,15	0.44	0	11,11,14	0.32	0
3	CO3	L	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	R5X	L	1004	2	26,28,28	2.17	5 (19%)	35,38,38	2.31	10 (28%)
6	1PE	L	1005	-	6,6,15	0.41	0	5,5,14	0.38	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
3	CO3	A	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	A	1004	2	-	0/22/22/22	0/3/3/3
5	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
3	CO3	B	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	B	1004	2	-	0/22/22/22	0/3/3/3
6	1PE	B	1005	-	-	0/7/7/13	0/0/0/0
6	1PE	B	1006	-	-	0/6/6/13	0/0/0/0
3	CO3	C	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	C	1004	2	-	0/22/22/22	0/3/3/3
3	CO3	D	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	D	1004	2	-	0/22/22/22	0/3/3/3
3	CO3	E	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	E	1004	2	-	0/22/22/22	0/3/3/3
5	SO4	E	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	E	1006	-	-	0/7/7/13	0/0/0/0
6	1PE	E	1007	-	-	0/7/7/13	0/0/0/0
5	SO4	E	1008	-	-	0/0/0/0	0/0/0/0
3	CO3	F	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	F	1004	2	-	0/22/22/22	0/3/3/3
6	1PE	F	1005	-	-	0/5/5/13	0/0/0/0
6	1PE	F	1006	-	-	0/6/6/13	0/0/0/0
6	1PE	F	1007	-	-	0/6/6/13	0/0/0/0
5	SO4	F	1008	-	-	0/0/0/0	0/0/0/0
3	CO3	G	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	G	1004	2	-	0/22/22/22	0/3/3/3
6	1PE	G	1005	-	-	0/10/10/13	0/0/0/0
6	1PE	G	1006	-	-	0/7/7/13	0/0/0/0
3	CO3	H	1002	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	R5X	H	1004	2	-	0/22/22/22	0/3/3/3
5	SO4	H	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	H	1006	-	-	0/7/7/13	0/0/0/0
3	CO3	I	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	I	1004	2	-	0/22/22/22	0/3/3/3
6	1PE	I	1005	-	-	0/7/7/13	0/0/0/0
6	1PE	I	1006	-	-	0/8/8/13	0/0/0/0
3	CO3	J	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	J	1004	2	-	0/22/22/22	0/3/3/3
6	1PE	J	1005	-	-	0/7/7/13	0/0/0/0
3	CO3	K	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	K	1004	2	-	0/22/22/22	0/3/3/3
5	SO4	K	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	K	1006	-	-	0/10/10/13	0/0/0/0
3	CO3	L	1002	-	-	0/0/0/0	0/0/0/0
4	R5X	L	1004	2	-	0/22/22/22	0/3/3/3
6	1PE	L	1005	-	-	0/4/4/13	0/0/0/0

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1004	R5X	C03-C12	-7.69	1.39	1.52
4	I	1004	R5X	C03-C12	-7.50	1.39	1.52
4	J	1004	R5X	C03-C12	-7.45	1.39	1.52
4	E	1004	R5X	C03-C12	-7.45	1.39	1.52
4	D	1004	R5X	C03-C12	-7.22	1.40	1.52
4	F	1004	R5X	C03-C12	-7.21	1.40	1.52
4	L	1004	R5X	C03-C12	-7.21	1.40	1.52
4	C	1004	R5X	C03-C12	-7.15	1.40	1.52
4	B	1004	R5X	C03-C12	-7.13	1.40	1.52
4	H	1004	R5X	C03-C12	-7.11	1.40	1.52
4	A	1004	R5X	C03-C12	-7.06	1.40	1.52
4	G	1004	R5X	C03-C12	-6.97	1.40	1.52
4	K	1004	R5X	C06-N07	-5.44	1.33	1.44
4	I	1004	R5X	C06-N07	-5.37	1.33	1.44
4	E	1004	R5X	C06-N07	-5.33	1.33	1.44
4	D	1004	R5X	C06-N07	-5.33	1.33	1.44
4	J	1004	R5X	C06-N07	-5.31	1.33	1.44
4	H	1004	R5X	C06-N07	-5.30	1.33	1.44
4	C	1004	R5X	C06-N07	-5.28	1.33	1.44
4	L	1004	R5X	C06-N07	-5.26	1.33	1.44
4	A	1004	R5X	C06-N07	-5.26	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1004	R5X	C06-N07	-5.26	1.33	1.44
4	B	1004	R5X	C06-N07	-5.17	1.33	1.44
4	G	1004	R5X	C06-N07	-5.17	1.33	1.44
4	I	1004	R5X	C19-C18	-5.11	1.39	1.50
4	E	1004	R5X	C19-C18	-5.11	1.39	1.50
4	G	1004	R5X	C19-C18	-5.10	1.39	1.50
4	D	1004	R5X	C19-C18	-5.08	1.39	1.50
4	H	1004	R5X	C19-C18	-5.08	1.39	1.50
4	A	1004	R5X	C19-C18	-5.04	1.39	1.50
4	K	1004	R5X	C19-C18	-5.02	1.39	1.50
4	J	1004	R5X	C19-C18	-5.01	1.39	1.50
4	L	1004	R5X	C19-C18	-5.00	1.39	1.50
4	F	1004	R5X	C19-C18	-4.99	1.39	1.50
4	C	1004	R5X	C19-C18	-4.98	1.39	1.50
4	B	1004	R5X	C19-C18	-4.97	1.39	1.50
4	A	1004	R5X	C11-C10	-2.23	1.32	1.37
4	C	1004	R5X	C11-C10	-2.20	1.32	1.37
4	I	1004	R5X	C11-C10	-2.17	1.33	1.37
4	G	1004	R5X	C11-C10	-2.15	1.33	1.37
4	K	1004	R5X	C11-C10	-2.14	1.33	1.37
4	E	1004	R5X	C11-C10	-2.14	1.33	1.37
4	J	1004	R5X	C11-C10	-2.11	1.33	1.37
4	K	1004	R5X	C11-N07	-2.11	1.33	1.36
4	B	1004	R5X	C11-C10	-2.09	1.33	1.37
4	F	1004	R5X	C11-C10	-2.08	1.33	1.37
4	D	1004	R5X	C11-C10	-2.08	1.33	1.37
4	H	1004	R5X	C11-C10	-2.08	1.33	1.37
4	E	1004	R5X	C11-N07	-2.07	1.33	1.36
4	L	1004	R5X	C11-C10	-2.06	1.33	1.37
4	D	1004	R5X	C11-N07	-2.05	1.33	1.36
4	I	1004	R5X	C11-N07	-2.05	1.33	1.36
4	H	1004	R5X	C11-N07	-2.02	1.33	1.36
4	J	1004	R5X	C11-N07	-2.02	1.33	1.36
4	L	1004	R5X	C11-N07	-2.01	1.33	1.36
4	B	1004	R5X	O17-N16	2.02	1.43	1.39
4	J	1004	R5X	O17-N16	2.32	1.44	1.39
4	F	1004	R5X	O17-N16	2.36	1.44	1.39
4	H	1004	R5X	O17-N16	2.46	1.44	1.39
4	G	1004	R5X	O17-N16	2.96	1.45	1.39
4	I	1004	R5X	O17-N16	4.30	1.47	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1004	R5X	C11-N07-N08	-3.74	109.36	111.94
4	F	1004	R5X	C11-N07-N08	-3.74	109.36	111.94
4	L	1004	R5X	C02-C03-C12	-3.67	114.69	120.80
4	D	1004	R5X	C11-N07-N08	-3.60	109.46	111.94
4	F	1004	R5X	C02-C03-C12	-3.57	114.86	120.80
4	H	1004	R5X	C11-N07-N08	-3.57	109.48	111.94
4	H	1004	R5X	C02-C03-C12	-3.54	114.91	120.80
4	J	1004	R5X	C11-N07-N08	-3.47	109.54	111.94
4	G	1004	R5X	C11-N07-N08	-3.40	109.59	111.94
4	E	1004	R5X	C11-N07-N08	-3.28	109.68	111.94
4	C	1004	R5X	C02-C03-C12	-3.27	115.37	120.80
4	B	1004	R5X	C11-N07-N08	-3.25	109.70	111.94
4	G	1004	R5X	C02-C03-C12	-3.13	115.59	120.80
4	B	1004	R5X	C02-C03-C12	-3.12	115.61	120.80
4	K	1004	R5X	C11-N07-N08	-2.97	109.89	111.94
4	A	1004	R5X	C02-C03-C12	-2.96	115.88	120.80
4	A	1004	R5X	C11-N07-N08	-2.90	109.94	111.94
4	I	1004	R5X	C11-N07-N08	-2.87	109.96	111.94
4	J	1004	R5X	C02-C03-C12	-2.85	116.06	120.80
4	K	1004	R5X	C02-C03-C12	-2.75	116.23	120.80
4	D	1004	R5X	C02-C03-C12	-2.75	116.23	120.80
4	C	1004	R5X	C11-N07-N08	-2.68	110.09	111.94
4	E	1004	R5X	C02-C03-C12	-2.67	116.36	120.80
4	L	1004	R5X	C19-C18-N13	-2.35	112.73	116.93
4	L	1004	R5X	O17-N16-C14	-2.25	116.68	119.86
4	L	1004	R5X	C05-C04-C03	-2.23	118.91	121.20
4	B	1004	R5X	O17-N16-C14	-2.22	116.73	119.86
4	E	1004	R5X	O17-N16-C14	-2.19	116.76	119.86
4	F	1004	R5X	C05-C04-C03	-2.14	119.00	121.20
4	H	1004	R5X	O17-N16-C14	-2.11	116.88	119.86
4	C	1004	R5X	C05-C04-C03	-2.11	119.04	121.20
4	K	1004	R5X	C05-C04-C03	-2.07	119.08	121.20
4	A	1004	R5X	O17-N16-C14	-2.05	116.97	119.86
4	C	1004	R5X	C03-C12-N13	2.03	118.33	112.94
4	A	1004	R5X	C03-C12-N13	2.14	118.63	112.94
4	G	1004	R5X	C03-C12-N13	2.17	118.69	112.94
4	L	1004	R5X	C12-N13-C18	2.17	126.10	122.55
4	B	1004	R5X	C03-C12-N13	2.20	118.77	112.94
4	A	1004	R5X	C04-C03-C12	2.20	124.46	120.80
4	F	1004	R5X	C03-C12-N13	2.31	119.08	112.94
4	B	1004	R5X	C04-C03-C12	2.41	124.82	120.80
4	C	1004	R5X	C04-C03-C12	2.44	124.87	120.80
4	H	1004	R5X	C03-C12-N13	2.52	119.64	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1004	R5X	C04-C03-C12	2.57	125.08	120.80
4	L	1004	R5X	C03-C12-N13	2.73	120.18	112.94
4	F	1004	R5X	C04-C03-C12	2.75	125.38	120.80
4	H	1004	R5X	C04-C03-C12	2.80	125.46	120.80
4	L	1004	R5X	C04-C03-C12	2.89	125.61	120.80
4	F	1004	R5X	C06-N07-N08	5.74	123.96	118.89
4	L	1004	R5X	C06-N07-N08	5.77	123.98	118.89
4	H	1004	R5X	C06-N07-N08	5.79	124.00	118.89
4	J	1004	R5X	C06-N07-N08	5.90	124.10	118.89
4	D	1004	R5X	C06-N07-N08	6.24	124.39	118.89
4	E	1004	R5X	C06-N07-N08	6.51	124.63	118.89
4	K	1004	R5X	C06-N07-N08	6.62	124.73	118.89
4	I	1004	R5X	C06-N07-N08	7.04	125.10	118.89
4	A	1004	R5X	C09-N08-N07	8.09	109.78	103.70
4	C	1004	R5X	C09-N08-N07	8.30	109.94	103.70
4	G	1004	R5X	C09-N08-N07	8.40	110.02	103.70
4	E	1004	R5X	C09-N08-N07	8.40	110.02	103.70
4	I	1004	R5X	C09-N08-N07	8.41	110.03	103.70
4	B	1004	R5X	C09-N08-N07	8.49	110.08	103.70
4	H	1004	R5X	C09-N08-N07	8.50	110.10	103.70
4	D	1004	R5X	C09-N08-N07	8.54	110.12	103.70
4	K	1004	R5X	C09-N08-N07	8.55	110.13	103.70
4	B	1004	R5X	C06-N07-N08	8.58	126.46	118.89
4	L	1004	R5X	C09-N08-N07	8.61	110.18	103.70
4	F	1004	R5X	C09-N08-N07	8.67	110.23	103.70
4	J	1004	R5X	C09-N08-N07	8.71	110.25	103.70
4	G	1004	R5X	C06-N07-N08	8.87	126.72	118.89
4	C	1004	R5X	C06-N07-N08	9.18	127.00	118.89
4	A	1004	R5X	C06-N07-N08	9.66	127.42	118.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	R5X	1	0
5	A	1005	SO4	2	0
4	B	1004	R5X	1	0
6	B	1005	1PE	1	0
4	C	1004	R5X	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1004	R5X	1	0
4	E	1004	R5X	1	0
4	F	1004	R5X	1	0
6	F	1005	1PE	1	0
6	G	1005	1PE	1	0
6	G	1006	1PE	1	0
4	I	1004	R5X	2	0
4	J	1004	R5X	3	0
4	K	1004	R5X	2	0
4	L	1004	R5X	2	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	515/528 (97%)	-0.39	5 (0%) 84 86	15, 23, 43, 75	0
1	B	511/528 (96%)	-0.15	13 (2%) 61 65	15, 26, 62, 82	1 (0%)
1	C	518/528 (98%)	-0.30	7 (1%) 78 80	15, 24, 53, 88	0
1	D	514/528 (97%)	-0.39	6 (1%) 81 83	16, 23, 45, 99	0
1	E	510/528 (96%)	-0.38	5 (0%) 84 86	16, 23, 39, 68	0
1	F	509/528 (96%)	-0.10	11 (2%) 65 69	16, 28, 55, 85	0
1	G	517/528 (97%)	-0.38	7 (1%) 78 80	18, 25, 45, 67	0
1	H	515/528 (97%)	-0.09	15 (2%) 55 60	17, 28, 64, 100	1 (0%)
1	I	516/528 (97%)	-0.26	5 (0%) 84 86	17, 26, 53, 79	0
1	J	511/528 (96%)	-0.34	2 (0%) 93 93	19, 25, 45, 66	0
1	K	509/528 (96%)	-0.31	3 (0%) 90 91	20, 25, 41, 69	0
1	L	510/528 (96%)	-0.14	7 (1%) 78 80	20, 27, 52, 66	0
All	All	6155/6336 (97%)	-0.27	86 (1%) 78 80	15, 25, 52, 100	2 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	363	GLY	7.3
1	D	260	ASN	7.0
1	L	363	GLY	4.9
1	H	136	GLY	4.9
1	F	141	PRO	4.9
1	H	603	ASP	4.6
1	B	363	GLY	4.4
1	H	259	VAL	3.8
1	H	196	ALA	3.6
1	E	550	SER	3.5
1	H	260	ASN	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	136	GLY	3.4
1	C	194	SER	3.4
1	I	195	VAL	3.3
1	A	362	LYS	3.3
1	H	400	MET	3.2
1	C	603	ASP	3.2
1	G	365	VAL	3.1
1	A	365	VAL	3.0
1	B	196	ALA	3.0
1	B	181	ASN	3.0
1	I	400	MET	3.0
1	F	550	SER	2.9
1	K	550	SER	2.9
1	H	195	VAL	2.8
1	H	398	PHE	2.8
1	F	161	ASN	2.8
1	A	136	GLY	2.8
1	J	603	ASP	2.8
1	L	119	GLY	2.7
1	L	141	PRO	2.7
1	G	259	VAL	2.7
1	B	123	VAL	2.7
1	F	439	TYR	2.7
1	C	137	LYS	2.6
1	C	400	MET	2.6
1	F	364	ASP	2.6
1	H	549	SER	2.5
1	L	375	GLY	2.5
1	G	258	ASN	2.5
1	G	195	VAL	2.5
1	A	364	ASP	2.5
1	H	276	THR	2.5
1	E	363	GLY	2.4
1	I	550	SER	2.4
1	B	183	ASN	2.4
1	B	549	SER	2.4
1	H	178	PHE	2.4
1	C	195	VAL	2.4
1	B	195	VAL	2.4
1	L	439	TYR	2.3
1	I	135	PRO	2.3
1	L	485	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	362	LYS	2.3
1	F	255	THR	2.2
1	E	439	TYR	2.2
1	F	419	GLU	2.2
1	L	376	ILE	2.2
1	C	136	GLY	2.2
1	G	257	LYS	2.2
1	B	276	THR	2.2
1	J	549	SER	2.2
1	F	375	GLY	2.2
1	D	398	PHE	2.2
1	K	406	VAL	2.2
1	B	194	SER	2.2
1	D	261	MET	2.1
1	A	257	LYS	2.1
1	B	180	ASP	2.1
1	D	255	THR	2.1
1	D	322	ASN	2.1
1	I	138	GLU	2.1
1	B	178	PHE	2.1
1	C	139	ASN	2.1
1	E	398	PHE	2.1
1	H	181	ASN	2.1
1	K	576	ILE	2.1
1	E	255	THR	2.1
1	H	363	GLY	2.1
1	D	603	ASP	2.1
1	F	508	GLU	2.1
1	G	160	GLU	2.1
1	H	483	ASP	2.1
1	G	363	GLY	2.1
1	H	180	ASP	2.0
1	F	160	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	1006	5/5	0.92	0.23	4.99	62,63,63,63	0
6	1PE	F	1007	9/16	0.91	0.22	3.15	39,40,42,43	0
6	1PE	H	1006	10/16	0.86	0.23	2.79	39,42,47,47	0
6	1PE	K	1006	13/16	0.94	0.23	2.78	34,36,39,40	0
6	1PE	B	1006	9/16	0.89	0.19	2.71	35,38,47,48	0
6	1PE	G	1005	13/16	0.92	0.15	2.32	38,39,45,45	0
6	1PE	G	1006	10/16	0.81	0.21	2.19	56,57,58,58	0
6	1PE	F	1006	9/16	0.79	0.19	2.18	39,39,41,41	0
6	1PE	L	1005	7/16	0.89	0.15	1.38	37,38,38,38	0
6	1PE	E	1006	10/16	0.95	0.15	1.04	27,28,29,30	0
6	1PE	J	1005	10/16	0.88	0.17	0.94	42,43,45,46	0
4	R5X	K	1004	26/26	0.93	0.16	0.93	31,36,48,48	0
6	1PE	I	1006	11/16	0.91	0.14	0.78	33,38,42,43	0
4	R5X	E	1004	26/26	0.94	0.17	0.75	26,44,50,51	0
3	CO3	K	1002	4/4	0.97	0.17	0.69	29,29,29,30	0
4	R5X	A	1004	26/26	0.93	0.15	0.67	26,28,43,44	0
3	CO3	H	1002	4/4	0.97	0.17	0.54	22,23,23,24	0
4	R5X	I	1004	26/26	0.93	0.16	0.53	20,28,38,41	0
3	CO3	L	1002	4/4	0.96	0.22	0.53	19,20,24,25	0
3	CO3	E	1002	4/4	0.97	0.14	0.45	22,23,24,24	0
4	R5X	B	1004	26/26	0.92	0.16	0.45	22,28,36,36	0
3	CO3	B	1002	4/4	0.98	0.17	0.26	19,19,19,20	0
4	R5X	F	1004	26/26	0.93	0.16	0.23	23,29,45,45	0
4	R5X	G	1004	26/26	0.95	0.13	0.16	24,27,38,39	0
4	R5X	D	1004	26/26	0.94	0.15	0.15	26,30,43,43	0
4	R5X	J	1004	26/26	0.94	0.15	0.15	25,34,44,44	0
3	CO3	C	1002	4/4	0.97	0.14	0.01	19,21,21,22	0
4	R5X	C	1004	26/26	0.95	0.13	-0.07	21,31,35,35	0
3	CO3	A	1002	4/4	0.96	0.13	-0.08	22,22,23,23	0
4	R5X	L	1004	26/26	0.94	0.13	-0.30	24,28,43,43	0
3	CO3	F	1002	4/4	0.94	0.13	-0.35	15,18,18,19	0
4	R5X	H	1004	26/26	0.94	0.14	-0.36	27,31,39,39	0
3	CO3	J	1002	4/4	0.98	0.15	-0.52	20,20,20,20	0
3	CO3	G	1002	4/4	0.98	0.11	-0.68	23,23,23,24	0
3	CO3	I	1002	4/4	0.98	0.12	-0.90	21,21,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CO3	D	1002	4/4	0.98	0.10	-1.14	17,18,18,19	0
2	ZN	F	1001	1/1	0.99	0.07	-1.62	28,28,28,28	0
2	ZN	D	1001	1/1	0.99	0.06	-1.88	24,24,24,24	0
2	ZN	L	1001	1/1	1.00	0.07	-1.89	29,29,29,29	0
2	ZN	J	1001	1/1	0.99	0.06	-1.90	23,23,23,23	0
2	ZN	E	1001	1/1	1.00	0.05	-2.02	26,26,26,26	0
2	ZN	K	1003	1/1	1.00	0.04	-2.09	28,28,28,28	0
5	SO4	K	1005	5/5	0.99	0.09	-2.16	23,24,25,25	0
2	ZN	K	1001	1/1	1.00	0.04	-2.36	27,27,27,27	0
2	ZN	I	1001	1/1	0.99	0.07	-2.37	32,32,32,32	0
2	ZN	B	1001	1/1	0.99	0.05	-2.41	35,35,35,35	0
5	SO4	A	1005	5/5	0.99	0.07	-2.52	14,17,19,20	0
2	ZN	F	1003	1/1	0.99	0.05	-2.54	26,26,26,26	0
2	ZN	H	1003	1/1	0.99	0.08	-2.64	34,34,34,34	0
5	SO4	E	1005	5/5	1.00	0.07	-2.67	22,22,22,23	0
2	ZN	B	1003	1/1	0.99	0.05	-2.81	29,29,29,29	0
5	SO4	H	1005	5/5	0.99	0.08	-2.86	16,20,20,21	0
2	ZN	G	1001	1/1	0.99	0.05	-2.97	30,30,30,30	0
2	ZN	A	1001	1/1	0.99	0.04	-3.31	27,27,27,27	0
2	ZN	I	1003	1/1	0.98	0.04	-3.39	29,29,29,29	0
2	ZN	J	1003	1/1	1.00	0.05	-3.42	28,28,28,28	0
2	ZN	E	1003	1/1	0.98	0.04	-3.42	32,32,32,32	0
2	ZN	L	1003	1/1	0.99	0.07	-3.53	30,30,30,30	0
2	ZN	A	1003	1/1	1.00	0.04	-3.58	23,23,23,23	0
2	ZN	C	1003	1/1	0.98	0.05	-3.98	32,32,32,32	0
2	ZN	C	1001	1/1	1.00	0.05	-4.08	28,28,28,28	0
2	ZN	D	1003	1/1	0.99	0.05	-4.24	28,28,28,28	0
2	ZN	G	1003	1/1	0.99	0.07	-4.29	33,33,33,33	0
2	ZN	H	1001	1/1	0.98	0.06	-4.72	30,30,30,30	0
6	1PE	I	1005	10/16	0.89	0.21	-	38,42,43,43	0
6	1PE	B	1005	10/16	0.79	0.25	-	58,61,62,62	0
5	SO4	F	1008	5/5	0.86	0.28	-	92,92,92,92	0
6	1PE	F	1005	8/16	0.88	0.32	-	47,47,48,48	0
6	1PE	E	1007	10/16	0.84	0.22	-	56,59,61,61	0
5	SO4	E	1008	5/5	0.88	0.35	-	87,87,88,88	0

## 6.5 Other polymers

There are no such residues in this entry.