



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 PM GMT

PDB ID : 4K3N
Title : Phosphonic Arginine Mimetics as Inhibitors of the M17 Aminopeptidases from Plasmodium falciparum
Authors : McGowan, S.
Deposited on : 2013-04-11
Resolution : 2.00 Å(reported)

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

The following versions of software and data (see [references ⓘ](#)) 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

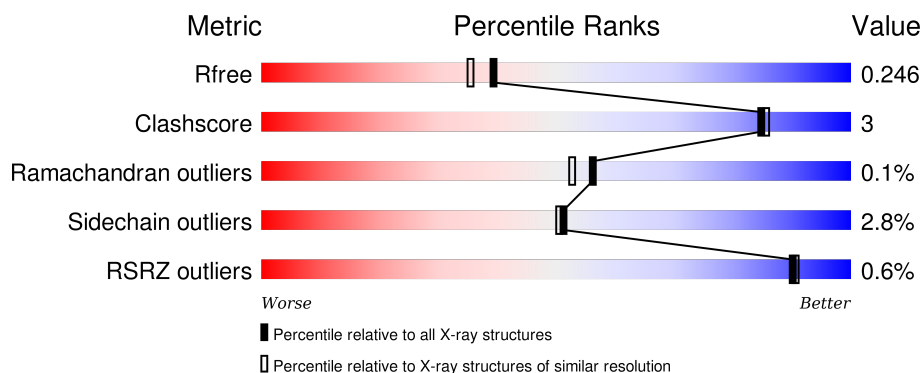
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>91%</div> <div>8%</div> <div>.</div> </div>
1	B	528	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	C	528	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	D	528	<div> <div>%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	E	528	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

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
2	ZN	B	1003	-	-	-	X
2	ZN	C	1001	-	-	-	X
2	ZN	D	1003	-	-	-	X
2	ZN	E	1003	-	-	-	X
2	ZN	H	1003	-	-	-	X
2	ZN	I	1001	-	-	-	X
2	ZN	I	1003	-	-	-	X
2	ZN	J	1003	-	-	-	X
2	ZN	K	1001	-	-	-	X
2	ZN	K	1003	-	-	-	X
3	CO3	C	1002	-	-	-	X
4	1OT	E	1004	-	-	-	X
4	1OT	F	1004	-	-	-	X
4	1OT	I	1004	-	-	-	X
4	1OT	J	1004	-	-	-	X
4	1OT	K	1004	-	-	-	X
4	1OT	L	1004	-	-	-	X
5	SO4	A	1007	-	-	-	X
5	SO4	A	1008	-	-	-	X
5	SO4	E	1006	-	-	-	X
5	SO4	G	1005	-	-	-	X
5	SO4	G	1007	-	-	-	X
5	SO4	I	1006	-	-	-	X
6	1PE	C	1008	-	-	-	X
6	1PE	D	1008	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	D	1009	-	-	-	X
6	1PE	E	1008	-	-	-	X
6	1PE	E	1009	-	-	-	X
6	1PE	F	1008	-	-	-	X
6	1PE	F	1009	-	-	-	X
6	1PE	G	1008	-	-	-	X
6	1PE	G	1011	-	-	-	X
6	1PE	I	1009	-	-	-	X
6	1PE	J	1006	-	-	-	X
6	1PE	J	1008	-	-	-	X
6	1PE	J	1009	-	-	-	X
6	1PE	K	1008	-	-	-	X
6	1PE	K	1010	-	-	-	X
6	1PE	L	1006	-	-	-	X
6	1PE	L	1007	-	-	-	X
6	1PE	L	1008	-	-	-	X
6	1PE	L	1009	-	-	-	X
7	2PE	B	1006	-	-	-	X
7	2PE	B	1007	-	-	-	X
7	2PE	C	1009	-	-	-	X
7	2PE	D	1012	-	-	-	X
7	2PE	E	1010	-	-	-	X
7	2PE	F	1010	-	-	-	X
7	2PE	H	1006	-	-	-	X
7	2PE	H	1007	-	-	-	X
7	2PE	I	1010	-	-	-	X
7	2PE	J	1010	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3995	2564	642	769	20			
1	B	518	Total	C	N	O	S	0	0	0
			3939	2529	638	752	20			
1	C	518	Total	C	N	O	S	0	1	0
			3960	2547	639	754	20			
1	D	514	Total	C	N	O	S	0	0	0
			3947	2539	635	753	20			
1	E	510	Total	C	N	O	S	0	0	0
			3905	2513	626	747	19			
1	F	511	Total	C	N	O	S	0	0	0
			3849	2472	624	734	19			
1	G	519	Total	C	N	O	S	0	0	0
			3993	2562	642	770	19			
1	H	516	Total	C	N	O	S	0	0	0
			3914	2513	632	750	19			
1	I	518	Total	C	N	O	S	0	0	0
			3964	2549	638	757	20			
1	J	513	Total	C	N	O	S	0	0	0
			3939	2536	636	747	20			
1	K	509	Total	C	N	O	S	0	0	0
			3906	2515	625	747	19			
1	L	513	Total	C	N	O	S	0	0	0
			3885	2494	628	744	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	607	HIS	-	EXPRESSION TAG	UNP Q8IL11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
F	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
F	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	610	HIS	-	EXPRESSION TAG	UNP Q8IL11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	611	HIS	-	EXPRESSION TAG	UNP Q8IL11

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

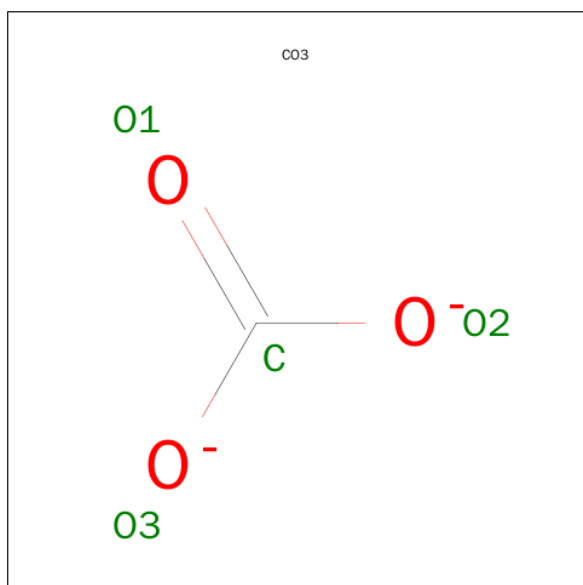
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



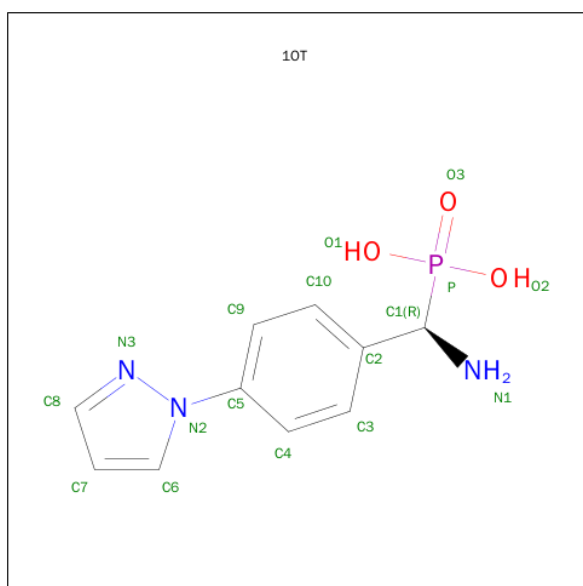
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 {(R)-AMINO[4-(1H-PYRAZOL-1-YL)PHENYL]METHYL}PHOSPHONIC ACID (three-letter code: 1OT) (formula: C₁₀H₁₂N₃O₃P).



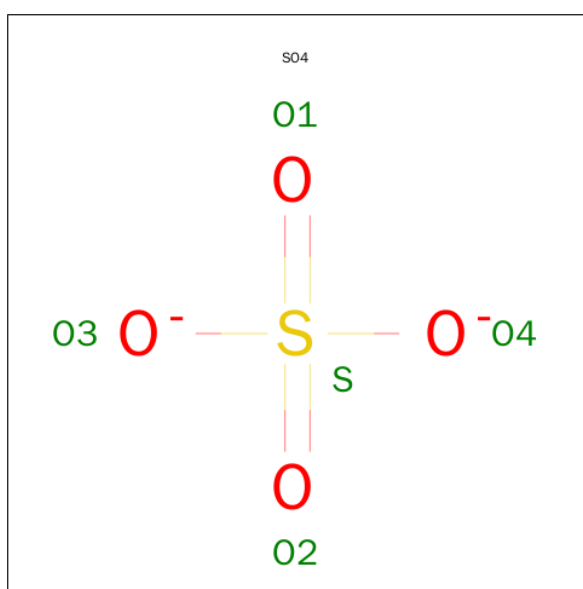
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	B	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	C	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	D	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	E	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	F	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	G	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	H	1	Total	C	N	O	P	0	0
			17	10	3	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	J	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	K	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	L	1	Total	C	N	O	P	0	0
			17	10	3	3	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



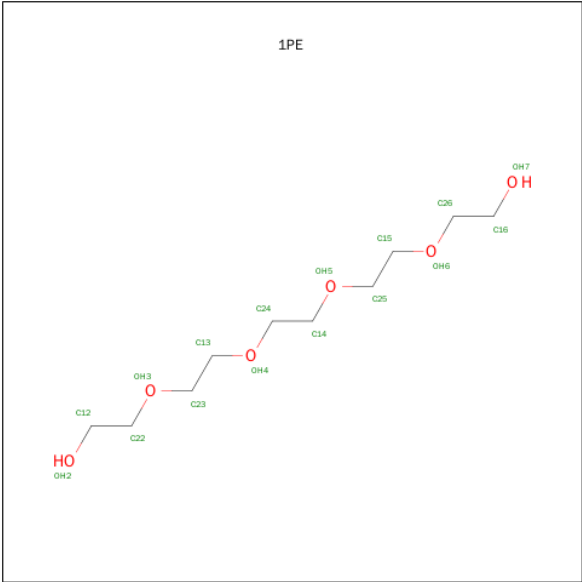
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	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: C₁₀H₂₂O₆).



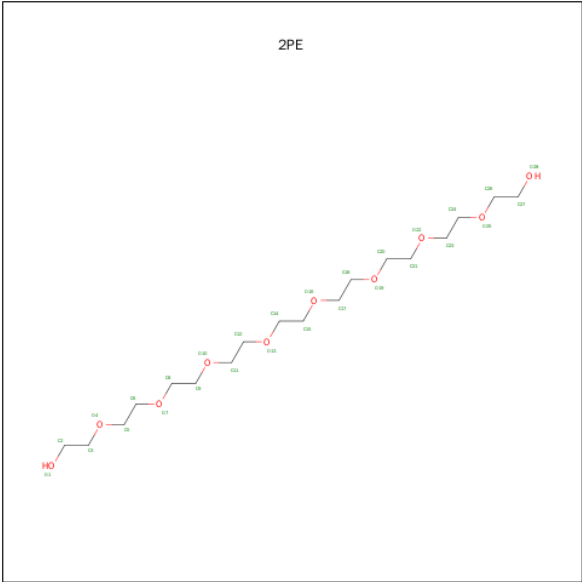
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	A	1	Total	C	O	0	0
			12	8	4		
6	C	1	Total	C	O	0	0
			13	9	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			7	5	2		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			11	8	3		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			26	17	9		
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			9	6	3		
7	D	1	Total	C	O	0	0
			13	9	4		
7	D	1	Total	C	O	0	0
			5	3	2		
7	D	1	Total	C	O	0	0
			9	6	3		
7	E	1	Total	C	O	0	0
			9	6	3		
7	F	1	Total	C	O	0	0
			9	6	3		
7	H	1	Total	C	O	0	0
			25	16	9		
7	H	1	Total	C	O	0	0
			10	7	3		
7	I	1	Total	C	O	0	0
			8	5	3		
7	J	1	Total	C	O	0	0
			10	7	3		

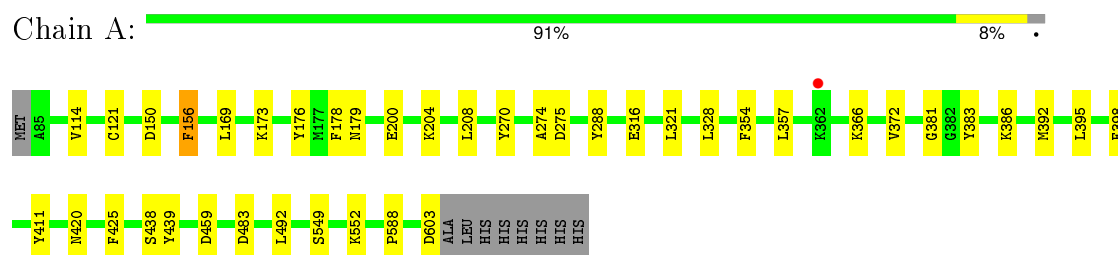
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	173	Total 173	O 173	0	0
8	B	125	Total 125	O 125	0	0
8	C	168	Total 168	O 168	0	0
8	D	150	Total 150	O 150	0	0
8	E	193	Total 193	O 193	0	0
8	F	117	Total 117	O 117	0	0
8	G	145	Total 145	O 145	0	0
8	H	129	Total 129	O 129	0	0
8	I	146	Total 146	O 146	0	0
8	J	137	Total 137	O 137	0	0
8	K	175	Total 175	O 175	0	0
8	L	126	Total 126	O 126	0	0

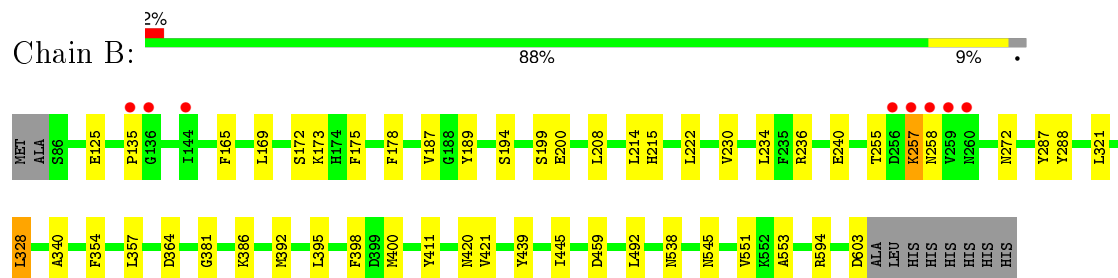
3 Residue-property plots

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.

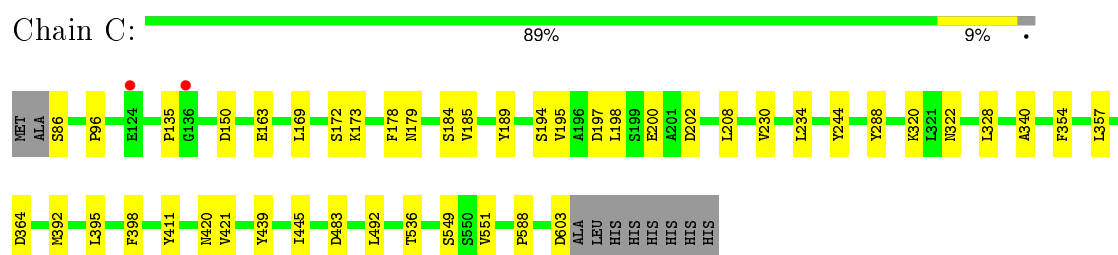
• Molecule 1: M17 leucyl aminopeptidase



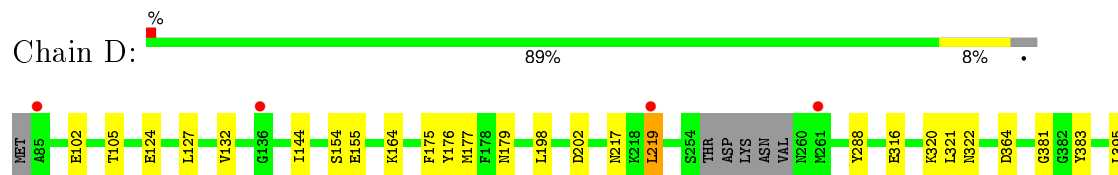
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase

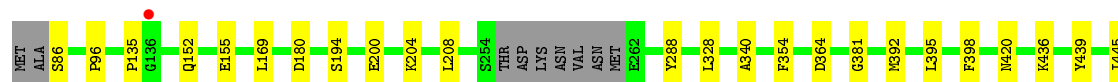


• Molecule 1: M17 leucyl aminopeptidase

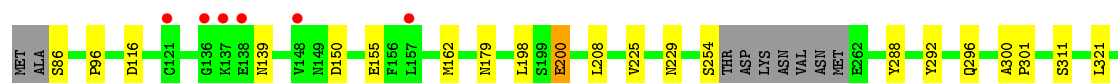
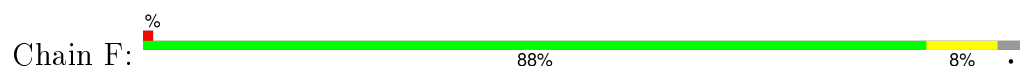




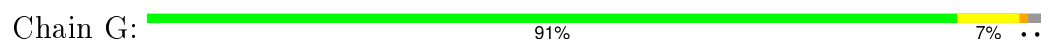
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



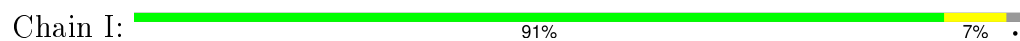
- Molecule 1: M17 leucyl aminopeptidase

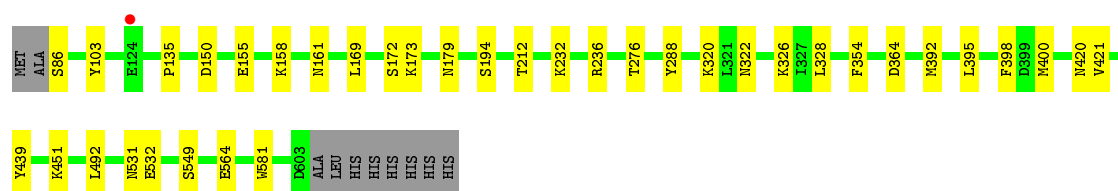


- Molecule 1: M17 leucyl aminopeptidase

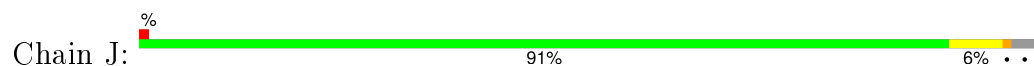


- Molecule 1: M17 leucyl aminopeptidase





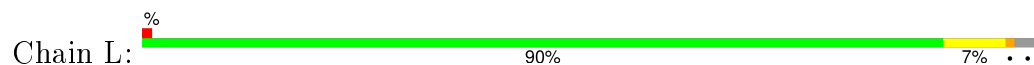
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.72Å 177.08Å 229.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.11 – 2.00 62.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.11-2.00) 99.9 (62.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.196 , 0.240 0.208 , 0.246	Depositor DCC
R_{free} test set	23744 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 472093 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49847	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 43.71 % 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 1.6963e-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, 0.375 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: ZN, 1OT, CO3, 1PE, 2PE, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/4075	0.53	1/5525 (0.0%)
1	B	0.35	0/4017	0.53	0/5455
1	C	0.37	0/4041	0.53	0/5483
1	D	0.36	0/4024	0.53	0/5455
1	E	0.37	0/3982	0.53	0/5403
1	F	0.35	0/3925	0.53	1/5336 (0.0%)
1	G	0.39	0/4071	0.53	0/5521
1	H	0.35	0/3991	0.53	0/5422
1	I	0.36	0/4042	0.52	0/5484
1	J	0.36	0/4016	0.53	0/5443
1	K	0.37	0/3982	0.53	0/5400
1	L	0.37	0/3962	0.52	0/5384
All	All	0.37	0/48128	0.53	2/65311 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	PHE	CG-CD1-CE1	5.96	127.35	120.80
1	F	139	ASN	N-CA-C	5.81	126.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	LYS	Peptide

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	3995	0	3929	20	0
1	B	3939	0	3835	21	0
1	C	3960	0	3890	18	0
1	D	3947	0	3887	37	0
1	E	3905	0	3830	20	0
1	F	3849	0	3722	24	0
1	G	3993	0	3922	26	0
1	H	3914	0	3793	18	0
1	I	3964	0	3897	20	0
1	J	3939	0	3892	27	0
1	K	3906	0	3837	16	0
1	L	3885	0	3760	24	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	1	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
4	A	17	0	10	3	0
4	B	17	0	11	4	0
4	C	17	0	11	2	0
4	D	17	0	12	2	0
4	E	17	0	11	4	0
4	F	17	0	12	3	0
4	G	17	0	10	3	0
4	H	17	0	12	2	0
4	I	17	0	12	2	0
4	J	17	0	11	2	0
4	K	17	0	12	3	0
4	L	17	0	11	4	0
5	A	20	0	0	0	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	15	0	0	0	0
5	H	5	0	0	0	0
5	I	10	0	0	0	0
5	J	5	0	0	1	0
5	K	10	0	0	0	0
5	L	5	0	0	0	0
6	A	21	0	22	1	0
6	C	29	0	30	2	0
6	D	30	0	30	7	0
6	E	32	0	36	3	0
6	F	41	0	51	2	0
6	G	36	0	39	8	0
6	I	31	0	35	3	0
6	J	41	0	48	8	0
6	K	41	0	44	3	0
6	L	41	0	48	9	0
7	B	36	0	45	0	0
7	C	9	0	10	2	0
7	D	27	0	28	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	9	0	10	1	0
7	F	9	0	10	1	0
7	H	35	0	43	2	0
7	I	8	0	8	0	0
7	J	10	0	10	0	0
8	A	173	0	0	0	0
8	B	125	0	0	0	0
8	C	168	0	0	1	0
8	D	150	0	0	5	0
8	E	193	0	0	0	0
8	F	117	0	0	2	0
8	G	145	0	0	0	0
8	H	129	0	0	1	0
8	I	146	0	0	3	0
8	J	137	0	0	3	0
8	K	175	0	0	3	0
8	L	126	0	0	2	0
All	All	49847	0	46876	275	0

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

All (275) 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:I:155:GLU:O	8:I:1103:HOH:O	1.97	0.82
1:I:161:ASN:ND2	8:I:1103:HOH:O	2.17	0.77
1:J:526:TRP:HB3	6:J:1009:1PE:H242	1.67	0.76
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.53	0.73
1:J:536:THR:OG1	8:J:1221:HOH:O	2.06	0.73
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.54	0.72
1:J:411:TYR:HE1	6:J:1006:1PE:H151	1.54	0.71
1:J:525:TRP:HA	6:J:1009:1PE:H132	1.70	0.71
1:J:392:MET:HE3	1:J:395:LEU:HD22	1.73	0.71
1:K:316:GLU:HG3	6:K:1007:1PE:H152	1.73	0.70
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.72	0.69
1:J:320:LYS:HB3	6:J:1006:1PE:H161	1.74	0.69
1:H:320:LYS:HB3	7:H:1006:2PE:H211	1.75	0.69
1:D:320:LYS:HZ1	7:D:1010:2PE:H121	1.59	0.67
1:J:533:TYR:O	1:J:536:THR:HG22	1.96	0.66
1:B:236:ARG:NE	1:B:240:GLU:OE2	2.21	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:567:GLN:OE1	1:G:567:GLN:HA	1.95	0.65
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.79	0.64
1:F:546:GLN:O	8:F:1209:HOH:O	2.15	0.64
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.62	0.62
1:G:316:GLU:HG3	6:G:1011:1PE:H231	1.80	0.62
1:J:411:TYR:CE1	6:J:1006:1PE:H151	2.32	0.62
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.81	0.62
1:D:320:LYS:HZ3	7:D:1010:2PE:H201	1.63	0.62
1:A:156:PHE:CD2	1:A:156:PHE:CZ	2.86	0.61
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.80	0.61
1:E:543:ASP:HB3	6:E:1009:1PE:H232	1.81	0.61
1:D:533:TYR:O	1:D:536:THR:HG22	2.01	0.61
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.84	0.60
1:A:366:LYS:HG2	1:A:420:ASN:HB3	1.84	0.60
1:J:451:LYS:HE3	6:J:1008:1PE:H261	1.82	0.60
1:L:492:LEU:HD11	4:L:1004:1OT:C7	2.33	0.59
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.84	0.59
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.84	0.59
1:D:124:GLU:HA	1:D:179:ASN:HD22	1.67	0.59
1:G:411:TYR:HE1	6:G:1008:1PE:H132	1.68	0.59
1:D:411:TYR:HE1	6:D:1007:1PE:H232	1.68	0.59
1:L:320:LYS:NZ	6:L:1009:1PE:H252	2.18	0.58
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.85	0.58
1:L:320:LYS:HE2	6:L:1009:1PE:H141	1.86	0.58
1:D:492:LEU:HD11	4:D:1004:1OT:C7	2.34	0.58
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.86	0.58
1:F:514:LEU:HD22	6:F:1009:1PE:H142	1.85	0.58
1:A:392:MET:HE3	1:A:395:LEU:HD22	1.86	0.57
1:H:331:LYS:O	1:H:335:GLU:HG3	2.02	0.57
1:F:533:TYR:O	1:F:536:THR:HG22	2.04	0.57
1:A:173:LYS:NZ	1:D:217:ASN:OD1	2.36	0.57
1:E:451:LYS:HG2	6:E:1009:1PE:H231	1.85	0.57
1:B:538:ASN:O	1:B:545:ASN:ND2	2.38	0.57
1:L:320:LYS:HZ1	6:L:1009:1PE:H252	1.69	0.57
1:F:451:LYS:HG2	6:F:1008:1PE:H141	1.87	0.57
1:B:492:LEU:HD11	4:B:1004:1OT:H12	1.87	0.57
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.85	0.56
1:L:533:TYR:O	1:L:536:THR:HG22	2.05	0.56
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.06	0.56
1:B:492:LEU:HD11	4:B:1004:1OT:C7	2.35	0.56
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:NZ	7:D:1010:2PE:H121	2.21	0.55
1:E:492:LEU:HD11	4:E:1004:1OT:C7	2.35	0.55
1:K:96:PRO:HA	6:K:1010:1PE:H141	1.87	0.55
1:H:492:LEU:HD11	4:H:1004:1OT:H12	1.88	0.55
1:F:96:PRO:HA	7:F:1010:2PE:H111	1.88	0.55
1:C:172:SER:O	1:C:173:LYS:HD2	2.06	0.55
1:K:492:LEU:HD11	4:K:1004:1OT:H12	1.89	0.55
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.87	0.55
1:K:174:HIS:HB3	1:K:213:MET:HE2	1.88	0.55
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.86	0.55
1:F:392:MET:HE3	1:F:395:LEU:HD22	1.89	0.55
1:G:392:MET:HE3	1:G:395:LEU:HD22	1.89	0.55
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.87	0.55
1:B:392:MET:HE3	1:B:395:LEU:HD22	1.89	0.55
1:L:436:LYS:NZ	8:L:1226:HOH:O	2.17	0.55
1:K:492:LEU:HD11	4:K:1004:1OT:C7	2.38	0.54
1:D:451:LYS:NZ	6:D:1009:1PE:H242	2.22	0.54
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.39	0.54
1:G:320:LYS:HZ2	6:G:1011:1PE:H251	1.72	0.54
1:G:492:LEU:HD11	4:G:1004:1OT:H12	1.90	0.54
1:E:96:PRO:HA	7:E:1010:2PE:H182	1.90	0.54
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.90	0.54
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.90	0.53
1:A:176:TYR:HB3	8:D:1131:HOH:O	2.08	0.53
1:K:320:LYS:HD3	6:K:1007:1PE:H222	1.91	0.53
1:D:164:LYS:HE2	8:D:1240:HOH:O	2.08	0.53
1:G:326:LYS:HG2	1:G:328:LEU:HD12	1.91	0.53
1:I:392:MET:HE3	1:I:395:LEU:HD22	1.90	0.53
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.90	0.52
1:L:326:LYS:HE3	1:L:328:LEU:HD11	1.90	0.52
1:J:217:ASN:HB2	1:J:219:LEU:HD21	1.90	0.52
1:B:178:PHE:HZ	1:F:155:GLU:HG2	1.75	0.52
1:D:514:LEU:O	1:D:518:LYS:HG2	2.09	0.52
1:B:135:PRO:HA	1:B:194:SER:O	2.08	0.52
1:D:543:ASP:HB3	6:D:1009:1PE:H132	1.90	0.52
4:H:1004:1OT:O2	4:H:1004:1OT:H10	2.10	0.52
1:D:217:ASN:HB3	1:D:219:LEU:HD21	1.92	0.52
1:B:172:SER:O	1:B:173:LYS:HD2	2.10	0.51
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.92	0.51
1:J:492:LEU:HD11	4:J:1004:1OT:C7	2.40	0.51
1:D:175:PHE:HB3	8:D:1131:HOH:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:TYR:OH	1:F:512:LYS:NZ	2.40	0.51
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.10	0.51
1:G:117:ILE:HG13	1:G:270:TYR:HB3	1.92	0.51
1:I:150:ASP:OD1	1:I:179:ASN:HB2	2.10	0.51
1:J:324:GLU:CG	1:J:358:THR:HB	2.41	0.51
1:L:103:TYR:HB2	6:L:1009:IPE:H161	1.93	0.50
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.94	0.50
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.94	0.50
1:G:320:LYS:NZ	6:G:1011:IPE:H251	2.26	0.50
1:H:254:SER:OG	1:H:255:THR:N	2.44	0.49
1:E:200:GLU:O	1:E:204:LYS:HG3	2.12	0.49
1:A:492:LEU:HD11	4:A:1004:IOT:H12	1.93	0.49
1:C:411:TYR:HE1	6:C:1007:IPE:H231	1.76	0.49
1:I:395:LEU:HD11	1:I:581:TRP:CG	2.48	0.49
1:J:104:ASN:N	5:J:1005:SO4:O2	2.40	0.49
1:D:217:ASN:HB2	1:D:219:LEU:HD11	1.95	0.49
1:F:200:GLU:HG3	8:F:1122:HOH:O	2.13	0.49
1:C:364:ASP:O	1:C:420:ASN:HA	2.12	0.49
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.42	0.49
1:J:548:SER:OG	8:J:1221:HOH:O	2.19	0.48
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.48	0.48
1:B:364:ASP:O	1:B:420:ASN:HA	2.13	0.48
1:K:164:LYS:NZ	8:K:1188:HOH:O	2.46	0.48
1:C:392:MET:HE3	1:C:395:LEU:HD22	1.94	0.48
1:L:492:LEU:HD11	4:L:1004:IOT:H12	1.96	0.48
1:H:364:ASP:O	1:H:420:ASN:HA	2.13	0.48
1:G:320:LYS:HD3	6:G:1011:IPE:H162	1.94	0.48
1:I:451:LYS:HE3	1:I:564:GLU:O	2.14	0.48
1:I:135:PRO:HA	1:I:194:SER:O	2.14	0.48
1:I:232:LYS:NZ	1:I:276:THR:O	2.46	0.48
1:G:320:LYS:HZ2	6:G:1011:IPE:H161	1.79	0.47
1:G:121:CYS:HA	1:G:270:TYR:CE2	2.49	0.47
1:A:316:GLU:HG3	6:A:1010:IPE:H131	1.95	0.47
4:B:1004:IOT:O2	4:B:1004:IOT:H10	2.14	0.47
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.95	0.47
1:J:364:ASP:O	1:J:420:ASN:HA	2.15	0.47
1:L:543:ASP:HB3	6:L:1007:IPE:H221	1.96	0.47
1:H:202:ASP:OD1	1:H:205:ARG:NH1	2.48	0.47
1:K:102:GLU:HG3	8:K:1272:HOH:O	2.15	0.47
1:G:103:TYR:CD1	6:G:1011:IPE:H252	2.50	0.47
4:J:1004:IOT:O2	4:J:1004:IOT:H10	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:492:LEU:HD11	4:F:1004:1OT:H12	1.96	0.47
1:I:531:ASN:HB2	6:I:1009:1PE:H241	1.94	0.47
1:G:367:LYS:HD3	1:G:480:TYR:CE2	2.50	0.47
1:H:104:ASN:HB3	8:H:1207:HOH:O	2.14	0.47
4:E:1004:1OT:O2	4:E:1004:1OT:H10	2.14	0.47
1:K:117:ILE:HG12	1:K:270:TYR:HB3	1.96	0.47
1:H:165:PHE:HB3	1:H:189:TYR:OH	2.14	0.47
7:D:1012:2PE:H121	8:D:1222:HOH:O	2.15	0.47
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.97	0.46
1:D:451:LYS:HG2	6:D:1009:1PE:H251	1.97	0.46
1:A:492:LEU:HD11	4:A:1004:1OT:C7	2.45	0.46
1:L:451:LYS:HZ3	6:L:1007:1PE:H141	1.80	0.46
1:C:195:VAL:HG12	1:C:197:ASP:H	1.81	0.46
1:D:364:ASP:O	1:D:420:ASN:HA	2.15	0.46
1:E:392:MET:HE3	1:E:395:LEU:HD22	1.97	0.46
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.97	0.46
1:L:518:LYS:NZ	6:L:1008:1PE:H131	2.31	0.46
1:F:150:ASP:OD1	1:F:179:ASN:HB2	2.16	0.46
1:C:536:THR:HG21	1:C:551:VAL:HG23	1.97	0.46
1:C:244:TYR:OH	1:C:588:PRO:O	2.32	0.46
1:E:543:ASP:CB	6:E:1009:1PE:H232	2.45	0.46
1:D:177:MET:HB3	8:D:1131:HOH:O	2.16	0.46
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.98	0.46
3:D:1002:CO3:O1	4:D:1004:1OT:O3	2.33	0.45
1:I:172:SER:O	1:I:173:LYS:HD2	2.15	0.45
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.97	0.45
1:J:320:LYS:NZ	6:J:1007:1PE:OH5	2.49	0.45
1:F:492:LEU:HD11	4:F:1004:1OT:C7	2.46	0.45
1:H:135:PRO:HA	1:H:194:SER:O	2.17	0.45
1:E:492:LEU:HD11	4:E:1004:1OT:H12	1.97	0.45
1:H:122:ASN:HD22	7:H:1007:2PE:H171	1.81	0.45
1:F:292:TYR:O	1:F:296:GLN:HG3	2.17	0.45
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.16	0.45
1:C:320:LYS:NZ	6:C:1006:1PE:OH6	2.50	0.45
1:D:411:TYR:CE1	6:D:1007:1PE:H232	2.51	0.44
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.17	0.44
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.98	0.44
1:D:451:LYS:HE3	1:D:564:GLU:O	2.17	0.44
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.53	0.44
1:K:364:ASP:O	1:K:420:ASN:HA	2.18	0.44
4:K:1004:1OT:H10	4:K:1004:1OT:O1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:LYS:HZ2	6:D:1009:1PE:H242	1.82	0.44
1:I:532:GLU:HG3	1:J:205:ARG:HH22	1.82	0.44
1:E:518:LYS:HE2	1:E:518:LYS:HB2	1.56	0.44
1:G:164:LYS:HD3	1:G:165:PHE:CE1	2.52	0.44
1:H:150:ASP:O	1:H:154:SER:HB2	2.17	0.44
1:K:172:SER:HB2	1:K:213:MET:HE1	2.00	0.44
1:A:383:TYR:HE2	1:A:438:SER:HB2	1.83	0.44
1:B:173:LYS:HB2	1:B:189:TYR:CE1	2.52	0.44
1:I:320:LYS:HD3	6:I:1007:1PE:H161	2.00	0.43
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.99	0.43
1:B:287:TYR:CD2	1:B:594:ARG:HG2	2.53	0.43
1:I:103:TYR:HB3	6:I:1008:1PE:H142	2.00	0.43
1:L:518:LYS:HZ1	6:L:1008:1PE:H131	1.83	0.43
1:C:135:PRO:HA	1:C:194:SER:O	2.19	0.43
1:H:117:ILE:HD11	1:H:146:SER:OG	2.18	0.43
4:C:1004:1OT:O2	4:C:1004:1OT:H10	2.17	0.43
1:C:492:LEU:HD11	4:C:1004:1OT:H12	2.00	0.43
1:I:326:LYS:HE3	1:I:328:LEU:HD11	2.00	0.43
1:E:579:VAL:O	1:E:589:LYS:HD2	2.18	0.43
1:D:127:LEU:HB2	1:D:219:LEU:HD22	1.99	0.43
1:E:536:THR:HG21	1:E:551:VAL:CG2	2.47	0.43
1:C:96:PRO:HA	7:C:1009:2PE:H172	2.00	0.43
1:B:381:GLY:HA2	1:B:459:ASP:OD1	2.18	0.43
4:G:1004:1OT:H10	4:G:1004:1OT:O2	2.19	0.43
1:E:364:ASP:O	1:E:420:ASN:HA	2.19	0.43
1:I:492:LEU:HD11	4:I:1004:1OT:H12	2.01	0.43
1:L:360:LYS:HD2	1:L:361:SER:O	2.18	0.43
1:A:381:GLY:HA2	1:A:459:ASP:OD1	2.18	0.43
1:B:175:PHE:N	1:B:187:VAL:O	2.41	0.42
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.01	0.42
1:L:311:SER:O	1:L:315:VAL:HG23	2.19	0.42
1:J:381:GLY:HA2	1:J:459:ASP:OD1	2.19	0.42
1:D:219:LEU:H	1:D:219:LEU:HG	1.30	0.42
1:J:219:LEU:HG	1:J:219:LEU:H	1.16	0.42
1:E:392:MET:HE2	4:E:1004:1OT:C8	2.50	0.42
1:I:492:LEU:HD23	1:I:492:LEU:HA	1.82	0.42
1:L:498:SER:O	1:L:523:PRO:HG2	2.19	0.42
1:D:198:LEU:HD22	1:D:202:ASP:HB3	2.02	0.42
1:D:321:LEU:HD11	1:D:411:TYR:HA	2.01	0.42
1:F:386:LYS:NZ	4:F:1004:1OT:O2	2.41	0.42
4:I:1004:1OT:H10	4:I:1004:1OT:O2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:TYR:HE2	1:D:438:SER:HB2	1.85	0.42
1:G:411:TYR:CE1	6:G:1008:1PE:H132	2.50	0.42
1:D:176:TYR:OH	1:D:217:ASN:OD1	2.20	0.42
1:C:173:LYS:HB2	1:C:189:TYR:CE1	2.55	0.42
1:L:200:GLU:HG3	8:L:1158:HOH:O	2.19	0.42
1:I:364:ASP:O	1:I:420:ASN:HA	2.19	0.42
1:D:381:GLY:HA2	1:D:459:ASP:OD1	2.20	0.42
1:F:360:LYS:HA	1:F:360:LYS:HD2	1.91	0.42
1:D:451:LYS:CG	6:D:1009:1PE:H251	2.50	0.42
1:C:230:VAL:HG12	1:C:234:LEU:HD23	2.02	0.42
1:D:597:THR:HG22	1:D:601:LEU:HD22	2.02	0.42
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.55	0.42
3:L:1002:CO3:O1	4:L:1004:1OT:O3	2.38	0.41
1:E:135:PRO:HA	1:E:194:SER:O	2.20	0.41
1:A:386:LYS:NZ	4:A:1004:1OT:O2	2.43	0.41
1:G:488:THR:HG21	1:G:555:SER:HA	2.02	0.41
1:J:332:GLU:HG3	8:J:1209:HOH:O	2.20	0.41
1:F:341:TYR:CE1	1:F:428:ALA:HB1	2.55	0.41
1:J:451:LYS:HE3	6:J:1008:1PE:H151	2.02	0.41
1:G:386:LYS:NZ	4:G:1004:1OT:O2	2.38	0.41
1:F:360:LYS:HD2	1:F:361:SER:N	2.34	0.41
1:D:132:VAL:HG21	1:D:144:ILE:HD13	2.03	0.41
1:D:395:LEU:HD11	1:D:581:TRP:CG	2.56	0.41
1:K:514:LEU:O	1:K:518:LYS:HG2	2.20	0.41
1:L:198:LEU:HD12	1:L:198:LEU:HA	1.84	0.41
1:I:158:LYS:HB2	8:I:1103:HOH:O	2.20	0.41
1:K:213:MET:HE3	8:K:1179:HOH:O	2.19	0.41
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.02	0.41
1:E:152:GLN:HG2	1:E:180:ASP:OD1	2.20	0.41
1:L:451:LYS:HE2	6:L:1007:1PE:H251	2.03	0.41
1:K:102:GLU:HG2	1:K:105:THR:HG22	2.02	0.41
1:D:102:GLU:HG2	1:D:105:THR:HG22	2.03	0.41
1:A:372:VAL:O	1:A:483:ASP:HA	2.21	0.41
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.03	0.41
1:B:386:LYS:NZ	4:B:1004:1OT:O2	2.42	0.41
7:C:1009:2PE:H141	8:C:1146:HOH:O	2.20	0.41
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.03	0.41
1:L:127:LEU:HD11	1:L:129:ILE:HD11	2.03	0.41
1:D:316:GLU:HG2	1:D:320:LYS:HE2	2.02	0.40
1:B:551:VAL:HG12	1:B:553:ALA:H	1.87	0.40
1:F:162:MET:HA	1:F:162:MET:HE2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:236:ARG:HH11	1:I:236:ARG:HD3	1.75	0.40
1:J:262:GLU:OE1	1:J:262:GLU:HA	2.21	0.40
1:F:360:LYS:HZ2	1:F:361:SER:HB2	1.86	0.40
1:D:320:LYS:HZ1	7:D:1010:2PE:C15	2.34	0.40
4:L:1004:1OT:H10	4:L:1004:1OT:O1	2.22	0.40
1:B:165:PHE:CE2	1:B:173:LYS:HG2	2.56	0.40
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.87	0.40
1:J:579:VAL:O	1:J:589:LYS:HD2	2.22	0.40
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.04	0.40
1:G:492:LEU:HD23	1:G:492:LEU:HA	1.89	0.40
1:H:488:THR:HG21	1:H:555:SER:HA	2.03	0.40
1:F:311:SER:HB2	1:F:327:ILE:HD12	2.03	0.40
1:C:198:LEU:HD22	1:C:202:ASP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/528 (98%)	507 (98%)	11 (2%)	0	100	100
1	B	516/528 (98%)	503 (98%)	11 (2%)	2 (0%)	39	33
1	C	517/528 (98%)	505 (98%)	12 (2%)	0	100	100
1	D	510/528 (97%)	498 (98%)	12 (2%)	0	100	100
1	E	506/528 (96%)	495 (98%)	11 (2%)	0	100	100
1	F	507/528 (96%)	497 (98%)	10 (2%)	0	100	100
1	G	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
1	H	512/528 (97%)	502 (98%)	9 (2%)	1 (0%)	52	48
1	I	516/528 (98%)	505 (98%)	11 (2%)	0	100	100
1	J	509/528 (96%)	498 (98%)	11 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	503/528 (95%)	494 (98%)	8 (2%)	1 (0%)	52	48
1	L	509/528 (96%)	500 (98%)	8 (2%)	1 (0%)	52	48
All	All	6140/6336 (97%)	6011 (98%)	124 (2%)	5 (0%)	56	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	GLU
1	L	137	LYS
1	B	257	LYS
1	B	258	ASN
1	K	363	GLY

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	429/455 (94%)	417 (97%)	12 (3%)	51	50
1	B	415/455 (91%)	399 (96%)	16 (4%)	39	35
1	C	421/455 (92%)	405 (96%)	16 (4%)	40	36
1	D	421/455 (92%)	414 (98%)	7 (2%)	68	71
1	E	416/455 (91%)	409 (98%)	7 (2%)	68	71
1	F	401/455 (88%)	389 (97%)	12 (3%)	48	47
1	G	428/455 (94%)	415 (97%)	13 (3%)	48	47
1	H	411/455 (90%)	395 (96%)	16 (4%)	39	35
1	I	423/455 (93%)	413 (98%)	10 (2%)	57	58
1	J	420/455 (92%)	412 (98%)	8 (2%)	65	67
1	K	417/455 (92%)	409 (98%)	8 (2%)	65	67
1	L	407/455 (90%)	393 (97%)	14 (3%)	44	41
All	All	5009/5460 (92%)	4870 (97%)	139 (3%)	51	50

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	200	GLU
1	A	204	LYS
1	A	208	LEU
1	A	275	ASP
1	A	288	TYR
1	A	398	PHE
1	A	439	TYR
1	A	549	SER
1	A	552	LYS
1	A	588	PRO
1	A	603	ASP
1	B	125	GLU
1	B	169	LEU
1	B	199	SER
1	B	200	GLU
1	B	208	LEU
1	B	215	HIS
1	B	255	THR
1	B	272	ASN
1	B	288	TYR
1	B	328	LEU
1	B	357	LEU
1	B	398	PHE
1	B	400	MET
1	B	421	VAL
1	B	439	TYR
1	B	603	ASP
1	C	86	SER
1	C	163	GLU
1	C	169	LEU
1	C	184	SER
1	C	185	VAL
1	C	200	GLU
1	C	208	LEU
1	C	288	TYR
1	C	322	ASN
1	C	357	LEU
1	C	398	PHE
1	C	421	VAL
1	C	439	TYR
1	C	483	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	549	SER
1	C	603	ASP
1	D	154	SER
1	D	219	LEU
1	D	288	TYR
1	D	322	ASN
1	D	398	PHE
1	D	439	TYR
1	D	552	LYS
1	E	86	SER
1	E	169	LEU
1	E	208	LEU
1	E	288	TYR
1	E	398	PHE
1	E	436	LYS
1	E	439	TYR
1	F	86	SER
1	F	116	ASP
1	F	198	LEU
1	F	200	GLU
1	F	208	LEU
1	F	225	VAL
1	F	229	ASN
1	F	254	SER
1	F	288	TYR
1	F	364	ASP
1	F	398	PHE
1	F	439	TYR
1	G	117	ILE
1	G	164	LYS
1	G	169	LEU
1	G	200	GLU
1	G	204	LYS
1	G	208	LEU
1	G	288	TYR
1	G	367	LYS
1	G	398	PHE
1	G	436	LYS
1	G	439	TYR
1	G	588	PRO
1	G	603	ASP
1	H	86	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	125	GLU
1	H	154	SER
1	H	164	LYS
1	H	173	LYS
1	H	181	ASN
1	H	200	GLU
1	H	208	LEU
1	H	215	HIS
1	H	254	SER
1	H	288	TYR
1	H	357	LEU
1	H	398	PHE
1	H	421	VAL
1	H	439	TYR
1	H	603	ASP
1	I	86	SER
1	I	169	LEU
1	I	212	THR
1	I	288	TYR
1	I	322	ASN
1	I	398	PHE
1	I	400	MET
1	I	421	VAL
1	I	439	TYR
1	I	549	SER
1	J	200	GLU
1	J	205	ARG
1	J	219	LEU
1	J	262	GLU
1	J	288	TYR
1	J	398	PHE
1	J	439	TYR
1	J	518	LYS
1	K	86	SER
1	K	132	VAL
1	K	145	SER
1	K	169	LEU
1	K	216	ASP
1	K	288	TYR
1	K	398	PHE
1	K	439	TYR
1	L	86	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	113	GLN
1	L	116	ASP
1	L	169	LEU
1	L	198	LEU
1	L	200	GLU
1	L	254	SER
1	L	288	TYR
1	L	295	SER
1	L	398	PHE
1	L	421	VAL
1	L	436	LYS
1	L	439	TYR
1	L	603	ASP

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

Mol	Chain	Res	Type
1	J	531	ASN
1	K	229	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 115 ligands modelled in this entry, 24 are monoatomic - leaving 91 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	1OT	A	1004	2	16,18,18	2.80	6 (37%)	21,26,26	2.87	11 (52%)
5	SO4	A	1005	-	4,4,4	0.16	0	6,6,6	0.20	0
5	SO4	A	1006	-	4,4,4	0.23	0	6,6,6	0.23	0
5	SO4	A	1007	-	4,4,4	0.24	0	6,6,6	0.26	0
5	SO4	A	1008	-	4,4,4	0.10	0	6,6,6	0.21	0
6	1PE	A	1009	-	8,8,15	0.44	0	7,7,14	0.29	0
6	1PE	A	1010	-	11,11,15	0.52	0	10,10,14	0.15	0
3	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	B	1004	2	16,18,18	2.81	6 (37%)	21,26,26	2.75	10 (47%)
5	SO4	B	1005	-	4,4,4	0.18	0	6,6,6	0.07	0
7	2PE	B	1006	-	25,25,27	0.19	0	24,24,26	0.17	0
7	2PE	B	1007	-	9,9,27	0.07	0	8,8,26	0.24	0
3	CO3	C	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	C	1004	2	16,18,18	2.71	6 (37%)	21,26,26	2.71	11 (52%)
5	SO4	C	1005	-	4,4,4	0.31	0	6,6,6	0.23	0
6	1PE	C	1006	-	12,12,15	0.55	0	11,11,14	0.21	0
6	1PE	C	1007	-	8,8,15	0.43	0	7,7,14	0.22	0
6	1PE	C	1008	-	6,6,15	0.50	0	5,5,14	0.25	0
7	2PE	C	1009	-	8,8,27	0.17	0	7,7,26	0.25	0
3	CO3	D	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	D	1004	2	16,18,18	2.86	6 (37%)	21,26,26	3.01	12 (57%)
5	SO4	D	1005	-	4,4,4	0.34	0	6,6,6	0.17	0
5	SO4	D	1006	-	4,4,4	0.25	0	6,6,6	0.08	0
6	1PE	D	1007	-	9,9,15	0.45	0	8,8,14	0.43	0
6	1PE	D	1008	-	8,8,15	0.51	0	7,7,14	0.22	0
6	1PE	D	1009	-	10,10,15	0.54	0	9,9,14	0.39	0
7	2PE	D	1010	-	12,12,27	0.21	0	11,11,26	0.15	0
7	2PE	D	1011	-	4,4,27	0.25	0	3,3,26	0.36	0
7	2PE	D	1012	-	8,8,27	0.19	0	7,7,26	0.17	0
3	CO3	E	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	E	1004	2	16,18,18	2.82	6 (37%)	21,26,26	2.86	12 (57%)
5	SO4	E	1005	-	4,4,4	0.28	0	6,6,6	0.20	0
5	SO4	E	1006	-	4,4,4	0.21	0	6,6,6	0.34	0
6	1PE	E	1007	-	11,11,15	0.49	0	10,10,14	0.34	0
6	1PE	E	1008	-	11,11,15	0.50	0	10,10,14	0.31	0
6	1PE	E	1009	-	7,7,15	0.44	0	6,6,14	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	2PE	E	1010	-	8,8,27	0.15	0	7,7,26	0.18	0
3	CO3	F	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	F	1004	2	16,18,18	2.78	6 (37%)	21,26,26	2.77	11 (52%)
5	SO4	F	1005	-	4,4,4	0.22	0	6,6,6	0.08	0
6	1PE	F	1006	-	9,9,15	0.44	0	8,8,14	0.25	0
6	1PE	F	1007	-	9,9,15	0.48	0	8,8,14	0.15	0
6	1PE	F	1008	-	9,9,15	0.47	0	8,8,14	0.21	0
6	1PE	F	1009	-	10,10,15	0.48	0	9,9,14	0.23	0
7	2PE	F	1010	-	8,8,27	0.22	0	7,7,26	0.21	0
3	CO3	G	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	G	1004	2	16,18,18	2.76	6 (37%)	21,26,26	2.64	8 (38%)
5	SO4	G	1005	-	4,4,4	0.25	0	6,6,6	0.25	0
5	SO4	G	1006	-	4,4,4	0.26	0	6,6,6	0.31	0
5	SO4	G	1007	-	4,4,4	0.13	0	6,6,6	0.15	0
6	1PE	G	1008	-	8,8,15	0.42	0	7,7,14	0.36	0
6	1PE	G	1009	-	5,5,15	0.45	0	4,4,14	0.51	0
6	1PE	G	1010	-	5,5,15	0.49	0	4,4,14	0.34	0
6	1PE	G	1011	-	14,14,15	0.42	0	13,13,14	0.58	0
3	CO3	H	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	H	1004	2	16,18,18	2.82	6 (37%)	21,26,26	2.63	8 (38%)
5	SO4	H	1005	-	4,4,4	0.08	0	6,6,6	0.29	0
7	2PE	H	1006	-	24,24,27	0.21	0	23,23,26	0.16	0
7	2PE	H	1007	-	9,9,27	0.22	0	8,8,26	0.09	0
3	CO3	I	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	I	1004	2	16,18,18	2.66	6 (37%)	21,26,26	2.84	13 (61%)
5	SO4	I	1005	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	I	1006	-	4,4,4	0.31	0	6,6,6	0.16	0
6	1PE	I	1007	-	14,14,15	0.40	0	13,13,14	0.49	0
6	1PE	I	1008	-	10,10,15	0.47	0	9,9,14	0.33	0
6	1PE	I	1009	-	4,4,15	0.39	0	3,3,14	0.29	0
7	2PE	I	1010	-	7,7,27	0.16	0	6,6,26	0.12	0
3	CO3	J	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	J	1004	2	16,18,18	2.77	6 (37%)	21,26,26	2.75	10 (47%)
5	SO4	J	1005	-	4,4,4	0.26	0	6,6,6	0.10	0
6	1PE	J	1006	-	10,10,15	0.44	0	9,9,14	0.45	0
6	1PE	J	1007	-	9,9,15	0.52	0	8,8,14	0.29	0
6	1PE	J	1008	-	10,10,15	0.55	0	9,9,14	0.28	0
6	1PE	J	1009	-	8,8,15	0.55	0	7,7,14	0.37	0
7	2PE	J	1010	-	9,9,27	0.23	0	8,8,26	0.12	0
3	CO3	K	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	K	1004	2	16,18,18	2.70	6 (37%)	21,26,26	2.75	11 (52%)
5	SO4	K	1005	-	4,4,4	0.25	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	K	1006	-	4,4,4	0.27	0	6,6,6	0.07	0
6	1PE	K	1007	-	11,11,15	0.53	0	10,10,14	0.44	0
6	1PE	K	1008	-	11,11,15	0.47	0	10,10,14	0.22	0
6	1PE	K	1009	-	10,10,15	0.48	0	9,9,14	0.15	0
6	1PE	K	1010	-	5,5,15	0.48	0	4,4,14	0.16	0
3	CO3	L	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	1OT	L	1004	2	16,18,18	2.78	6 (37%)	21,26,26	2.88	11 (52%)
5	SO4	L	1005	-	4,4,4	0.21	0	6,6,6	0.14	0
6	1PE	L	1006	-	9,9,15	0.37	0	8,8,14	0.69	0
6	1PE	L	1007	-	11,11,15	0.53	0	10,10,14	0.21	0
6	1PE	L	1008	-	7,7,15	0.46	0	6,6,14	0.38	0
6	1PE	L	1009	-	10,10,15	0.51	0	9,9,14	0.50	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	1OT	A	1004	2	-	0/13/14/14	0/2/2/2
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
5	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
6	1PE	A	1009	-	-	0/6/6/13	0/0/0/0
6	1PE	A	1010	-	-	0/9/9/13	0/0/0/0
3	CO3	B	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	B	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
7	2PE	B	1006	-	-	0/23/23/25	0/0/0/0
7	2PE	B	1007	-	-	0/7/7/25	0/0/0/0
3	CO3	C	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	C	1004	2	-	0/13/14/14	0/2/2/2
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
6	1PE	C	1008	-	-	0/4/4/13	0/0/0/0
7	2PE	C	1009	-	-	0/6/6/25	0/0/0/0
3	CO3	D	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	D	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	D	1005	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/6/6/13	0/0/0/0
6	1PE	D	1009	-	-	0/8/8/13	0/0/0/0
7	2PE	D	1010	-	-	0/10/10/25	0/0/0/0
7	2PE	D	1011	-	-	0/2/2/25	0/0/0/0
7	2PE	D	1012	-	-	0/6/6/25	0/0/0/0
3	CO3	E	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	E	1004	2	-	0/13/14/14	0/2/2/2
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
6	1PE	E	1009	-	-	0/5/5/13	0/0/0/0
7	2PE	E	1010	-	-	0/6/6/25	0/0/0/0
3	CO3	F	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	F	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	F	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	F	1006	-	-	0/7/7/13	0/0/0/0
6	1PE	F	1007	-	-	0/7/7/13	0/0/0/0
6	1PE	F	1008	-	-	0/7/7/13	0/0/0/0
6	1PE	F	1009	-	-	0/8/8/13	0/0/0/0
7	2PE	F	1010	-	-	0/6/6/25	0/0/0/0
3	CO3	G	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	G	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	G	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	G	1006	-	-	0/0/0/0	0/0/0/0
5	SO4	G	1007	-	-	0/0/0/0	0/0/0/0
6	1PE	G	1008	-	-	0/6/6/13	0/0/0/0
6	1PE	G	1009	-	-	0/3/3/13	0/0/0/0
6	1PE	G	1010	-	-	0/3/3/13	0/0/0/0
6	1PE	G	1011	-	-	0/12/12/13	0/0/0/0
3	CO3	H	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	H	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	H	1005	-	-	0/0/0/0	0/0/0/0
7	2PE	H	1006	-	-	0/22/22/25	0/0/0/0
7	2PE	H	1007	-	-	0/7/7/25	0/0/0/0
3	CO3	I	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	I	1004	2	-	0/13/14/14	0/2/2/2
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	-	-	0/12/12/13	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	I	1008	-	-	0/8/8/13	0/0/0/0
6	1PE	I	1009	-	-	0/2/2/13	0/0/0/0
7	2PE	I	1010	-	-	0/5/5/25	0/0/0/0
3	CO3	J	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	J	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	J	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	J	1006	-	-	0/8/8/13	0/0/0/0
6	1PE	J	1007	-	-	0/7/7/13	0/0/0/0
6	1PE	J	1008	-	-	0/8/8/13	0/0/0/0
6	1PE	J	1009	-	-	0/6/6/13	0/0/0/0
7	2PE	J	1010	-	-	0/7/7/25	0/0/0/0
3	CO3	K	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	K	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	K	1005	-	-	0/0/0/0	0/0/0/0
5	SO4	K	1006	-	-	0/0/0/0	0/0/0/0
6	1PE	K	1007	-	-	0/9/9/13	0/0/0/0
6	1PE	K	1008	-	-	0/9/9/13	0/0/0/0
6	1PE	K	1009	-	-	0/8/8/13	0/0/0/0
6	1PE	K	1010	-	-	0/3/3/13	0/0/0/0
3	CO3	L	1002	-	-	0/0/0/0	0/0/0/0
4	1OT	L	1004	2	-	0/13/14/14	0/2/2/2
5	SO4	L	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	L	1006	-	-	0/7/7/13	0/0/0/0
6	1PE	L	1007	-	-	0/9/9/13	0/0/0/0
6	1PE	L	1008	-	-	0/5/5/13	0/0/0/0
6	1PE	L	1009	-	-	0/8/8/13	0/0/0/0

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1004	1OT	C5-N2	-5.50	1.33	1.44
4	E	1004	1OT	C5-N2	-5.47	1.33	1.44
4	A	1004	1OT	C5-N2	-5.31	1.33	1.44
4	B	1004	1OT	C5-N2	-5.27	1.33	1.44
4	J	1004	1OT	C5-N2	-5.27	1.33	1.44
4	D	1004	1OT	C5-N2	-5.26	1.33	1.44
4	G	1004	1OT	C5-N2	-5.26	1.33	1.44
4	F	1004	1OT	C5-N2	-5.25	1.33	1.44
4	K	1004	1OT	C5-N2	-5.25	1.33	1.44
4	H	1004	1OT	C5-N2	-5.23	1.33	1.44
4	C	1004	1OT	C5-N2	-5.10	1.33	1.44
4	I	1004	1OT	C5-N2	-4.99	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1004	1OT	P-O1	-3.95	1.48	1.54
4	H	1004	1OT	P-O1	-3.92	1.48	1.54
4	I	1004	1OT	P-O1	-3.76	1.48	1.54
4	E	1004	1OT	P-O1	-3.75	1.48	1.54
4	A	1004	1OT	P-O1	-3.67	1.48	1.54
4	C	1004	1OT	P-O1	-3.52	1.49	1.54
4	L	1004	1OT	P-O1	-3.50	1.49	1.54
4	A	1004	1OT	C2-C1	-3.43	1.47	1.52
4	K	1004	1OT	C2-C1	-3.42	1.47	1.52
4	H	1004	1OT	C2-C1	-3.39	1.47	1.52
4	F	1004	1OT	P-O1	-3.36	1.49	1.54
4	G	1004	1OT	C2-C1	-3.36	1.47	1.52
4	G	1004	1OT	P-O1	-3.26	1.49	1.54
4	J	1004	1OT	C2-C1	-3.25	1.47	1.52
4	I	1004	1OT	C2-C1	-3.23	1.47	1.52
4	L	1004	1OT	C2-C1	-3.18	1.48	1.52
4	D	1004	1OT	P-O1	-3.14	1.49	1.54
4	J	1004	1OT	P-O1	-3.10	1.49	1.54
4	D	1004	1OT	C2-C1	-3.06	1.48	1.52
4	E	1004	1OT	C2-C1	-3.03	1.48	1.52
4	B	1004	1OT	C2-C1	-3.02	1.48	1.52
4	K	1004	1OT	P-O1	-2.91	1.50	1.54
4	F	1004	1OT	C2-C1	-2.81	1.48	1.52
4	C	1004	1OT	C2-C1	-2.73	1.48	1.52
4	F	1004	1OT	C6-N2	-2.55	1.32	1.36
4	J	1004	1OT	C6-N2	-2.49	1.33	1.36
4	K	1004	1OT	C6-N2	-2.46	1.33	1.36
4	E	1004	1OT	C6-N2	-2.40	1.33	1.36
4	L	1004	1OT	C6-N2	-2.32	1.33	1.36
4	B	1004	1OT	C6-N2	-2.31	1.33	1.36
4	H	1004	1OT	C6-N2	-2.29	1.33	1.36
4	A	1004	1OT	C6-N2	-2.27	1.33	1.36
4	G	1004	1OT	C6-N2	-2.27	1.33	1.36
4	C	1004	1OT	C6-N2	-2.25	1.33	1.36
4	I	1004	1OT	C6-N2	-2.22	1.33	1.36
4	D	1004	1OT	C6-N2	-2.17	1.33	1.36
4	J	1004	1OT	P-O2	3.82	1.61	1.54
4	H	1004	1OT	P-O2	3.87	1.61	1.54
4	C	1004	1OT	P-O2	4.11	1.61	1.54
4	I	1004	1OT	P-O2	4.12	1.61	1.54
4	B	1004	1OT	P-O2	4.15	1.61	1.54
4	A	1004	1OT	P-O2	4.17	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1004	1OT	P-O2	4.18	1.61	1.54
4	E	1004	1OT	P-O2	4.19	1.61	1.54
4	F	1004	1OT	P-O2	4.21	1.61	1.54
4	K	1004	1OT	P-O2	4.31	1.61	1.54
4	L	1004	1OT	P-O2	4.46	1.62	1.54
4	D	1004	1OT	P-O2	4.64	1.62	1.54
4	I	1004	1OT	P-O3	6.16	1.61	1.49
4	K	1004	1OT	P-O3	6.30	1.61	1.49
4	L	1004	1OT	P-O3	6.40	1.61	1.49
4	A	1004	1OT	P-O3	6.58	1.61	1.49
4	G	1004	1OT	P-O3	6.63	1.61	1.49
4	B	1004	1OT	P-O3	6.71	1.62	1.49
4	C	1004	1OT	P-O3	6.72	1.62	1.49
4	E	1004	1OT	P-O3	6.83	1.62	1.49
4	H	1004	1OT	P-O3	6.85	1.62	1.49
4	J	1004	1OT	P-O3	6.85	1.62	1.49
4	F	1004	1OT	P-O3	6.87	1.62	1.49
4	D	1004	1OT	P-O3	7.05	1.62	1.49

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1004	1OT	C7-C6-N2	-5.51	102.63	107.07
4	K	1004	1OT	C7-C6-N2	-5.42	102.70	107.07
4	F	1004	1OT	C7-C6-N2	-5.42	102.71	107.07
4	G	1004	1OT	C7-C6-N2	-5.39	102.72	107.07
4	B	1004	1OT	C7-C6-N2	-5.28	102.82	107.07
4	A	1004	1OT	C7-C6-N2	-5.28	102.82	107.07
4	J	1004	1OT	C7-C6-N2	-5.27	102.82	107.07
4	H	1004	1OT	C7-C6-N2	-5.24	102.85	107.07
4	C	1004	1OT	C7-C6-N2	-5.22	102.86	107.07
4	I	1004	1OT	C7-C6-N2	-5.22	102.87	107.07
4	E	1004	1OT	C7-C6-N2	-5.17	102.91	107.07
4	D	1004	1OT	C10-C2-C1	-4.79	115.65	120.69
4	D	1004	1OT	C7-C6-N2	-4.55	103.40	107.07
4	I	1004	1OT	C2-C1-N1	-4.20	102.01	113.18
4	A	1004	1OT	C10-C2-C1	-4.14	116.34	120.69
4	E	1004	1OT	C10-C2-C1	-3.78	116.72	120.69
4	L	1004	1OT	C2-C1-N1	-3.72	103.28	113.18
4	C	1004	1OT	C2-C1-N1	-3.68	103.40	113.18
4	J	1004	1OT	C10-C2-C1	-3.66	116.85	120.69
4	L	1004	1OT	C10-C2-C1	-3.64	116.87	120.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1004	1OT	C2-C1-N1	-3.37	104.22	113.18
4	I	1004	1OT	C10-C2-C1	-3.34	117.18	120.69
4	D	1004	1OT	C4-C5-C9	-3.31	116.07	121.21
4	D	1004	1OT	C2-C1-N1	-3.31	104.38	113.18
4	I	1004	1OT	C4-C5-C9	-3.30	116.09	121.21
4	F	1004	1OT	C4-C5-C9	-3.29	116.09	121.21
4	B	1004	1OT	C2-C1-N1	-3.28	104.46	113.18
4	H	1004	1OT	C2-C1-N1	-3.24	104.55	113.18
4	G	1004	1OT	C2-C1-N1	-3.19	104.70	113.18
4	G	1004	1OT	C4-C5-C9	-3.19	116.26	121.21
4	C	1004	1OT	C4-C5-C9	-3.18	116.28	121.21
4	F	1004	1OT	C10-C2-C1	-3.18	117.35	120.69
4	H	1004	1OT	C4-C5-C9	-3.16	116.30	121.21
4	F	1004	1OT	C2-C1-N1	-3.15	104.80	113.18
4	E	1004	1OT	C2-C1-N1	-3.15	104.80	113.18
4	B	1004	1OT	C10-C2-C1	-3.12	117.41	120.69
4	A	1004	1OT	C2-C1-N1	-3.12	104.88	113.18
4	B	1004	1OT	C4-C5-C9	-3.09	116.41	121.21
4	K	1004	1OT	C4-C5-C9	-3.09	116.41	121.21
4	J	1004	1OT	C4-C5-C9	-2.99	116.56	121.21
4	L	1004	1OT	C4-C5-C9	-2.98	116.58	121.21
4	J	1004	1OT	C2-C1-N1	-2.98	105.25	113.18
4	G	1004	1OT	C10-C2-C1	-2.98	117.56	120.69
4	A	1004	1OT	C4-C5-C9	-2.89	116.73	121.21
4	E	1004	1OT	C4-C5-C9	-2.84	116.80	121.21
4	K	1004	1OT	C10-C2-C1	-2.66	117.89	120.69
4	H	1004	1OT	C10-C2-C1	-2.62	117.94	120.69
4	C	1004	1OT	C10-C2-C1	-2.59	117.97	120.69
4	D	1004	1OT	C6-N2-C5	-2.55	120.72	124.48
4	C	1004	1OT	O1-P-O3	-2.51	106.81	113.49
4	E	1004	1OT	C6-N2-C5	-2.50	120.80	124.48
4	A	1004	1OT	C6-N2-C5	-2.42	120.92	124.48
4	D	1004	1OT	C4-C3-C2	-2.40	118.74	121.20
4	B	1004	1OT	C6-N2-C5	-2.27	121.14	124.48
4	F	1004	1OT	C6-N2-C5	-2.20	121.24	124.48
4	J	1004	1OT	C6-N2-C5	-2.18	121.27	124.48
4	E	1004	1OT	C8-N3-N2	-2.12	102.10	103.70
4	I	1004	1OT	O1-P-O3	-2.10	107.90	113.49
4	I	1004	1OT	C4-C3-C2	-2.06	119.08	121.20
4	A	1004	1OT	C4-C3-C2	-2.06	119.09	121.20
4	I	1004	1OT	C6-N2-C5	-2.06	121.45	124.48
4	K	1004	1OT	O2-P-O3	-2.05	108.04	113.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1004	1OT	C6-N2-C5	-2.04	121.47	124.48
4	K	1004	1OT	C4-C3-C2	-2.04	119.11	121.20
4	E	1004	1OT	O1-P-O3	-2.02	108.11	113.49
4	C	1004	1OT	C6-N2-C5	-2.02	121.50	124.48
4	L	1004	1OT	O1-P-O3	-2.01	108.15	113.49
4	F	1004	1OT	C6-C7-C8	2.01	109.96	105.38
4	C	1004	1OT	P-C1-C2	2.05	115.39	111.82
4	D	1004	1OT	P-C1-C2	2.10	115.49	111.82
4	K	1004	1OT	P-C1-C2	2.15	115.57	111.82
4	I	1004	1OT	P-C1-C2	2.19	115.63	111.82
4	H	1004	1OT	C3-C4-C5	2.23	121.50	119.23
4	L	1004	1OT	C3-C2-C1	2.27	123.08	120.69
4	A	1004	1OT	C3-C4-C5	2.28	121.56	119.23
4	J	1004	1OT	C3-C2-C1	2.34	123.15	120.69
4	B	1004	1OT	C3-C4-C5	2.35	121.62	119.23
4	F	1004	1OT	C3-C2-C1	2.36	123.17	120.69
4	I	1004	1OT	C3-C2-C1	2.39	123.20	120.69
4	A	1004	1OT	C3-C2-C1	2.42	123.23	120.69
4	B	1004	1OT	C3-C2-C1	2.45	123.27	120.69
4	E	1004	1OT	C3-C4-C5	2.53	121.81	119.23
4	E	1004	1OT	C3-C2-C1	2.57	123.40	120.69
4	J	1004	1OT	C3-C4-C5	2.63	121.90	119.23
4	L	1004	1OT	C3-C4-C5	2.80	122.08	119.23
4	G	1004	1OT	C3-C4-C5	2.84	122.12	119.23
4	F	1004	1OT	C3-C4-C5	2.93	122.21	119.23
4	K	1004	1OT	C10-C9-C5	3.00	122.29	119.23
4	K	1004	1OT	C3-C4-C5	3.03	122.32	119.23
4	C	1004	1OT	C3-C4-C5	3.08	122.37	119.23
4	L	1004	1OT	C10-C9-C5	3.14	122.43	119.23
4	C	1004	1OT	C10-C9-C5	3.17	122.45	119.23
4	E	1004	1OT	C10-C9-C5	3.22	122.51	119.23
4	J	1004	1OT	C10-C9-C5	3.25	122.54	119.23
4	I	1004	1OT	C3-C4-C5	3.30	122.59	119.23
4	D	1004	1OT	C10-C9-C5	3.31	122.60	119.23
4	D	1004	1OT	C3-C4-C5	3.31	122.60	119.23
4	I	1004	1OT	C10-C9-C5	3.34	122.63	119.23
4	G	1004	1OT	C10-C9-C5	3.40	122.69	119.23
4	F	1004	1OT	C10-C9-C5	3.42	122.71	119.23
4	B	1004	1OT	C10-C9-C5	3.51	122.80	119.23
4	A	1004	1OT	C10-C9-C5	3.57	122.87	119.23
4	H	1004	1OT	C10-C9-C5	3.70	123.00	119.23
4	D	1004	1OT	C3-C2-C1	3.84	124.73	120.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1004	1OT	C5-N2-N3	3.87	122.31	118.89
4	L	1004	1OT	C5-N2-N3	4.05	122.47	118.89
4	K	1004	1OT	C5-N2-N3	4.30	122.68	118.89
4	H	1004	1OT	C5-N2-N3	4.42	122.80	118.89
4	J	1004	1OT	C5-N2-N3	4.53	122.89	118.89
4	C	1004	1OT	C5-N2-N3	4.58	122.93	118.89
4	F	1004	1OT	C5-N2-N3	4.77	123.10	118.89
4	I	1004	1OT	C6-N2-N3	4.80	115.26	111.94
4	E	1004	1OT	C5-N2-N3	4.89	123.21	118.89
4	D	1004	1OT	C6-N2-N3	4.91	115.34	111.94
4	I	1004	1OT	C5-N2-N3	4.98	123.29	118.89
4	B	1004	1OT	C5-N2-N3	5.03	123.33	118.89
4	A	1004	1OT	C5-N2-N3	5.12	123.41	118.89
4	H	1004	1OT	C6-N2-N3	5.14	115.50	111.94
4	B	1004	1OT	C6-N2-N3	5.17	115.52	111.94
4	G	1004	1OT	C6-N2-N3	5.19	115.53	111.94
4	C	1004	1OT	C6-N2-N3	5.24	115.57	111.94
4	F	1004	1OT	C6-N2-N3	5.37	115.66	111.94
4	A	1004	1OT	C6-N2-N3	5.39	115.67	111.94
4	K	1004	1OT	C6-N2-N3	5.44	115.71	111.94
4	J	1004	1OT	C6-N2-N3	5.63	115.84	111.94
4	D	1004	1OT	C5-N2-N3	5.72	123.94	118.89
4	E	1004	1OT	C6-N2-N3	5.85	115.99	111.94
4	L	1004	1OT	C6-N2-N3	5.95	116.06	111.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

44 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	1OT	3	0
6	A	1010	1PE	1	0
4	B	1004	1OT	4	0
4	C	1004	1OT	2	0
6	C	1006	1PE	1	0
6	C	1007	1PE	1	0
7	C	1009	2PE	2	0
3	D	1002	CO3	1	0
4	D	1004	1OT	2	0
6	D	1007	1PE	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1009	1PE	5	0
7	D	1010	2PE	4	0
7	D	1012	2PE	1	0
4	E	1004	1OT	4	0
6	E	1009	1PE	3	0
7	E	1010	2PE	1	0
4	F	1004	1OT	3	0
6	F	1008	1PE	1	0
6	F	1009	1PE	1	0
7	F	1010	2PE	1	0
4	G	1004	1OT	3	0
6	G	1008	1PE	2	0
6	G	1011	1PE	6	0
4	H	1004	1OT	2	0
7	H	1006	2PE	1	0
7	H	1007	2PE	1	0
4	I	1004	1OT	2	0
6	I	1007	1PE	1	0
6	I	1008	1PE	1	0
6	I	1009	1PE	1	0
4	J	1004	1OT	2	0
5	J	1005	SO4	1	0
6	J	1006	1PE	3	0
6	J	1007	1PE	1	0
6	J	1008	1PE	2	0
6	J	1009	1PE	2	0
4	K	1004	1OT	3	0
6	K	1007	1PE	2	0
6	K	1010	1PE	1	0
3	L	1002	CO3	1	0
4	L	1004	1OT	4	0
6	L	1007	1PE	3	0
6	L	1008	1PE	2	0
6	L	1009	1PE	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9	
1	A	519/528 (98%)	-0.30	1 (0%)	95	95	6, 13, 30, 50	0
1	B	518/528 (98%)	-0.16	8 (1%)	76	77	5, 14, 43, 65	1 (0%)
1	C	518/528 (98%)	-0.29	2 (0%)	93	93	4, 13, 33, 48	0
1	D	514/528 (97%)	-0.35	5 (0%)	84	84	5, 12, 31, 54	0
1	E	510/528 (96%)	-0.44	2 (0%)	93	93	4, 11, 25, 50	0
1	F	511/528 (96%)	-0.16	7 (1%)	78	78	6, 16, 37, 69	0
1	G	519/528 (98%)	-0.30	0	100	100	5, 12, 31, 52	0
1	H	516/528 (97%)	-0.22	2 (0%)	93	93	5, 14, 41, 63	1 (0%)
1	I	518/528 (98%)	-0.30	1 (0%)	95	95	4, 13, 33, 56	0
1	J	513/528 (97%)	-0.36	5 (0%)	84	84	4, 13, 32, 57	0
1	K	509/528 (96%)	-0.43	2 (0%)	93	93	5, 12, 26, 52	0
1	L	513/528 (97%)	-0.22	3 (0%)	90	90	5, 14, 35, 52	0
All	All	6178/6336 (97%)	-0.29	38 (0%)	90	90	4, 13, 34, 69	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	VAL	6.2
1	H	136	GLY	4.1
1	B	257	LYS	3.9
1	J	136	GLY	3.8
1	J	85	ALA	3.7
1	F	136	GLY	3.6
1	L	136	GLY	3.6
1	B	136	GLY	3.5
1	F	121	CYS	3.5
1	K	550	SER	3.3
1	D	85	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	136	GLY	3.0
1	E	136	GLY	2.9
1	F	148	VAL	2.8
1	J	603	ASP	2.8
1	F	137	LYS	2.8
1	B	260	ASN	2.7
1	F	361	SER	2.7
1	B	256	ASP	2.6
1	D	603	ASP	2.6
1	C	136	GLY	2.6
1	B	144	ILE	2.5
1	A	362	LYS	2.4
1	F	138	GLU	2.4
1	K	363	GLY	2.4
1	J	219	LEU	2.4
1	I	124	GLU	2.3
1	E	550	SER	2.3
1	L	363	GLY	2.3
1	F	157	LEU	2.3
1	H	181	ASN	2.2
1	C	124	GLU	2.2
1	D	219	LEU	2.2
1	J	549	SER	2.1
1	B	258	ASN	2.1
1	L	134	ASN	2.1
1	D	261	MET	2.0
1	B	135	PRO	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
5	SO4	E	1006	5/5	0.90	0.27	14.81	46,53,54,62	0
6	1PE	K	1010	6/16	0.77	0.18	13.70	23,28,37,39	0
7	2PE	D	1012	9/28	0.86	0.21	13.40	36,42,45,47	0
6	1PE	C	1008	7/16	0.77	0.35	10.55	42,43,44,45	0
7	2PE	E	1010	9/28	0.84	0.19	9.75	36,39,42,46	0
5	SO4	I	1006	5/5	0.94	0.24	9.39	53,55,56,60	0
6	1PE	G	1011	15/16	0.81	0.22	9.37	26,38,47,51	0
7	2PE	J	1010	10/28	0.81	0.22	8.39	18,47,48,48	0
6	1PE	F	1009	11/16	0.82	0.29	8.12	46,51,55,56	0
2	ZN	K	1003	1/1	0.98	0.19	8.00	46,46,46,46	0
7	2PE	B	1007	10/28	0.87	0.17	6.93	45,49,53,55	0
2	ZN	E	1003	1/1	0.99	0.17	6.68	49,49,49,49	0
5	SO4	G	1005	5/5	0.95	0.18	5.69	32,32,33,40	0
6	1PE	L	1009	11/16	0.76	0.20	5.43	36,39,43,45	0
5	SO4	A	1007	5/5	0.93	0.19	5.42	38,42,45,49	0
6	1PE	J	1009	9/16	0.73	0.25	5.07	26,32,38,39	0
6	1PE	I	1009	5/16	0.92	0.15	5.05	14,20,20,21	0
6	1PE	G	1008	9/16	0.88	0.15	5.00	17,25,29,30	0
2	ZN	J	1003	1/1	0.94	0.16	4.97	53,53,53,53	0
6	1PE	J	1008	11/16	0.75	0.23	4.83	26,32,42,42	0
6	1PE	F	1008	10/16	0.87	0.17	4.71	26,32,35,36	0
6	1PE	J	1006	11/16	0.92	0.16	4.38	20,25,35,37	0
2	ZN	D	1003	1/1	0.99	0.14	4.32	45,45,45,45	0
4	1OT	J	1004	17/17	0.93	0.17	4.22	15,21,43,44	0
7	2PE	I	1010	8/28	0.82	0.18	4.18	32,39,48,49	0
7	2PE	C	1009	9/28	0.88	0.15	4.03	29,32,38,39	0
6	1PE	E	1009	8/16	0.81	0.22	3.90	29,42,43,43	0
2	ZN	C	1001	1/1	0.99	0.13	3.89	41,41,41,41	0
6	1PE	E	1008	12/16	0.90	0.16	3.71	19,23,39,39	0
5	SO4	A	1008	5/5	0.88	0.18	3.68	26,35,41,48	0
2	ZN	I	1001	1/1	0.99	0.12	3.60	40,40,40,40	0
6	1PE	K	1008	12/16	0.94	0.14	3.55	16,25,38,39	0
2	ZN	I	1003	1/1	1.00	0.15	3.54	42,42,42,42	0
7	2PE	F	1010	9/28	0.88	0.14	3.48	35,38,39,42	0
6	1PE	D	1008	9/16	0.75	0.22	3.36	46,49,60,60	0
6	1PE	L	1007	12/16	0.78	0.18	3.26	28,35,39,41	0
4	1OT	L	1004	17/17	0.92	0.15	3.10	7,25,34,34	0
6	1PE	L	1006	10/16	0.92	0.15	2.92	19,25,29,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	1PE	L	1008	8/16	0.67	0.20	2.85	48,51,53,53	0
2	ZN	H	1003	1/1	0.96	0.15	2.85	46,46,46,46	0
2	ZN	K	1001	1/1	0.99	0.11	2.57	35,35,35,35	0
4	1OT	F	1004	17/17	0.92	0.15	2.57	10,24,32,32	0
7	2PE	H	1007	10/28	0.81	0.19	2.56	36,45,53,53	0
4	1OT	E	1004	17/17	0.94	0.15	2.55	14,20,41,42	0
7	2PE	B	1006	26/28	0.86	0.18	2.54	17,43,51,51	0
4	1OT	K	1004	17/17	0.94	0.15	2.50	12,20,40,40	0
2	ZN	B	1003	1/1	0.98	0.14	2.50	38,38,38,38	0
3	CO3	C	1002	4/4	0.98	0.12	2.36	8,10,12,17	0
5	SO4	G	1007	5/5	0.92	0.16	2.24	43,48,51,56	0
7	2PE	H	1006	25/28	0.85	0.15	2.21	21,31,39,44	0
6	1PE	D	1009	11/16	0.82	0.19	2.08	23,35,40,43	0
4	1OT	I	1004	17/17	0.93	0.14	2.07	9,24,37,37	0
4	1OT	D	1004	17/17	0.95	0.14	1.83	12,21,39,39	0
6	1PE	I	1008	11/16	0.90	0.14	1.79	18,24,31,33	0
3	CO3	F	1002	4/4	0.98	0.12	1.77	7,12,14,15	0
4	1OT	H	1004	17/17	0.92	0.15	1.77	10,24,37,37	0
6	1PE	K	1009	11/16	0.85	0.17	1.75	30,33,36,38	0
2	ZN	F	1003	1/1	0.98	0.12	1.67	51,51,51,51	0
2	ZN	L	1003	1/1	0.98	0.13	1.59	45,45,45,45	0
6	1PE	G	1010	6/16	0.91	0.14	1.58	30,32,32,33	0
6	1PE	D	1007	10/16	0.92	0.12	1.53	17,24,28,32	0
7	2PE	D	1011	5/28	0.91	0.25	1.49	21,21,28,28	0
3	CO3	E	1002	4/4	0.98	0.11	1.34	8,10,11,17	0
2	ZN	C	1003	1/1	0.96	0.13	1.31	41,41,41,41	0
3	CO3	J	1002	4/4	0.97	0.11	1.19	5,6,11,15	0
6	1PE	G	1009	6/16	0.96	0.19	1.17	21,22,26,33	0
5	SO4	B	1005	5/5	0.93	0.18	1.14	67,68,68,69	0
4	1OT	G	1004	17/17	0.94	0.13	1.09	8,20,32,35	0
3	CO3	B	1002	4/4	0.98	0.12	0.97	5,6,7,11	0
4	1OT	C	1004	17/17	0.94	0.13	0.91	9,18,36,37	0
3	CO3	L	1002	4/4	0.98	0.12	0.83	6,8,10,12	0
6	1PE	C	1007	9/16	0.90	0.13	0.83	13,22,29,31	0
2	ZN	E	1001	1/1	0.99	0.10	0.69	36,36,36,36	0
4	1OT	B	1004	17/17	0.94	0.12	0.58	9,18,39,41	0
2	ZN	H	1001	1/1	0.98	0.10	0.55	36,36,36,36	0
2	ZN	F	1001	1/1	0.97	0.11	0.34	39,39,39,39	0
3	CO3	I	1002	4/4	0.98	0.11	0.34	7,8,8,15	0
6	1PE	F	1006	10/16	0.92	0.13	0.26	29,32,36,37	0
3	CO3	H	1002	4/4	0.98	0.10	0.21	4,10,10,12	0
4	1OT	A	1004	17/17	0.94	0.12	-0.01	5,20,33,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	G	1003	1/1	0.99	0.11	-0.11	39,39,39,39	0
2	ZN	D	1001	1/1	0.99	0.09	-0.11	36,36,36,36	0
3	CO3	G	1002	4/4	0.98	0.10	-0.23	7,8,8,17	0
3	CO3	D	1002	4/4	0.98	0.09	-0.33	6,7,10,12	0
6	1PE	A	1009	9/16	0.93	0.09	-0.53	18,21,25,34	0
5	SO4	K	1005	5/5	0.99	0.08	-0.96	9,11,11,12	0
5	SO4	D	1005	5/5	0.99	0.08	-1.09	9,9,11,12	0
2	ZN	L	1001	1/1	0.99	0.09	-1.11	41,41,41,41	0
2	ZN	A	1003	1/1	0.98	0.09	-1.21	46,46,46,46	0
3	CO3	A	1002	4/4	0.99	0.09	-1.33	7,10,12,18	0
2	ZN	A	1001	1/1	0.99	0.07	-1.82	37,37,37,37	0
2	ZN	B	1001	1/1	0.99	0.08	-2.08	36,36,36,36	0
5	SO4	A	1005	5/5	0.99	0.07	-2.24	6,7,11,13	0
5	SO4	H	1005	5/5	0.99	0.09	-2.25	7,8,10,11	0
2	ZN	J	1001	1/1	1.00	0.07	-2.53	36,36,36,36	0
3	CO3	K	1002	4/4	0.98	0.08	-2.87	8,12,13,18	0
2	ZN	G	1001	1/1	0.99	0.06	-7.11	39,39,39,39	0
5	SO4	A	1006	5/5	0.96	0.20	-	45,46,50,50	0
5	SO4	F	1005	5/5	0.96	0.21	-	44,46,49,51	0
5	SO4	I	1005	5/5	0.95	0.29	-	50,51,54,55	0
5	SO4	G	1006	5/5	0.94	0.21	-	40,41,45,49	0
5	SO4	D	1006	5/5	0.94	0.23	-	44,51,54,55	0
5	SO4	K	1006	5/5	0.96	0.22	-	42,45,47,53	0
6	1PE	C	1006	13/16	0.85	0.17	-	12,34,44,45	0
5	SO4	L	1005	5/5	0.94	0.17	-	33,40,45,48	0
6	1PE	K	1007	12/16	0.85	0.17	-	31,37,40,41	0
6	1PE	I	1007	15/16	0.86	0.21	-	20,31,40,40	0
6	1PE	A	1010	12/16	0.75	0.23	-	32,38,46,48	0
5	SO4	C	1005	5/5	0.91	0.26	-	41,47,51,54	0
6	1PE	E	1007	12/16	0.83	0.15	-	29,32,34,34	0
6	1PE	F	1007	10/16	0.82	0.18	-	40,42,49,51	0
5	SO4	J	1005	5/5	0.94	0.28	-	51,51,55,56	0
7	2PE	D	1010	13/28	0.84	0.20	-	28,38,49,51	0
5	SO4	E	1005	5/5	0.96	0.22	-	42,45,49,50	0
6	1PE	J	1007	10/16	0.80	0.22	-	28,32,39,41	0

6.5 Other polymers

There are no such residues in this entry.