Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:56 AM GMT

PDB ID	:	3Q9F
Title	:	Crystal Structure of APAH complexed with CAPS
Authors	:	Lombardi, P.M.; Christianson, D.W.
Deposited on	:	2011-01-07
Resolution	:	2.35 Å(reported)

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

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

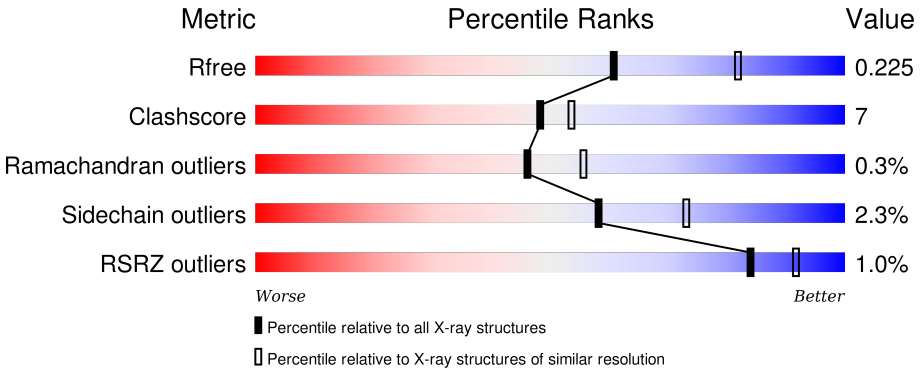
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	81% 18% •
1	B	341	% 83% 16% •
1	C	341	83% 16% •
1	D	341	82% 16% •
1	E	341	% 79% 20% •

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Mol	Chain	Length	Quality of chain
1	F	341	2% 84% 15%
1	G	341	% 81% 19%
1	H	341	2% 84% 15%
1	I	341	80% 19%
1	J	341	% 81% 18%
1	K	341	% 82% 18%
1	L	341	% 81% 18%

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	CXS	A	401	-	-	-	X
2	CXS	B	402	-	-	-	X
2	CXS	C	403	-	-	-	X
2	CXS	D	404	-	-	-	X
2	CXS	F	406	-	-	-	X
2	CXS	G	407	-	-	-	X
2	CXS	H	408	-	-	-	X
2	CXS	I	409	-	-	-	X
2	CXS	J	410	-	-	-	X
2	CXS	K	411	-	-	-	X
2	CXS	L	412	-	-	-	X
5	NA	A	343	-	-	-	X
5	NA	B	343	-	-	-	X
5	NA	C	343	-	-	-	X
5	NA	D	343	-	-	-	X
5	NA	E	343	-	-	-	X
5	NA	G	343	-	-	-	X
5	NA	I	343	-	-	-	X
5	NA	K	343	-	-	-	X

2 Entry composition

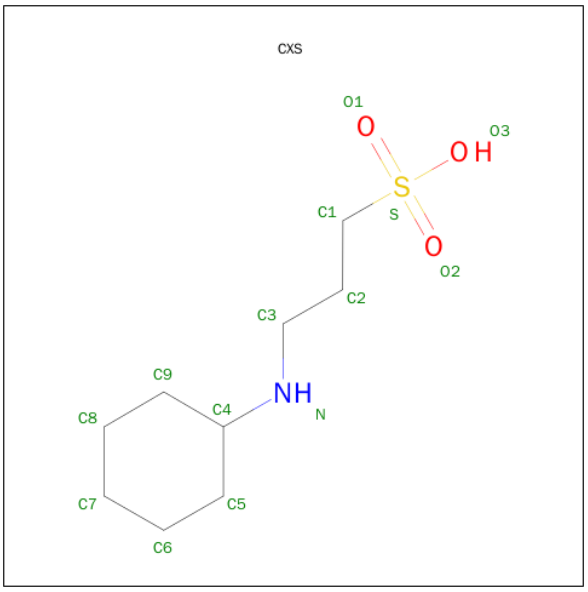
There are 7 unique types of molecules in this entry. The entry contains 32471 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylpolyamine amidohydrolase.

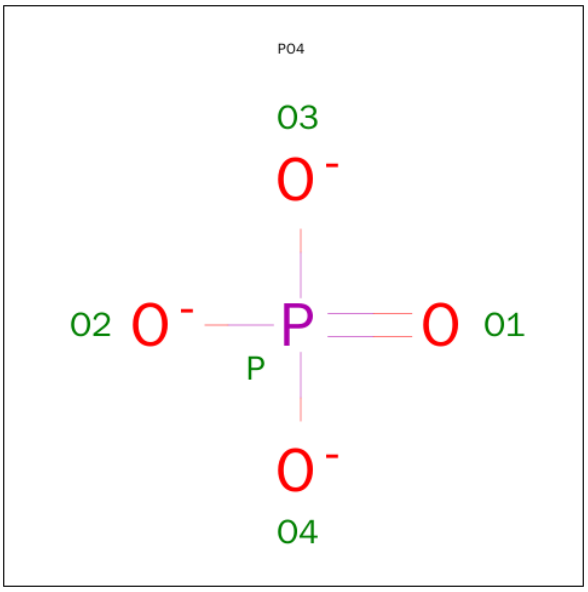
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	B	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	C	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	D	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	E	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	F	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	G	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	H	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	I	340	Total	C	N	O	S	0	0	0
			2563	1642	434	478	9			
1	J	340	Total	C	N	O	S	0	0	0
			2563	1642	434	478	9			
1	K	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	L	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			

- Molecule 2 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Na 1 1	0	0
5	J	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	K	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0
5	H	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	I	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0
5	L	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	129	Total O 129 129	0	0

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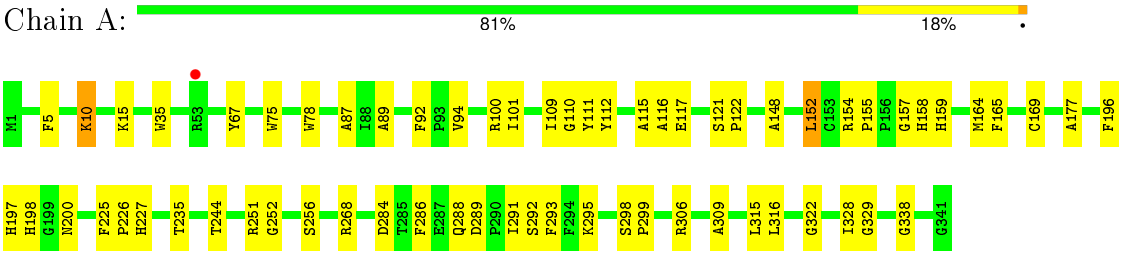
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	117	Total O 117 117	0	0
7	C	124	Total O 124 124	0	0
7	D	125	Total O 125 125	0	0
7	E	115	Total O 115 115	0	0
7	F	107	Total O 107 107	0	0
7	G	106	Total O 106 106	0	0
7	H	112	Total O 112 112	0	0
7	I	132	Total O 132 132	0	0
7	J	98	Total O 98 98	0	0
7	K	113	Total O 113 113	0	0
7	L	115	Total O 115 115	0	0

3 Residue-property plots (i)

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

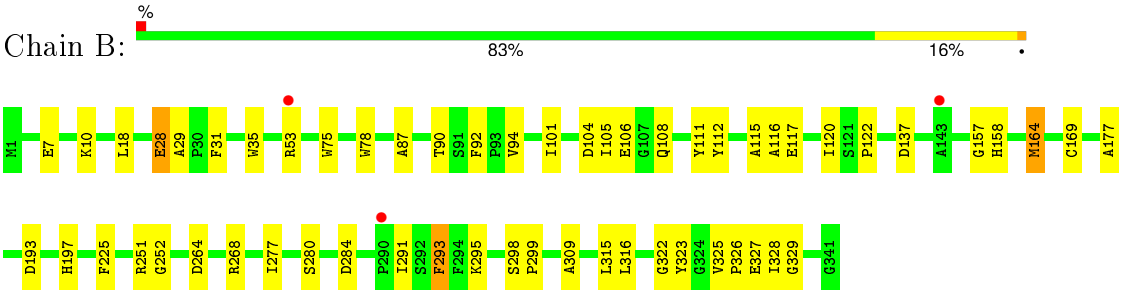
- Molecule 1: Acetylpolyamine amidohydrolase

Chain A:



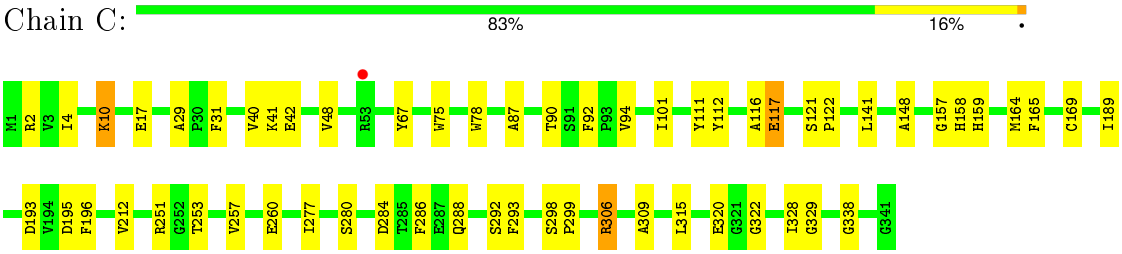
- Molecule 1: Acetylpolyamine amidohydrolase

Chain B:



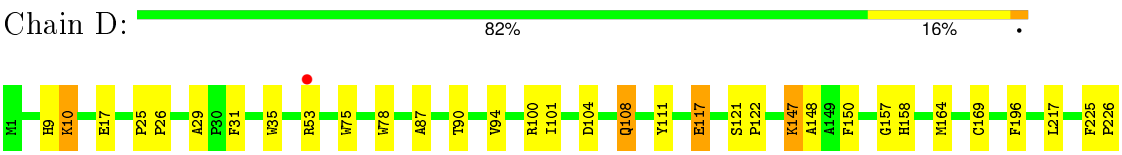
- Molecule 1: Acetylpolyamine amidohydrolase

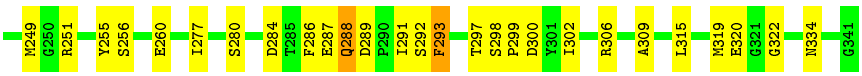
Chain C:



- Molecule 1: Acetylpolyamine amidohydrolase

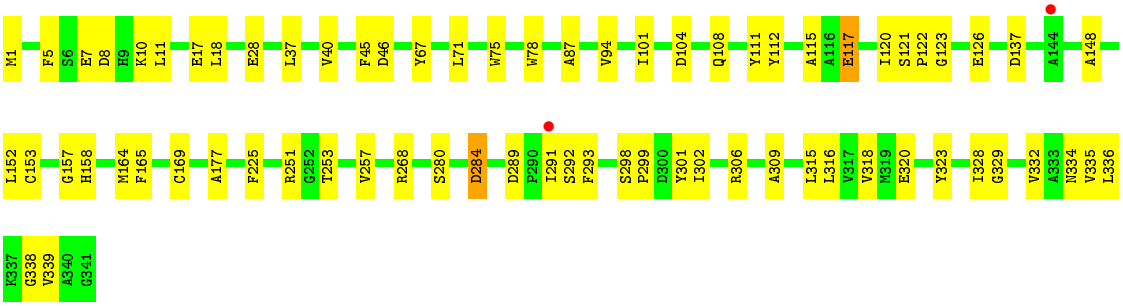
Chain D:





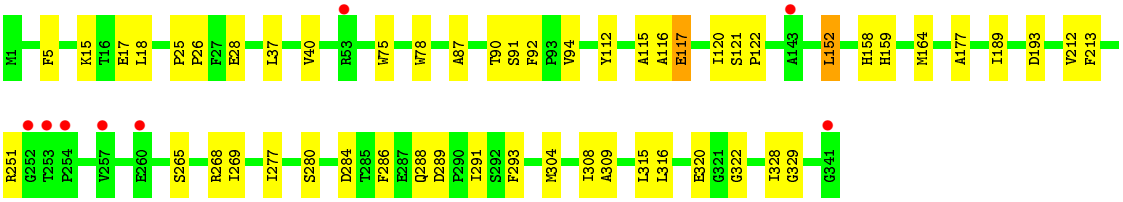
• Molecule 1: Acetylpolyamine amidohydrolase

Chain E:



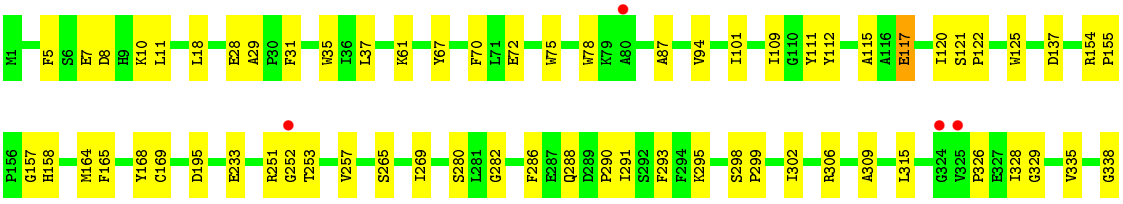
• Molecule 1: Acetylpolyamine amidohydrolase

Chain F:



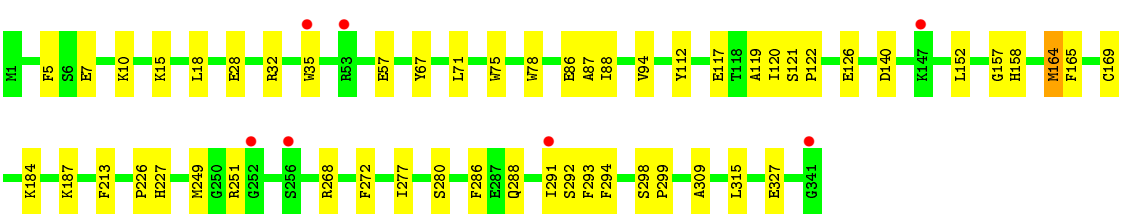
• Molecule 1: Acetylpolyamine amidohydrolase

Chain G:



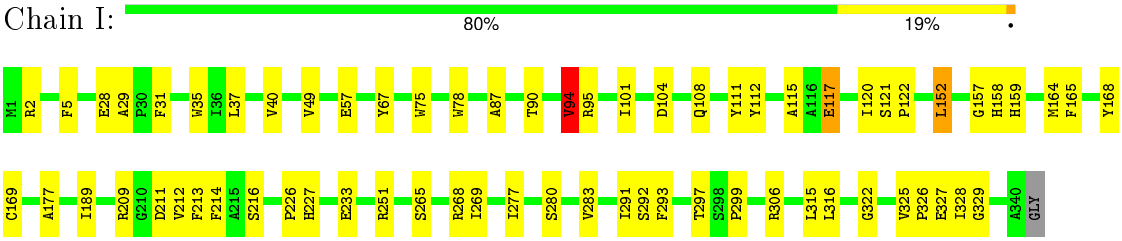
• Molecule 1: Acetylpolyamine amidohydrolase

Chain H:



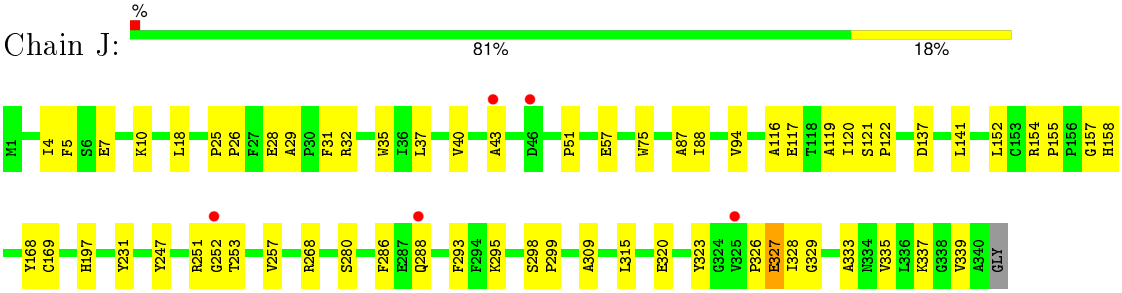
• Molecule 1: Acetylpolyamine amidohydrolase

Chain I:



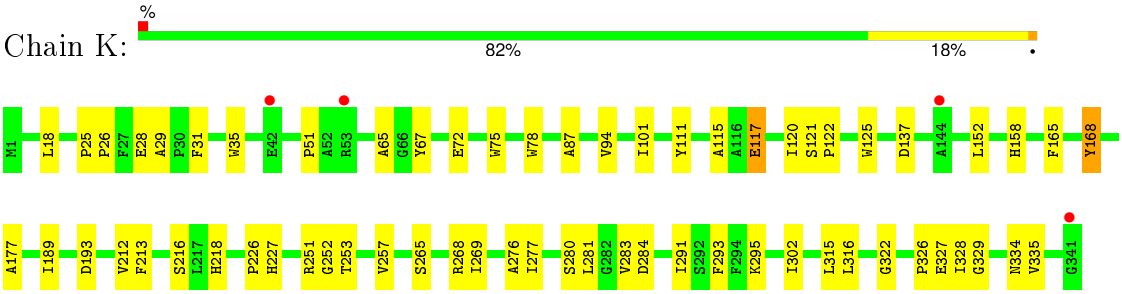
• Molecule 1: Acetylpolyamine amidohydrolase

Chain J:



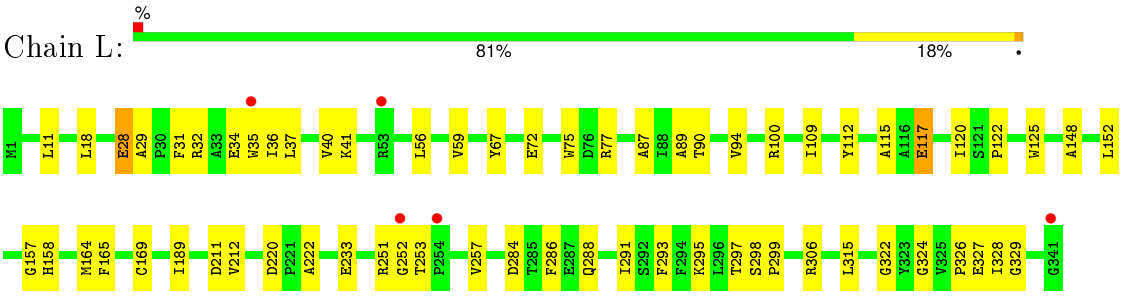
• Molecule 1: Acetylpolyamine amidohydrolase

Chain K:



• Molecule 1: Acetylpolyamine amidohydrolase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	118.25Å 119.65Å 119.57Å 98.34° 94.94° 114.95°	Depositor
Resolution (Å)	50.00 – 2.35 46.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-2.35) 85.3 (46.62-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.225 0.189 , 0.225	Depositor DCC
R_{free} test set	11007 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.0	EDS
Estimated twinning fraction	0.001 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 235850 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32471	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, NA, ZN, CXS, PO4

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	0.41	0/2636	0.59	0/3582
1	B	0.39	0/2636	0.58	0/3582
1	C	0.41	0/2636	0.59	0/3582
1	D	0.41	0/2636	0.59	0/3582
1	E	0.39	0/2636	0.58	0/3582
1	F	0.39	0/2636	0.57	0/3582
1	G	0.39	0/2636	0.59	0/3582
1	H	0.39	0/2636	0.56	0/3582
1	I	0.41	0/2631	0.58	0/3577
1	J	0.37	0/2631	0.56	0/3577
1	K	0.40	0/2636	0.58	0/3582
1	L	0.39	0/2636	0.58	0/3582
All	All	0.40	0/31622	0.58	0/42974

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2568	0	2490	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2568	0	2492	37	0
1	C	2568	0	2491	37	0
1	D	2568	0	2491	44	0
1	E	2568	0	2491	44	0
1	F	2568	0	2490	36	0
1	G	2568	0	2492	38	0
1	H	2568	0	2492	34	0
1	I	2563	0	2488	40	0
1	J	2563	0	2488	38	0
1	K	2568	0	2491	36	0
1	L	2568	0	2492	41	0
2	A	14	0	19	1	0
2	B	14	0	18	4	0
2	C	14	0	18	1	0
2	D	14	0	18	6	0
2	E	14	0	18	3	0
2	F	14	0	19	1	0
2	G	14	0	18	1	0
2	H	14	0	19	0	0
2	I	14	0	18	4	0
2	J	14	0	18	1	0
2	K	14	0	18	3	0
2	L	14	0	18	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
7	A	129	0	0	1	0
7	B	117	0	0	1	0
7	C	124	0	0	1	0
7	D	125	0	0	0	0
7	E	115	0	0	3	0
7	F	107	0	0	1	0
7	G	106	0	0	1	0
7	H	112	0	0	1	0
7	I	132	0	0	2	0
7	J	98	0	0	1	0
7	K	113	0	0	0	0
7	L	115	0	0	2	0
All	All	32471	0	30107	449	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 7.

All (449) 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:L:157:GLY:HA2	1:L:169:CYS:HB3	1.63	0.79
1:E:306:ARG:HD2	1:E:338:GLY:O	1.87	0.75
1:D:289:ASP:OD1	1:D:291:ILE:HG12	1.88	0.74
1:I:291:ILE:HD12	2:I:409:CXS:H51	1.71	0.73
1:H:157:GLY:HA2	1:H:169:CYS:HB3	1.70	0.72
1:J:157:GLY:HA2	1:J:169:CYS:HB3	1.70	0.72
1:A:15:LYS:HE2	1:A:15:LYS:HA	1.73	0.70
1:L:75:TRP:CE2	1:L:122:PRO:HG3	2.25	0.70
1:A:286:PHE:CE2	1:A:288:GLN:HB2	2.27	0.69
1:L:72:GLU:HG3	1:L:125:TRP:NE1	2.07	0.69
1:G:306:ARG:HD2	1:G:338:GLY:O	1.91	0.69
1:I:159:HIS:CD2	2:I:409:CXS:H11	2.28	0.68
1:G:328:ILE:HG13	1:G:329:GLY:N	2.09	0.67
1:D:225:PHE:CE2	2:D:404:CXS:H31	2.30	0.67
1:K:302:ILE:HG13	1:K:334:ASN:HB3	1.78	0.66
1:E:251:ARG:HA	1:E:293:PHE:CD2	2.31	0.66
1:E:157:GLY:HA2	1:E:169:CYS:HB3	1.78	0.66
1:C:251:ARG:HA	1:C:293:PHE:CD2	2.30	0.66
1:L:31:PHE:HA	1:L:34:GLU:HG2	1.77	0.65
1:E:291:ILE:HD12	2:E:405:CXS:H51	1.77	0.65
1:B:75:TRP:CE2	1:B:122:PRO:HG3	2.32	0.65
1:A:306:ARG:HD2	1:A:338:GLY:O	1.97	0.65
1:L:36:ILE:O	1:L:40:VAL:HG13	1.97	0.64
1:A:289:ASP:OD1	1:A:291:ILE:HG12	1.99	0.62
1:I:159:HIS:HD2	2:I:409:CXS:H11	1.64	0.62
2:E:405:CXS:H52	7:E:1003:HOH:O	2.00	0.62
1:K:168:TYR:CE2	2:K:411:CXS:H32	2.34	0.62
1:J:29:ALA:HB3	1:J:31:PHE:CE1	2.35	0.62
1:F:251:ARG:HA	1:F:293:PHE:CD2	2.34	0.62
1:F:286:PHE:CE2	1:F:288:GLN:HB2	2.34	0.62
1:B:87:ALA:HB3	1:B:120:ILE:HB	1.83	0.61
1:F:121:SER:HB2	1:F:122:PRO:CD	2.31	0.61
1:F:159:HIS:CD2	2:F:406:CXS:H11	2.37	0.60
1:D:286:PHE:CE2	1:D:288:GLN:HB2	2.37	0.60
1:H:309:ALA:HA	1:H:315:LEU:HD11	1.83	0.60
1:J:87:ALA:HB3	1:J:120:ILE:HB	1.84	0.60
1:G:115:ALA:HB1	1:G:117:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:ARG:HA	1:J:293:PHE:CD2	2.37	0.59
1:D:284:ASP:HB3	1:D:322:GLY:HA2	1.84	0.59
1:J:75:TRP:CE2	1:J:122:PRO:HG3	2.38	0.59
1:C:4:ILE:HD12	1:C:4:ILE:N	2.18	0.59
1:A:268:ARG:HB3	1:A:268:ARG:NH1	2.18	0.59
1:E:302:ILE:HG13	1:E:334:ASN:HB3	1.85	0.59
1:C:309:ALA:HA	1:C:315:LEU:HD11	1.83	0.58
1:B:309:ALA:HA	1:B:315:LEU:HD11	1.84	0.58
1:F:75:TRP:NE1	1:F:122:PRO:HG3	2.19	0.58
1:L:117:GLU:HG3	2:L:412:CXS:H92	1.84	0.58
1:L:35:TRP:CZ3	1:L:326:PRO:HA	2.39	0.58
1:E:75:TRP:CE2	1:E:122:PRO:HG3	2.39	0.58
1:E:323:TYR:HB3	7:E:864:HOH:O	2.03	0.58
1:K:251:ARG:HA	1:K:293:PHE:CD2	2.39	0.58
1:K:35:TRP:CE3	1:K:326:PRO:HA	2.39	0.57
1:E:8:ASP:HB3	1:E:11:LEU:HD12	1.86	0.57
1:L:286:PHE:CE2	1:L:288:GLN:HB2	2.40	0.57
1:I:117:GLU:HG3	2:I:409:CXS:H92	1.87	0.57
2:G:407:CXS:H71	7:G:1004:HOH:O	2.02	0.57
1:C:92:PHE:HZ	1:C:116:ALA:HB2	1.70	0.57
1:D:225:PHE:HB2	2:D:404:CXS:H81	1.86	0.56
1:A:251:ARG:HA	1:A:293:PHE:CD2	2.39	0.56
1:B:225:PHE:CD2	2:B:402:CXS:H31	2.40	0.56
1:A:309:ALA:HA	1:A:315:LEU:HD11	1.86	0.56
1:K:213:PHE:HZ	1:K:268:ARG:HD2	1.70	0.56
1:A:75:TRP:NE1	1:A:122:PRO:HG3	2.21	0.56
1:E:309:ALA:HA	1:E:315:LEU:HD11	1.86	0.56
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.40	0.56
1:D:298:SER:HB2	1:D:299:PRO:HD3	1.87	0.56
1:I:115:ALA:HB1	1:I:117:GLU:OE1	2.05	0.56
1:I:328:ILE:HG13	1:I:329:GLY:N	2.21	0.56
1:L:87:ALA:HB3	1:L:120:ILE:HB	1.88	0.56
1:G:72:GLU:HG3	1:G:125:TRP:NE1	2.21	0.56
1:A:35:TRP:HE3	1:A:35:TRP:HA	1.71	0.56
1:G:35:TRP:CE3	1:G:326:PRO:HA	2.41	0.56
1:L:306:ARG:HH11	1:L:306:ARG:HG3	1.71	0.55
1:E:115:ALA:HB1	1:E:117:GLU:OE1	2.06	0.55
1:C:2:ARG:HD2	1:C:141:LEU:HD11	1.87	0.55
1:G:87:ALA:HB3	1:G:120:ILE:HB	1.88	0.55
1:D:225:PHE:CG	2:D:404:CXS:H4	2.42	0.55
1:A:75:TRP:CE2	1:A:122:PRO:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASP:HB3	1:B:322:GLY:HA2	1.88	0.55
1:H:112:TYR:O	1:H:164:MET:HA	2.07	0.55
1:F:121:SER:HB2	1:F:122:PRO:HD2	1.89	0.55
1:C:284:ASP:HB3	1:C:322:GLY:HA2	1.88	0.55
1:C:298:SER:HB2	1:C:299:PRO:HD3	1.89	0.55
1:G:75:TRP:CE2	1:G:122:PRO:HG3	2.42	0.54
1:B:157:GLY:HA2	1:B:169:CYS:HB3	1.89	0.54
1:K:328:ILE:HG13	1:K:329:GLY:N	2.22	0.54
1:A:78:TRP:CE2	1:A:87:ALA:HA	2.41	0.54
1:G:298:SER:HB2	1:G:299:PRO:HD3	1.90	0.54
1:D:150:PHE:CZ	1:D:319:MET:HG2	2.42	0.54
1:G:251:ARG:HA	1:G:293:PHE:CD2	2.42	0.54
1:B:78:TRP:CE2	1:B:87:ALA:HA	2.43	0.54
1:D:277:ILE:HB	1:D:315:LEU:HD23	1.89	0.54
1:D:225:PHE:CD1	2:D:404:CXS:H61	2.43	0.54
1:K:67:TYR:OH	1:K:165:PHE:HB3	2.08	0.54
1:K:75:TRP:CE2	1:K:122:PRO:HG3	2.43	0.54
1:E:101:ILE:HG12	1:E:111:TYR:CZ	2.43	0.53
1:K:291:ILE:HD12	2:K:411:CXS:H51	1.89	0.53
1:I:78:TRP:CE2	1:I:87:ALA:HA	2.44	0.53
1:I:5:PHE:CD1	1:I:152:LEU:HD13	2.43	0.53
1:C:121:SER:HB2	1:C:122:PRO:HD2	1.90	0.53
1:L:112:TYR:O	1:L:164:MET:HA	2.08	0.53
1:H:75:TRP:NE1	1:H:122:PRO:HG3	2.24	0.53
1:D:196:PHE:CD1	1:D:292:SER:HB2	2.43	0.53
1:I:75:TRP:CE2	1:I:122:PRO:HG3	2.44	0.53
1:L:298:SER:HB2	1:L:299:PRO:HD3	1.91	0.53
1:J:309:ALA:HA	1:J:315:LEU:HD11	1.90	0.53
1:A:112:TYR:O	1:A:164:MET:HA	2.09	0.52
1:H:75:TRP:CE2	1:H:122:PRO:HG3	2.45	0.52
1:F:309:ALA:HA	1:F:315:LEU:HD11	1.92	0.52
1:B:328:ILE:HG13	1:B:329:GLY:N	2.24	0.52
1:G:157:GLY:HA2	1:G:169:CYS:HB3	1.92	0.52
1:G:29:ALA:HB3	1:G:31:PHE:CE1	2.44	0.52
1:K:72:GLU:HG3	1:K:125:TRP:NE1	2.25	0.52
1:K:117:GLU:HG3	2:K:411:CXS:H92	1.91	0.52
1:D:121:SER:HB2	1:D:122:PRO:CD	2.40	0.52
1:J:43:ALA:HB1	1:J:337:LYS:HE2	1.90	0.52
1:J:298:SER:HB2	1:J:299:PRO:HD3	1.91	0.52
1:I:157:GLY:HA2	1:I:169:CYS:HB3	1.92	0.52
1:K:277:ILE:HB	1:K:315:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ILE:HG12	1:H:119:ALA:HB2	1.92	0.52
1:B:298:SER:HB2	1:B:299:PRO:HD3	1.92	0.52
1:E:280:SER:HB3	1:E:320:GLU:HG3	1.91	0.52
1:G:252:GLY:HA2	1:G:295:LYS:HG3	1.92	0.51
1:E:328:ILE:HG13	1:E:329:GLY:N	2.25	0.51
1:A:268:ARG:HB3	1:A:268:ARG:HH11	1.76	0.51
1:C:121:SER:HB2	1:C:122:PRO:CD	2.40	0.51
1:G:35:TRP:CZ3	1:G:326:PRO:HA	2.45	0.51
1:B:53:ARG:HH11	1:B:53:ARG:HG2	1.76	0.51
1:H:226:PRO:O	1:H:227:HIS:HB2	2.11	0.51
1:C:280:SER:HB3	1:C:320:GLU:HG3	1.93	0.51
1:E:87:ALA:HB3	1:E:120:ILE:HB	1.93	0.51
1:H:35:TRP:HA	1:H:35:TRP:CE3	2.45	0.51
1:I:29:ALA:HB3	1:I:31:PHE:CE1	2.47	0.50
1:B:7:GLU:O	1:B:10:LYS:HG2	2.10	0.50
1:C:112:TYR:O	1:C:164:MET:HA	2.11	0.50
1:J:333:ALA:O	1:J:337:LYS:HG3	2.11	0.50
1:D:104:ASP:O	1:D:108:GLN:HB2	2.12	0.50
1:F:15:LYS:HA	1:F:15:LYS:HE2	1.93	0.50
1:J:326:PRO:HG2	1:J:327:GLU:OE1	2.12	0.50
1:C:29:ALA:HB3	1:C:31:PHE:CE1	2.46	0.50
1:A:252:GLY:O	1:A:295:LYS:HE2	2.12	0.50
1:D:302:ILE:HG13	1:D:334:ASN:HB3	1.94	0.50
1:D:78:TRP:CE2	1:D:87:ALA:HA	2.47	0.50
1:F:5:PHE:CD1	1:F:152:LEU:HD13	2.46	0.50
1:G:112:TYR:O	1:G:164:MET:HA	2.11	0.49
1:D:29:ALA:HB3	1:D:31:PHE:CE1	2.47	0.49
1:L:115:ALA:HB1	1:L:117:GLU:OE1	2.11	0.49
1:I:326:PRO:HG2	1:I:327:GLU:OE2	2.12	0.49
1:H:298:SER:HB2	1:H:299:PRO:HD3	1.94	0.49
1:L:37:LEU:O	1:L:41:LYS:HG3	2.12	0.49
1:B:264:ASP:O	1:B:268:ARG:HG2	2.13	0.49
1:E:123:GLY:HA2	1:E:126:GLU:OE1	2.12	0.49
1:F:78:TRP:CE2	1:F:87:ALA:HA	2.48	0.49
1:D:277:ILE:HB	1:D:315:LEU:CD2	2.42	0.49
1:A:196:PHE:CD1	1:A:292:SER:HB2	2.48	0.49
1:K:78:TRP:CE2	1:K:87:ALA:HA	2.48	0.49
1:H:87:ALA:HB3	1:H:120:ILE:HB	1.94	0.49
1:I:87:ALA:HB3	1:I:120:ILE:HB	1.94	0.49
1:I:214:PHE:CZ	1:I:216:SER:HB2	2.48	0.49
1:D:35:TRP:CE3	1:D:35:TRP:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:ILE:O	1:L:212:VAL:HA	2.13	0.49
1:C:10:LYS:HB3	1:C:10:LYS:NZ	2.28	0.49
1:J:5:PHE:CD1	1:J:152:LEU:HD13	2.48	0.49
1:D:225:PHE:CD1	2:D:404:CXS:H4	2.48	0.49
1:E:225:PHE:HB2	2:E:405:CXS:H91	1.95	0.49
1:C:328:ILE:HG23	1:C:329:GLY:N	2.28	0.48
1:H:67:TYR:CZ	1:H:71:LEU:HD11	2.48	0.48
1:A:157:GLY:HA2	1:A:169:CYS:HB3	1.95	0.48
1:K:189:ILE:O	1:K:212:VAL:HA	2.13	0.48
1:A:10:LYS:NZ	1:A:10:LYS:HB3	2.27	0.48
1:A:121:SER:HB2	1:A:122:PRO:CD	2.44	0.48
1:H:121:SER:HB2	1:H:122:PRO:CD	2.44	0.48
1:I:209:ARG:HB3	1:I:211:ASP:OD1	2.13	0.48
1:A:101:ILE:HG12	1:A:111:TYR:CZ	2.48	0.48
1:B:112:TYR:O	1:B:164:MET:HA	2.13	0.48
1:A:284:ASP:HB3	1:A:322:GLY:HA2	1.94	0.48
1:A:121:SER:HB2	1:A:122:PRO:HD2	1.95	0.48
1:G:72:GLU:HG3	1:G:125:TRP:CD1	2.48	0.48
1:K:101:ILE:HG12	1:K:111:TYR:CZ	2.49	0.48
1:L:284:ASP:HB3	1:L:322:GLY:HA2	1.95	0.48
1:B:277:ILE:HB	1:B:315:LEU:HD23	1.95	0.48
1:G:67:TYR:OH	1:G:165:PHE:HB3	2.14	0.48
1:E:18:LEU:HD22	1:H:18:LEU:HD12	1.95	0.48
1:F:115:ALA:HB1	1:F:117:GLU:OE1	2.13	0.48
1:F:328:ILE:HG23	1:F:329:GLY:N	2.29	0.48
1:D:256:SER:O	1:D:260:GLU:HG3	2.14	0.48
1:J:247:TYR:OH	1:J:268:ARG:HD2	2.14	0.47
1:I:189:ILE:O	1:I:212:VAL:HA	2.14	0.47
1:C:159:HIS:CD2	2:C:403:CXS:H11	2.49	0.47
1:J:7:GLU:O	1:J:10:LYS:HG2	2.14	0.47
1:G:328:ILE:HG13	1:G:329:GLY:H	1.76	0.47
1:F:75:TRP:CE2	1:F:122:PRO:HG3	2.49	0.47
1:G:5:PHE:CE2	1:G:37:LEU:HD22	2.50	0.47
1:J:328:ILE:HG13	1:J:329:GLY:N	2.28	0.47
1:A:67:TYR:OH	1:A:165:PHE:HB3	2.14	0.47
1:I:277:ILE:HB	1:I:315:LEU:CD2	2.45	0.47
1:F:280:SER:HB3	1:F:320:GLU:HG3	1.95	0.47
1:L:56:LEU:O	1:L:59:VAL:HG12	2.14	0.47
1:B:104:ASP:O	1:B:108:GLN:HG3	2.14	0.47
1:B:299:PRO:HB2	1:E:306:ARG:CG	2.45	0.47
1:I:35:TRP:CE3	1:I:326:PRO:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:THR:O	1:J:116:ALA:N	2.47	0.47
1:G:233:GLU:OE2	1:L:100:ARG:NH2	2.48	0.47
1:L:253:THR:HG23	1:L:257:VAL:HB	1.96	0.47
1:J:4:ILE:HD11	1:J:141:LEU:HD11	1.95	0.47
1:D:147:LYS:HD2	1:D:148:ALA:N	2.30	0.47
1:K:87:ALA:HB3	1:K:120:ILE:HB	1.96	0.47
1:B:35:TRP:CE3	1:B:326:PRO:HA	2.50	0.47
1:E:67:TYR:CZ	1:E:71:LEU:HD11	2.50	0.47
1:F:92:PHE:HZ	1:F:116:ALA:HB2	1.79	0.47
1:G:101:ILE:HG12	1:G:111:TYR:CZ	2.50	0.47
1:A:159:HIS:CD2	2:A:401:CXS:H11	2.50	0.47
1:A:268:ARG:NH2	7:A:360:HOH:O	2.47	0.47
1:D:121:SER:HB2	1:D:122:PRO:HD2	1.97	0.47
1:F:117:GLU:HG2	1:F:117:GLU:O	2.15	0.46
1:L:28:GLU:OE2	1:L:32:ARG:NH1	2.41	0.46
1:L:148:ALA:HA	1:L:315:LEU:O	2.14	0.46
1:H:268:ARG:HG2	1:H:268:ARG:HH11	1.80	0.46
1:J:29:ALA:HB3	1:J:31:PHE:CD1	2.50	0.46
1:B:29:ALA:HB3	1:B:31:PHE:CE1	2.50	0.46
1:L:291:ILE:HG13	1:L:291:ILE:O	2.15	0.46
1:D:302:ILE:HD13	1:G:302:ILE:HD13	1.96	0.46
1:F:265:SER:O	1:F:269:ILE:HG13	2.15	0.46
1:L:252:GLY:O	1:L:295:LYS:HE2	2.15	0.46
1:I:213:PHE:HZ	1:I:268:ARG:HD2	1.80	0.46
1:K:193:ASP:HA	1:K:280:SER:HB2	1.96	0.46
1:C:157:GLY:HA2	1:C:169:CYS:HB3	1.98	0.46
1:A:235:THR:HA	1:A:244:THR:O	2.15	0.46
1:J:121:SER:HB2	1:J:122:PRO:CD	2.46	0.46
1:K:281:LEU:HD11	1:K:335:VAL:HG21	1.96	0.46
1:K:252:GLY:HA2	1:K:295:LYS:HE2	1.98	0.46
1:I:67:TYR:OH	1:I:165:PHE:HB3	2.15	0.46
1:B:197:HIS:CE1	2:B:402:CXS:H22	2.51	0.46
1:H:251:ARG:HA	1:H:293:PHE:CD2	2.51	0.46
1:K:226:PRO:O	1:K:227:HIS:HB2	2.15	0.46
1:J:37:LEU:O	1:J:40:VAL:HG22	2.16	0.46
1:H:187:LYS:HA	1:H:187:LYS:HD3	1.79	0.46
1:J:35:TRP:CE3	1:J:326:PRO:HA	2.51	0.45
1:J:51:PRO:HA	1:J:137:ASP:OD1	2.16	0.45
1:E:253:THR:HG23	1:E:257:VAL:HB	1.98	0.45
1:L:251:ARG:HA	1:L:293:PHE:CD2	2.51	0.45
1:B:197:HIS:ND1	2:B:402:CXS:H22	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:ILE:HB	1:K:315:LEU:HD23	1.98	0.45
1:J:32:ARG:HD2	1:J:323:TYR:HD1	1.80	0.45
1:J:57:GLU:HB2	7:J:474:HOH:O	2.15	0.45
1:G:78:TRP:CE2	1:G:87:ALA:HA	2.51	0.45
1:C:75:TRP:NE1	1:C:122:PRO:HG3	2.31	0.45
1:J:4:ILE:HG22	1:J:51:PRO:HG3	1.98	0.45
1:H:7:GLU:O	1:H:10:LYS:HG2	2.16	0.45
1:D:306:ARG:HE	1:D:306:ARG:HA	1.81	0.45
1:A:148:ALA:HA	1:A:315:LEU:O	2.17	0.45
1:B:325:VAL:HB	1:B:327:GLU:OE2	2.16	0.45
1:F:284:ASP:N	1:F:284:ASP:OD1	2.50	0.45
1:G:195:ASP:HA	1:G:282:GLY:HA3	1.99	0.45
1:D:280:SER:HB3	1:D:320:GLU:HG3	1.98	0.45
1:D:225:PHE:CD2	2:D:404:CXS:H31	2.52	0.45
1:I:121:SER:HB2	1:I:122:PRO:CD	2.47	0.45
1:H:78:TRP:CE2	1:H:87:ALA:HA	2.52	0.45
1:H:67:TYR:OH	1:H:165:PHE:HB3	2.16	0.45
1:G:70:PHE:CZ	1:G:109:ILE:HA	2.52	0.45
1:G:121:SER:HB2	1:G:122:PRO:CD	2.47	0.45
1:A:177:ALA:HB1	1:A:316:LEU:HD23	1.98	0.45
1:I:283:VAL:HG23	1:I:322:GLY:HA3	1.97	0.45
1:B:323:TYR:HB3	7:B:695:HOH:O	2.16	0.45
1:L:72:GLU:HG3	1:L:125:TRP:CD1	2.52	0.45
1:G:335:VAL:O	1:G:339:VAL:HG23	2.17	0.45
1:B:18:LEU:HD22	1:F:18:LEU:HD22	1.99	0.45
1:C:306:ARG:HG2	1:C:338:GLY:O	2.17	0.45
1:L:77:ARG:HD3	7:L:355:HOH:O	2.15	0.45
1:H:213:PHE:HB2	1:H:272:PHE:CD2	2.52	0.45
1:G:7:GLU:O	1:G:10:LYS:HG2	2.17	0.44
1:D:75:TRP:CE2	1:D:122:PRO:HG3	2.52	0.44
1:K:216:SER:OG	1:K:218:HIS:ND1	2.47	0.44
1:L:37:LEU:HG	1:L:41:LYS:HE3	1.98	0.44
1:F:284:ASP:HB3	1:F:322:GLY:HA2	1.98	0.44
1:G:61:LYS:HD3	1:K:65:ALA:HB1	1.99	0.44
1:C:4:ILE:HD11	1:C:141:LEU:CD1	2.47	0.44
1:L:67:TYR:OH	1:L:165:PHE:HB3	2.17	0.44
1:J:327:GLU:N	1:J:327:GLU:OE1	2.50	0.44
1:B:28:GLU:HG2	1:B:323:TYR:HE1	1.82	0.44
1:E:284:ASP:HA	1:E:289:ASP:OD2	2.17	0.44
1:E:298:SER:HB2	1:E:299:PRO:HD3	2.00	0.44
1:K:25:PRO:HA	1:K:26:PRO:HD3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:SER:HB2	7:F:988:HOH:O	2.15	0.44
1:E:17:GLU:HG3	1:E:117:GLU:O	2.17	0.44
1:F:17:GLU:HG3	1:F:117:GLU:O	2.17	0.44
1:J:88:ILE:HG12	1:J:119:ALA:HB2	2.00	0.44
1:B:101:ILE:HG12	1:B:111:TYR:CZ	2.53	0.44
1:E:148:ALA:HA	1:E:315:LEU:O	2.18	0.44
1:B:29:ALA:HB3	1:B:31:PHE:CD1	2.53	0.44
1:B:105:ILE:HG23	1:B:106:GLU:N	2.33	0.44
1:F:112:TYR:O	1:F:164:MET:HA	2.18	0.44
1:E:153:CYS:SG	1:E:318:VAL:HG13	2.57	0.44
1:C:101:ILE:HG12	1:C:111:TYR:CZ	2.53	0.44
1:I:325:VAL:HB	1:I:327:GLU:OE1	2.18	0.44
1:C:90:THR:O	1:K:115:ALA:HA	2.18	0.44
1:F:304:MET:O	1:F:308:ILE:HG13	2.18	0.44
1:I:251:ARG:HA	1:I:293:PHE:CD2	2.53	0.43
1:E:5:PHE:CE2	1:E:37:LEU:HD22	2.53	0.43
1:K:121:SER:HB2	1:K:122:PRO:CD	2.48	0.43
1:K:177:ALA:HB1	1:K:316:LEU:HD23	2.00	0.43
1:A:298:SER:HB2	1:A:299:PRO:HD3	1.99	0.43
1:L:37:LEU:O	1:L:40:VAL:HG22	2.18	0.43
1:E:40:VAL:O	1:E:45:PHE:HB2	2.18	0.43
1:I:226:PRO:O	1:I:227:HIS:HB2	2.18	0.43
1:C:40:VAL:HG23	1:C:41:LYS:N	2.32	0.43
1:J:252:GLY:HA2	1:J:295:LYS:HG2	2.00	0.43
1:E:78:TRP:CE2	1:E:87:ALA:HA	2.53	0.43
1:E:1:MET:SD	1:E:336:LEU:HD22	2.58	0.43
1:H:5:PHE:CD1	1:H:152:LEU:HD13	2.53	0.43
1:I:265:SER:O	1:I:269:ILE:HG13	2.19	0.43
1:I:297:THR:OG1	1:I:299:PRO:HD2	2.18	0.43
1:B:115:ALA:HA	1:F:90:THR:O	2.17	0.43
1:F:284:ASP:HA	1:F:289:ASP:OD2	2.19	0.43
1:H:140:ASP:OD1	1:H:184:LYS:HE3	2.19	0.43
1:G:8:ASP:HB3	1:G:11:LEU:HD12	2.01	0.43
1:L:328:ILE:HG23	1:L:329:GLY:N	2.34	0.43
1:E:301:TYR:HB3	1:E:335:VAL:HG23	1.98	0.43
1:D:251:ARG:HA	1:D:293:PHE:CD2	2.53	0.43
1:E:121:SER:HB2	1:E:122:PRO:HD2	2.00	0.43
1:F:193:ASP:HA	1:F:280:SER:HB2	2.01	0.43
1:H:286:PHE:CE2	1:H:288:GLN:HB2	2.53	0.43
1:A:328:ILE:HG23	1:A:329:GLY:N	2.33	0.43
1:K:302:ILE:CG1	1:K:334:ASN:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:HB	2:B:402:CXS:H82	2.01	0.43
1:D:148:ALA:HA	1:D:315:LEU:O	2.18	0.43
1:A:100:ARG:NE	1:I:233:GLU:OE2	2.48	0.43
1:E:7:GLU:O	1:E:10:LYS:HG2	2.18	0.43
1:A:226:PRO:O	1:A:227:HIS:HB2	2.19	0.43
1:H:121:SER:HB2	1:H:122:PRO:HD2	2.00	0.43
1:B:251:ARG:HA	1:B:293:PHE:CD2	2.53	0.43
1:C:286:PHE:CE2	1:C:288:GLN:HB2	2.54	0.43
1:I:112:TYR:O	1:I:164:MET:HA	2.19	0.43
1:H:15:LYS:HG2	1:H:86:GLU:OE2	2.19	0.43
1:D:101:ILE:HG12	1:D:111:TYR:CZ	2.54	0.43
1:E:104:ASP:O	1:E:108:GLN:HG3	2.19	0.43
1:D:299:PRO:HB2	1:G:306:ARG:HD3	2.01	0.42
1:J:121:SER:HB2	1:J:122:PRO:HD2	2.00	0.42
1:C:148:ALA:HA	1:C:315:LEU:O	2.19	0.42
1:K:51:PRO:HA	1:K:137:ASP:OD1	2.18	0.42
1:E:268:ARG:HH11	1:E:268:ARG:HG3	1.84	0.42
1:L:211:ASP:OD1	1:L:212:VAL:HG23	2.19	0.42
1:C:41:LYS:CE	1:C:48:VAL:HG21	2.48	0.42
1:A:92:PHE:HZ	1:A:116:ALA:HB2	1.84	0.42
1:B:252:GLY:HA2	1:B:295:LYS:HG2	2.01	0.42
1:A:197:HIS:CD2	1:A:225:PHE:HB3	2.54	0.42
1:D:309:ALA:HA	1:D:315:LEU:HD11	2.01	0.42
1:C:75:TRP:CE2	1:C:122:PRO:HG3	2.55	0.42
1:F:189:ILE:O	1:F:212:VAL:HA	2.18	0.42
1:I:101:ILE:HG12	1:I:111:TYR:CZ	2.54	0.42
1:C:17:GLU:HG3	1:C:117:GLU:O	2.20	0.42
1:E:67:TYR:OH	1:E:165:PHE:HB3	2.20	0.42
1:C:189:ILE:O	1:C:212:VAL:HA	2.19	0.42
1:B:92:PHE:HZ	1:B:116:ALA:HB2	1.84	0.42
1:G:121:SER:HB2	1:G:122:PRO:HD2	2.01	0.42
1:D:150:PHE:HZ	1:D:319:MET:HG2	1.84	0.42
1:I:2:ARG:HD3	1:I:49:VAL:HG11	2.01	0.42
1:J:335:VAL:O	1:J:339:VAL:HG23	2.20	0.42
1:B:193:ASP:HA	1:B:280:SER:HB2	2.01	0.42
1:H:277:ILE:HB	1:H:315:LEU:CD2	2.50	0.42
1:E:121:SER:HB2	1:E:122:PRO:CD	2.50	0.42
1:E:335:VAL:O	1:E:339:VAL:HG23	2.19	0.42
1:L:233:GLU:HG2	7:L:504:HOH:O	2.20	0.42
1:A:5:PHE:CD1	1:A:152:LEU:HD13	2.54	0.42
1:G:309:ALA:HA	1:G:315:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLU:HG3	1:D:117:GLU:O	2.20	0.42
1:A:198:HIS:CE1	1:A:200:ASN:HA	2.54	0.42
1:B:90:THR:O	1:F:116:ALA:N	2.53	0.42
1:I:177:ALA:HB1	1:I:316:LEU:HD23	2.02	0.42
1:I:94:VAL:HB	1:I:95:ARG:H	1.62	0.42
1:F:87:ALA:HB3	1:F:120:ILE:HB	2.02	0.41
1:K:253:THR:HG23	1:K:257:VAL:HB	2.02	0.41
1:A:115:ALA:HA	1:I:90:THR:O	2.20	0.41
1:K:265:SER:O	1:K:269:ILE:HG13	2.20	0.41
1:I:104:ASP:O	1:I:108:GLN:HG3	2.20	0.41
1:B:53:ARG:NH1	1:B:53:ARG:HG2	2.36	0.41
1:G:265:SER:O	1:G:269:ILE:HG13	2.20	0.41
1:K:189:ILE:HD12	1:K:276:ALA:HB3	2.02	0.41
1:C:90:THR:HG22	1:K:18:LEU:HD23	2.02	0.41
1:K:29:ALA:HB3	1:K:31:PHE:CE1	2.55	0.41
1:L:157:GLY:HA2	1:L:169:CYS:CB	2.43	0.41
1:G:154:ARG:HA	1:G:155:PRO:C	2.41	0.41
1:C:78:TRP:CE2	1:C:87:ALA:HA	2.55	0.41
1:C:67:TYR:OH	1:C:165:PHE:HB3	2.20	0.41
1:J:154:ARG:HA	1:J:155:PRO:C	2.41	0.41
1:J:286:PHE:CE2	1:J:288:GLN:HB2	2.56	0.41
1:F:25:PRO:HA	1:F:26:PRO:HD3	1.96	0.41
1:G:253:THR:HG23	1:G:257:VAL:HB	2.00	0.41
1:E:292:SER:HB2	7:E:1288:HOH:O	2.20	0.41
1:J:25:PRO:HA	1:J:26:PRO:HD3	1.91	0.41
1:A:154:ARG:HA	1:A:155:PRO:C	2.41	0.41
1:D:255:TYR:CD1	1:D:300:ASP:HB3	2.55	0.41
1:C:257:VAL:HA	1:C:260:GLU:OE1	2.20	0.41
1:E:177:ALA:HB1	1:E:316:LEU:HD23	2.02	0.41
1:H:291:ILE:HG13	1:H:291:ILE:O	2.20	0.41
1:B:299:PRO:HB2	1:E:306:ARG:HG3	2.00	0.41
1:G:115:ALA:HA	1:L:90:THR:O	2.21	0.41
1:C:277:ILE:HB	1:C:315:LEU:CD2	2.51	0.41
1:I:37:LEU:O	1:I:40:VAL:HG22	2.20	0.41
1:C:253:THR:HG23	1:C:257:VAL:HB	2.02	0.41
1:D:217:LEU:HD23	1:D:249:MET:HE1	2.03	0.41
1:C:193:ASP:OD1	1:C:195:ASP:HB3	2.20	0.41
1:L:220:ASP:OD2	1:L:222:ALA:HB3	2.20	0.41
1:I:57:GLU:HB2	7:I:479:HOH:O	2.19	0.41
1:J:252:GLY:HA2	1:J:295:LYS:CG	2.51	0.41
1:E:7:GLU:O	1:E:10:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:GLU:HB2	7:H:359:HOH:O	2.21	0.41
1:H:35:TRP:HA	1:H:35:TRP:HE3	1.85	0.41
1:E:284:ASP:N	1:E:284:ASP:OD1	2.50	0.41
1:B:177:ALA:HB1	1:B:316:LEU:HD23	2.03	0.41
1:I:306:ARG:HG2	1:I:306:ARG:HH21	1.86	0.41
1:A:89:ALA:HB1	1:A:110:GLY:HA2	2.03	0.41
1:A:89:ALA:HB2	1:A:109:ILE:HG12	2.02	0.41
1:L:89:ALA:HB2	1:L:109:ILE:HG12	2.02	0.41
1:L:11:LEU:HD23	1:L:11:LEU:HA	1.93	0.41
1:J:32:ARG:HD2	1:J:323:TYR:CD1	2.56	0.41
1:H:213:PHE:HB2	1:H:272:PHE:CE2	2.56	0.41
1:D:225:PHE:CG	1:D:226:PRO:HA	2.56	0.40
1:D:25:PRO:HA	1:D:26:PRO:HD3	1.96	0.40
1:D:157:GLY:HA2	1:D:169:CYS:HB3	2.03	0.40
1:F:291:ILE:H	1:F:291:ILE:HG13	1.70	0.40
1:F:37:LEU:O	1:F:40:VAL:HG22	2.22	0.40
1:H:249:MET:HB2	1:H:294:PHE:CZ	2.55	0.40
1:F:213:PHE:HZ	1:F:268:ARG:HD2	1.86	0.40
1:J:253:THR:HG23	1:J:257:VAL:HB	2.03	0.40
1:F:177:ALA:HB1	1:F:316:LEU:HD23	2.04	0.40
1:E:112:TYR:O	1:E:164:MET:HA	2.20	0.40
1:H:327:GLU:OE1	1:H:327:GLU:N	2.54	0.40
1:C:196:PHE:CD1	1:C:292:SER:HB2	2.57	0.40
1:L:297:THR:OG1	1:L:299:PRO:HD2	2.21	0.40
1:F:277:ILE:HB	1:F:315:LEU:HD23	2.03	0.40
1:D:287:GLU:OE1	1:D:297:THR:HG22	2.21	0.40
1:G:286:PHE:CE2	1:G:288:GLN:HB2	2.57	0.40
1:L:29:ALA:HB3	1:L:31:PHE:CD2	2.57	0.40
1:L:31:PHE:CZ	1:L:324:GLY:HA3	2.56	0.40
1:E:328:ILE:O	1:E:332:VAL:HG23	2.22	0.40
1:C:164:MET:HE2	7:C:359:HOH:O	2.20	0.40
1:D:35:TRP:HA	1:D:35:TRP:HE3	1.86	0.40
1:D:100:ARG:HD2	1:J:231:TYR:CD2	2.56	0.40
1:H:28:GLU:OE2	1:H:32:ARG:NH1	2.52	0.40
1:D:9:HIS:CG	1:D:10:LYS:N	2.90	0.40
1:H:126:GLU:CD	1:H:126:GLU:H	2.24	0.40
1:I:292:SER:HB2	7:I:1279:HOH:O	2.20	0.40
1:G:18:LEU:HD22	1:L:18:LEU:HD22	2.03	0.40
1:I:5:PHE:CE2	1:I:37:LEU:HD22	2.56	0.40
1:K:283:VAL:CG2	1:K:322:GLY:HA3	2.51	0.40
1:J:197:HIS:CE1	2:J:410:CXS:H12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:327:GLU:N	1:K:327:GLU:OE1	2.54	0.40
1:J:280:SER:HB3	1:J:320:GLU:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/341 (99%)	322 (95%)	16 (5%)	1 (0%)	46	55
1	B	339/341 (99%)	321 (95%)	17 (5%)	1 (0%)	46	55
1	C	339/341 (99%)	322 (95%)	16 (5%)	1 (0%)	46	55
1	D	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	46	55
1	E	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	46	55
1	F	339/341 (99%)	318 (94%)	20 (6%)	1 (0%)	46	55
1	G	339/341 (99%)	319 (94%)	17 (5%)	3 (1%)	21	22
1	H	339/341 (99%)	322 (95%)	16 (5%)	1 (0%)	46	55
1	I	338/341 (99%)	324 (96%)	13 (4%)	1 (0%)	46	55
1	J	338/341 (99%)	319 (94%)	18 (5%)	1 (0%)	46	55
1	K	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	46	55
1	L	339/341 (99%)	319 (94%)	19 (6%)	1 (0%)	46	55
All	All	4066/4092 (99%)	3858 (95%)	194 (5%)	14 (0%)	46	55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	94	VAL
1	G	290	PRO

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Mol	Chain	Res	Type
1	G	291	ILE
1	D	94	VAL
1	A	94	VAL
1	H	94	VAL
1	B	94	VAL
1	I	94	VAL
1	K	94	VAL
1	C	94	VAL
1	J	94	VAL
1	L	94	VAL
1	E	94	VAL
1	G	94	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/253 (100%)	248 (98%)	5 (2%)	63	77
1	B	253/253 (100%)	247 (98%)	6 (2%)	57	71
1	C	253/253 (100%)	248 (98%)	5 (2%)	63	77
1	D	253/253 (100%)	244 (96%)	9 (4%)	42	55
1	E	253/253 (100%)	246 (97%)	7 (3%)	51	65
1	F	253/253 (100%)	249 (98%)	4 (2%)	70	83
1	G	253/253 (100%)	247 (98%)	6 (2%)	57	71
1	H	253/253 (100%)	248 (98%)	5 (2%)	63	77
1	I	253/253 (100%)	246 (97%)	7 (3%)	51	65
1	J	253/253 (100%)	247 (98%)	6 (2%)	57	71
1	K	253/253 (100%)	247 (98%)	6 (2%)	57	71
1	L	253/253 (100%)	248 (98%)	5 (2%)	63	77
All	All	3036/3036 (100%)	2965 (98%)	71 (2%)	58	73

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	117	GLU
1	A	152	LEU
1	A	158	HIS
1	A	256	SER
1	B	28	GLU
1	B	117	GLU
1	B	137	ASP
1	B	158	HIS
1	B	164	MET
1	B	293	PHE
1	C	10	LYS
1	C	42	GLU
1	C	117	GLU
1	C	158	HIS
1	C	306	ARG
1	D	10	LYS
1	D	53	ARG
1	D	108	GLN
1	D	117	GLU
1	D	147	LYS
1	D	158	HIS
1	D	164	MET
1	D	288	GLN
1	D	293	PHE
1	E	28	GLU
1	E	46	ASP
1	E	117	GLU
1	E	137	ASP
1	E	152	LEU
1	E	158	HIS
1	E	284	ASP
1	F	28	GLU
1	F	117	GLU
1	F	152	LEU
1	F	158	HIS
1	G	28	GLU
1	G	117	GLU
1	G	137	ASP
1	G	158	HIS
1	G	168	TYR
1	G	280	SER
1	H	117	GLU

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Mol	Chain	Res	Type
1	H	158	HIS
1	H	164	MET
1	H	280	SER
1	H	292	SER
1	I	28	GLU
1	I	94	VAL
1	I	117	GLU
1	I	152	LEU
1	I	158	HIS
1	I	168	TYR
1	I	280	SER
1	J	18	LEU
1	J	28	GLU
1	J	117	GLU
1	J	158	HIS
1	J	168	TYR
1	J	327	GLU
1	K	28	GLU
1	K	117	GLU
1	K	152	LEU
1	K	158	HIS
1	K	168	TYR
1	K	284	ASP
1	L	28	GLU
1	L	117	GLU
1	L	152	LEU
1	L	158	HIS
1	L	327	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	C	197	HIS
1	F	198	HIS
1	H	69	ASN
1	J	69	ASN
1	L	13	ASN
1	L	331	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 68 ligands modelled in this entry, 44 are monoatomic - leaving 24 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	PO4	A	353	-	4,4,4	1.10	0	6,6,6	0.27	0
2	CXS	A	401	6	13,14,14	1.11	1 (7%)	15,18,18	1.75	3 (20%)
3	PO4	B	352	-	4,4,4	1.15	0	6,6,6	0.27	0
2	CXS	B	402	6	13,14,14	0.95	1 (7%)	15,18,18	1.57	3 (20%)
3	PO4	C	353	-	4,4,4	1.12	0	6,6,6	0.27	0
2	CXS	C	403	6	13,14,14	1.06	1 (7%)	15,18,18	1.65	3 (20%)
3	PO4	D	352	-	4,4,4	1.14	0	6,6,6	0.27	0
2	CXS	D	404	6	13,14,14	1.03	0	15,18,18	1.66	4 (26%)
3	PO4	E	353	-	4,4,4	1.23	0	6,6,6	0.27	0
2	CXS	E	405	6	13,14,14	1.01	0	15,18,18	1.65	3 (20%)
3	PO4	F	352	-	4,4,4	1.12	0	6,6,6	0.27	0
2	CXS	F	406	6	13,14,14	1.03	0	15,18,18	1.63	3 (20%)
3	PO4	G	353	-	4,4,4	1.11	0	6,6,6	0.27	0
2	CXS	G	407	6	13,14,14	1.17	1 (7%)	15,18,18	1.68	2 (13%)
3	PO4	H	352	-	4,4,4	1.09	0	6,6,6	0.27	0
2	CXS	H	408	6	13,14,14	1.13	1 (7%)	15,18,18	1.71	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	I	353	-	4,4,4	1.15	0	6,6,6	0.27	0
2	CXS	I	409	6	13,14,14	1.01	1 (7%)	15,18,18	1.65	2 (13%)
3	PO4	J	352	-	4,4,4	1.07	0	6,6,6	0.27	0
2	CXS	J	410	6	13,14,14	1.07	1 (7%)	15,18,18	1.76	4 (26%)
3	PO4	K	353	-	4,4,4	1.12	0	6,6,6	0.27	0
2	CXS	K	411	6	13,14,14	0.96	0	15,18,18	1.64	2 (13%)
3	PO4	L	352	-	4,4,4	1.13	0	6,6,6	0.27	0
2	CXS	L	412	6	13,14,14	1.00	0	15,18,18	1.75	3 (20%)

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	PO4	A	353	-	-	0/0/0/0	0/0/0/0
2	CXS	A	401	6	-	0/8/16/16	0/1/1/1
3	PO4	B	352	-	-	0/0/0/0	0/0/0/0
2	CXS	B	402	6	-	0/8/16/16	0/1/1/1
3	PO4	C	353	-	-	0/0/0/0	0/0/0/0
2	CXS	C	403	6	-	0/8/16/16	0/1/1/1
3	PO4	D	352	-	-	0/0/0/0	0/0/0/0
2	CXS	D	404	6	-	0/8/16/16	0/1/1/1
3	PO4	E	353	-	-	0/0/0/0	0/0/0/0
2	CXS	E	405	6	-	0/8/16/16	0/1/1/1
3	PO4	F	352	-	-	0/0/0/0	0/0/0/0
2	CXS	F	406	6	-	0/8/16/16	0/1/1/1
3	PO4	G	353	-	-	0/0/0/0	0/0/0/0
2	CXS	G	407	6	-	0/8/16/16	0/1/1/1
3	PO4	H	352	-	-	0/0/0/0	0/0/0/0
2	CXS	H	408	6	-	0/8/16/16	0/1/1/1
3	PO4	I	353	-	-	0/0/0/0	0/0/0/0
2	CXS	I	409	6	-	0/8/16/16	0/1/1/1
3	PO4	J	352	-	-	0/0/0/0	0/0/0/0
2	CXS	J	410	6	-	0/8/16/16	0/1/1/1
3	PO4	K	353	-	-	0/0/0/0	0/0/0/0
2	CXS	K	411	6	-	0/8/16/16	0/1/1/1
3	PO4	L	352	-	-	0/0/0/0	0/0/0/0
2	CXS	L	412	6	-	0/8/16/16	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	CXS	C9-C4	2.02	1.57	1.51
2	I	409	CXS	C9-C4	2.22	1.57	1.51
2	J	410	CXS	C9-C4	2.28	1.57	1.51
2	H	408	CXS	C9-C4	2.40	1.58	1.51
2	C	403	CXS	C9-C4	2.41	1.58	1.51
2	G	407	CXS	C9-C4	2.42	1.58	1.51
2	A	401	CXS	C9-C4	2.46	1.58	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	412	CXS	O1-S-C1	-5.27	102.41	106.91
2	A	401	CXS	O1-S-C1	-5.25	102.43	106.91
2	G	407	CXS	O1-S-C1	-4.87	102.75	106.91
2	H	408	CXS	O1-S-C1	-4.87	102.75	106.91
2	I	409	CXS	O1-S-C1	-4.78	102.82	106.91
2	C	403	CXS	O1-S-C1	-4.71	102.89	106.91
2	K	411	CXS	O1-S-C1	-4.71	102.89	106.91
2	J	410	CXS	O1-S-C1	-4.68	102.91	106.91
2	F	406	CXS	O1-S-C1	-4.63	102.95	106.91
2	E	405	CXS	O1-S-C1	-4.51	103.06	106.91
2	B	402	CXS	O1-S-C1	-4.25	103.28	106.91
2	D	404	CXS	O1-S-C1	-4.00	103.49	106.91
2	D	404	CXS	C3-C2-C1	-2.80	107.65	112.24
2	E	405	CXS	C9-C4-C5	-2.40	106.73	110.82
2	G	407	CXS	C9-C4-C5	-2.39	106.75	110.82
2	J	410	CXS	C9-C4-C5	-2.34	106.83	110.82
2	H	408	CXS	C9-C4-C5	-2.34	106.83	110.82
2	B	402	CXS	C9-C4-C5	-2.29	106.91	110.82
2	K	411	CXS	C9-C4-C5	-2.16	107.13	110.82
2	F	406	CXS	C9-C4-C5	-2.13	107.20	110.82
2	A	401	CXS	C9-C4-C5	-2.08	107.27	110.82
2	D	404	CXS	C9-C4-C5	-2.05	107.32	110.82
2	C	403	CXS	C9-C4-C5	-2.04	107.34	110.82
2	L	412	CXS	C9-C4-C5	-2.03	107.37	110.82
2	F	406	CXS	C3-C2-C1	-2.02	108.93	112.24
2	J	410	CXS	C3-C2-C1	-2.01	108.95	112.24
2	J	410	CXS	C8-C9-C4	2.01	114.24	111.13
2	L	412	CXS	C8-C9-C4	2.06	114.31	111.13
2	C	403	CXS	C8-C9-C4	2.07	114.33	111.13
2	D	404	CXS	C8-C9-C4	2.10	114.38	111.13
2	A	401	CXS	C8-C9-C4	2.17	114.49	111.13
2	I	409	CXS	C8-C9-C4	2.18	114.50	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	405	CXS	C8-C9-C4	2.23	114.58	111.13
2	B	402	CXS	C8-C9-C4	2.38	114.81	111.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CXS	1	0
2	B	402	CXS	4	0
2	C	403	CXS	1	0
2	D	404	CXS	6	0
2	E	405	CXS	3	0
2	F	406	CXS	1	0
2	G	407	CXS	1	0
2	I	409	CXS	4	0
2	J	410	CXS	1	0
2	K	411	CXS	3	0
2	L	412	CXS	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	341/341 (100%)	-0.46	1 (0%) 94 97	22, 33, 46, 63	0
1	B	341/341 (100%)	-0.36	3 (0%) 85 92	24, 36, 52, 60	0
1	C	341/341 (100%)	-0.35	1 (0%) 94 97	21, 34, 47, 66	0
1	D	341/341 (100%)	-0.46	1 (0%) 94 97	23, 34, 46, 60	0
1	E	341/341 (100%)	-0.30	2 (0%) 90 95	25, 36, 52, 61	0
1	F	341/341 (100%)	-0.11	8 (2%) 64 76	23, 38, 57, 65	0
1	G	341/341 (100%)	-0.28	4 (1%) 81 89	24, 36, 52, 65	0
1	H	341/341 (100%)	-0.19	7 (2%) 67 79	23, 38, 53, 66	0
1	I	340/341 (99%)	-0.42	0 100 100	24, 36, 48, 66	0
1	J	340/341 (99%)	-0.15	5 (1%) 76 85	26, 41, 64, 76	0
1	K	341/341 (100%)	-0.37	4 (1%) 81 89	26, 36, 49, 66	0
1	L	341/341 (100%)	-0.25	5 (1%) 76 85	26, 38, 52, 67	0
All	All	4090/4092 (99%)	-0.31	41 (1%) 84 92	21, 36, 52, 76	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	341	GLY	4.6
1	F	341	GLY	3.8
1	F	254	PRO	3.5
1	F	257	VAL	3.5
1	L	341	GLY	3.4
1	G	325	VAL	3.3
1	A	53	ARG	3.3
1	F	252	GLY	3.3
1	L	53	ARG	3.3
1	C	53	ARG	3.1
1	F	53	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	143	ALA	3.1
1	H	291	ILE	2.9
1	J	325	VAL	2.9
1	G	324	GLY	2.9
1	D	53	ARG	2.8
1	K	144	ALA	2.8
1	J	43	ALA	2.7
1	H	53	ARG	2.7
1	G	252	GLY	2.7
1	J	252	GLY	2.6
1	G	80	ALA	2.6
1	E	291	ILE	2.6
1	H	256	SER	2.5
1	J	288	GLN	2.5
1	L	252	GLY	2.5
1	H	35	TRP	2.4
1	F	260	GLU	2.4
1	B	290	PRO	2.4
1	H	147	LYS	2.3
1	L	254	PRO	2.3
1	K	341	GLY	2.3
1	L	35	TRP	2.3
1	K	53	ARG	2.3
1	H	252	GLY	2.2
1	E	144	ALA	2.2
1	J	46	ASP	2.2
1	B	53	ARG	2.1
1	F	143	ALA	2.1
1	F	253	THR	2.0
1	K	42	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NA	C	343	1/1	0.99	0.18	9.63	14,14,14,14	0
5	NA	D	343	1/1	1.00	0.17	9.01	14,14,14,14	0
2	CXS	A	401	14/14	0.92	0.23	8.08	89,95,98,98	0
2	CXS	K	411	14/14	0.95	0.23	7.88	92,96,100,101	0
2	CXS	C	403	14/14	0.92	0.30	7.84	85,92,97,97	0
5	NA	E	343	1/1	0.99	0.14	5.32	16,16,16,16	0
5	NA	I	343	1/1	0.97	0.15	5.11	20,20,20,20	0
2	CXS	J	410	14/14	0.87	0.26	5.01	88,93,99,99	0
5	NA	A	343	1/1	0.99	0.16	4.98	14,14,14,14	0
2	CXS	F	406	14/14	0.90	0.27	4.87	97,102,106,106	0
5	NA	B	343	1/1	0.99	0.15	4.60	13,13,13,13	0
2	CXS	D	404	14/14	0.92	0.24	4.47	78,84,88,88	0
2	CXS	I	409	14/14	0.95	0.20	3.68	80,87,91,91	0
5	NA	G	343	1/1	0.99	0.19	3.61	16,16,16,16	0
2	CXS	B	402	14/14	0.94	0.20	3.32	85,92,96,96	0
2	CXS	L	412	14/14	0.93	0.23	3.24	85,90,96,96	0
5	NA	K	343	1/1	0.98	0.16	2.84	19,19,19,19	0
2	CXS	H	408	14/14	0.93	0.26	2.75	94,98,103,103	0
2	CXS	G	407	14/14	0.94	0.19	2.03	76,80,86,86	0
2	CXS	E	405	14/14	0.92	0.20	1.93	78,85,90,90	0
5	NA	J	343	1/1	0.97	0.13	1.77	22,22,22,22	0
5	NA	H	343	1/1	0.99	0.11	1.42	24,24,24,24	0
5	NA	L	343	1/1	0.92	0.12	0.56	25,25,25,25	0
3	PO4	K	353	5/5	0.91	0.16	0.26	87,87,88,89	0
3	PO4	L	352	5/5	0.83	0.17	0.20	102,102,103,103	0
5	NA	F	343	1/1	0.91	0.11	0.13	27,27,27,27	0
3	PO4	I	353	5/5	0.92	0.15	0.10	87,87,88,88	0
4	K	G	344	1/1	0.83	0.16	0.07	120,120,120,120	0
4	K	C	342	1/1	0.98	0.09	0.06	29,29,29,29	0
3	PO4	E	353	5/5	0.97	0.13	0.02	74,74,75,76	0
4	K	H	344	1/1	0.93	0.15	0.01	72,72,72,72	0
4	K	E	342	1/1	0.99	0.09	-0.17	33,33,33,33	0
3	PO4	A	353	5/5	0.94	0.12	-0.26	71,73,73,74	0
4	K	G	342	1/1	0.99	0.08	-0.32	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	D	352	5/5	0.91	0.11	-0.39	78,79,79,79	0
4	K	E	344	1/1	0.78	0.13	-0.56	96,96,96,96	0
4	K	B	342	1/1	0.98	0.08	-0.64	32,32,32,32	0
4	K	A	342	1/1	0.99	0.08	-0.71	29,29,29,29	0
4	K	K	342	1/1	0.99	0.09	-0.75	33,33,33,33	0
4	K	C	344	1/1	0.93	0.10	-0.88	77,77,77,77	0
6	ZN	C	345	1/1	0.98	0.09	-1.21	51,51,51,51	0
4	K	L	344	1/1	0.90	0.09	-1.23	84,84,84,84	0
4	K	J	342	1/1	1.00	0.10	-1.24	39,39,39,39	0
4	K	A	344	1/1	0.97	0.07	-1.39	73,73,73,73	0
4	K	F	344	1/1	0.34	0.10	-1.40	100,100,100,100	0
6	ZN	G	345	1/1	0.99	0.04	-1.71	48,48,48,48	0
6	ZN	D	345	1/1	0.99	0.04	-1.78	46,46,46,46	0
4	K	I	342	1/1	1.00	0.05	-1.99	32,32,32,32	0
6	ZN	I	344	1/1	0.96	0.05	-2.30	51,51,51,51	0
6	ZN	J	344	1/1	0.99	0.07	-2.30	58,58,58,58	0
6	ZN	H	345	1/1	0.97	0.05	-2.54	51,51,51,51	0
4	K	D	344	1/1	0.97	0.05	-2.64	69,69,69,69	0
4	K	D	342	1/1	0.99	0.04	-2.78	29,29,29,29	0
4	K	H	342	1/1	0.99	0.07	-2.91	34,34,34,34	0
6	ZN	E	345	1/1	0.99	0.05	-3.04	50,50,50,50	0
4	K	F	342	1/1	0.99	0.04	-3.10	31,31,31,31	0
6	ZN	B	344	1/1	0.98	0.05	-3.22	53,53,53,53	0
6	ZN	F	345	1/1	0.98	0.04	-3.53	58,58,58,58	0
6	ZN	A	345	1/1	0.99	0.04	-3.84	52,52,52,52	0
4	K	L	342	1/1	0.99	0.04	-4.26	31,31,31,31	0
6	ZN	K	344	1/1	0.96	0.05	-4.59	53,53,53,53	0
6	ZN	L	345	1/1	0.99	0.04	-5.62	49,49,49,49	0
3	PO4	C	353	5/5	0.95	0.08	-	75,76,77,77	0
3	PO4	G	353	5/5	0.95	0.13	-	77,77,79,79	0
3	PO4	H	352	5/5	0.89	0.12	-	97,97,98,98	0
3	PO4	J	352	5/5	0.96	0.08	-	84,84,85,85	0
3	PO4	B	352	5/5	0.97	0.11	-	65,66,67,68	0
3	PO4	F	352	5/5	0.91	0.11	-	90,91,92,92	0

6.5 Other polymers

There are no such residues in this entry.