



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:08 PM UTC

PDB ID : 2QUB / pdb_00002qub
Title : Crystal structure of extracellular lipase LipA from *Serratia marcescens*
Authors : Meier, R.; Baumann, U.
Deposited on : 2007-08-04
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

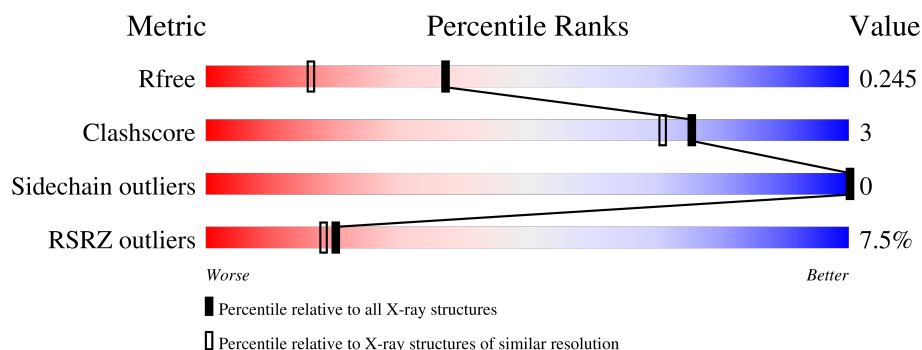
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	615	8% 96% .
1	C	615	3% 96% .
1	E	615	13% 93% 7%
1	G	615	6% 96% .
1	I	615	4% 96% .
1	K	615	11% 94% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29575 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 Extracellular lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4601	2883	779	936	3			
1	C	615	Total	C	N	O	S	0	0	0
			4601	2883	779	936	3			
1	E	615	Total	C	N	O	S	0	0	0
			4601	2883	779	936	3			
1	G	615	Total	C	N	O	S	0	0	0
			4601	2883	779	936	3			
1	I	615	Total	C	N	O	S	0	0	0
			4601	2883	779	936	3			
1	K	615	Total	C	N	O	S	0	0	0
			4601	2883	779	936	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q59933
A	0	HIS	-	expression tag	UNP Q59933
C	-1	SER	-	expression tag	UNP Q59933
C	0	HIS	-	expression tag	UNP Q59933
E	-1	SER	-	expression tag	UNP Q59933
E	0	HIS	-	expression tag	UNP Q59933
G	-1	SER	-	expression tag	UNP Q59933
G	0	HIS	-	expression tag	UNP Q59933
I	-1	SER	-	expression tag	UNP Q59933
I	0	HIS	-	expression tag	UNP Q59933
K	-1	SER	-	expression tag	UNP Q59933
K	0	HIS	-	expression tag	UNP Q59933

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total Ca 8 8	0	0
2	C	8	Total Ca 8 8	0	0
2	E	8	Total Ca 8 8	0	0
2	G	8	Total Ca 8 8	0	0
2	I	8	Total Ca 8 8	0	0
2	K	8	Total Ca 8 8	0	0

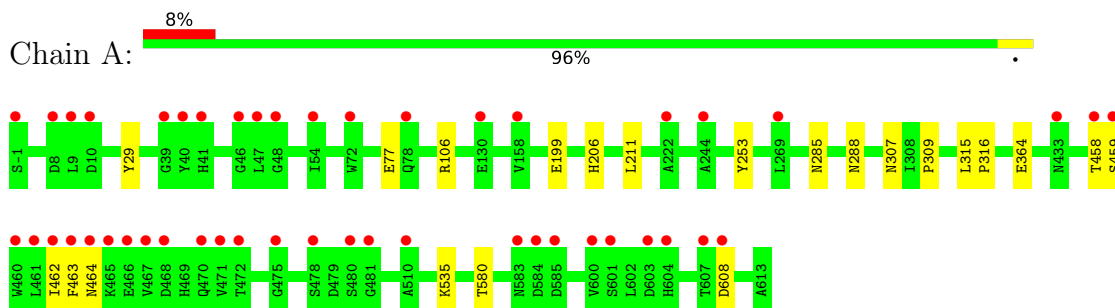
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	322	Total O 322 322	0	0
3	C	360	Total O 360 360	0	0
3	E	285	Total O 285 285	0	0
3	G	346	Total O 346 346	0	0
3	I	305	Total O 305 305	0	0
3	K	303	Total O 303 303	0	0

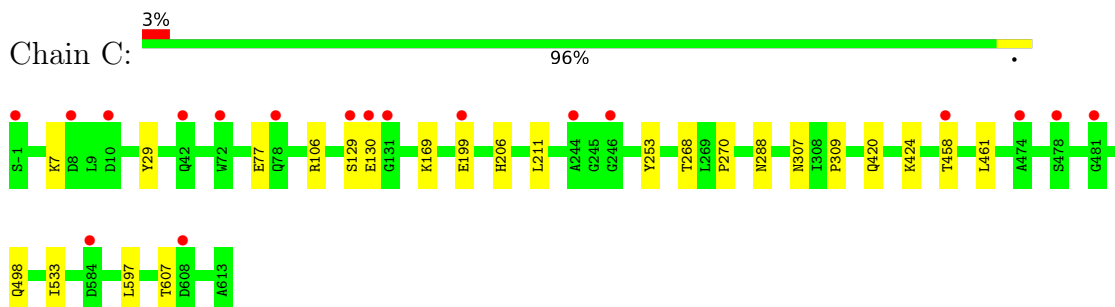
3 Residue-property plots [i](#)

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

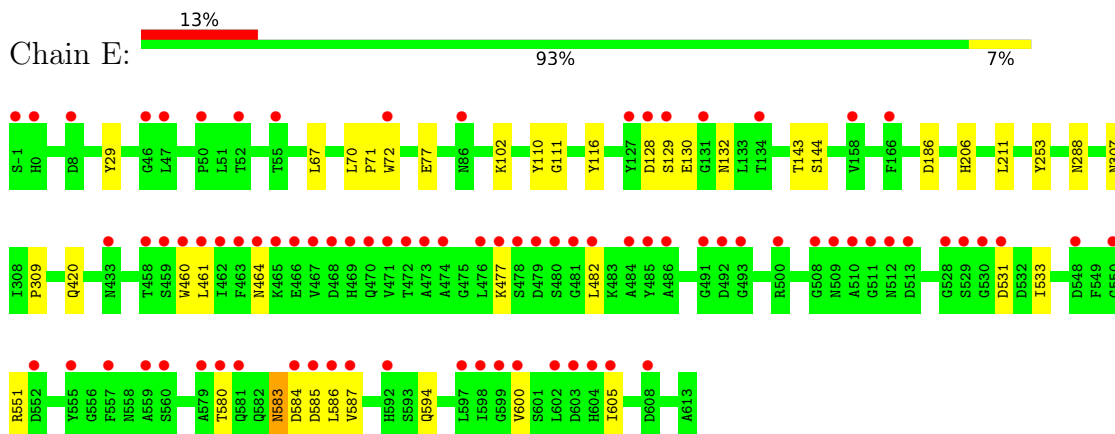
- Molecule 1: Extracellular lipase



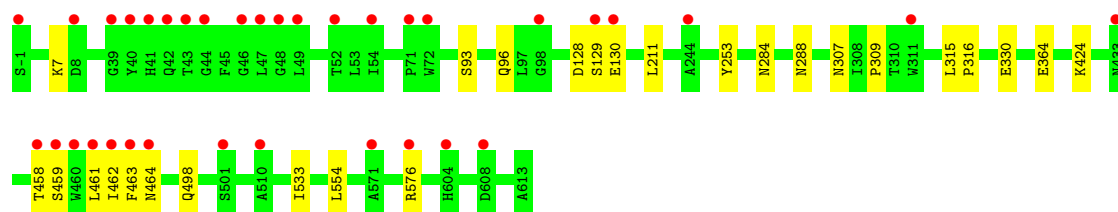
- Molecule 1: Extracellular lipase



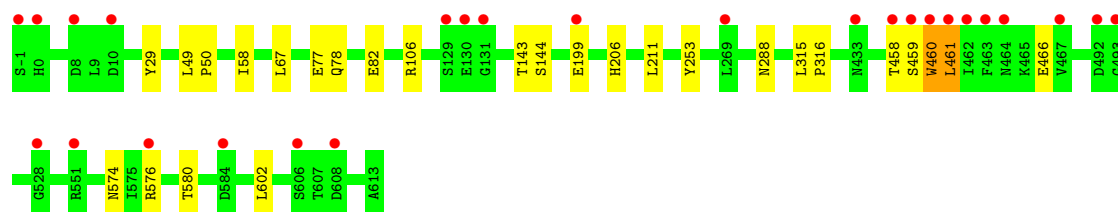
- Molecule 1: Extracellular lipase



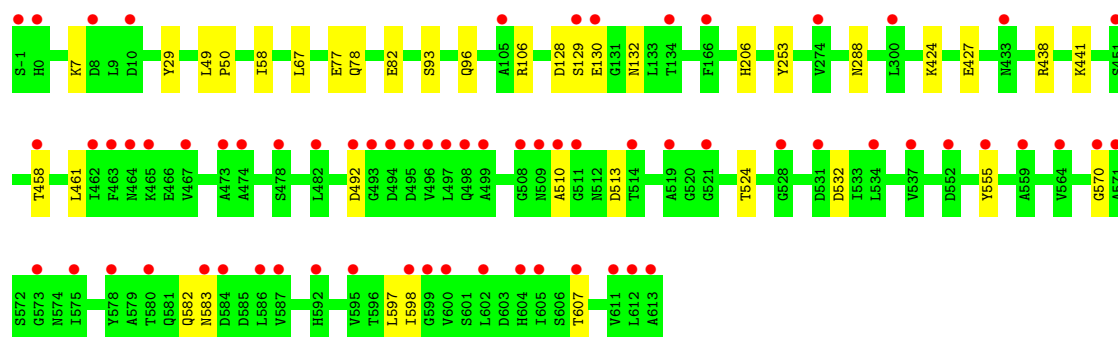
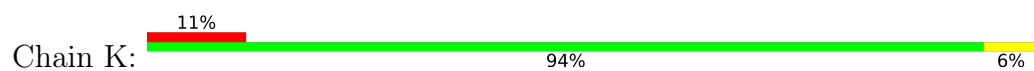
- Molecule 1: Extracellular lipase



- Molecule 1: Extracellular lipase



- Molecule 1: Extracellular lipase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	202.40Å 202.40Å 317.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.93 – 1.80 24.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.93-1.80) 95.6 (24.93-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.171 , 0.200 (Not available) , 0.245	Depositor DCC
R_{free} test set	1275 reflections (0.28%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29575	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 21.53 % 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 6.8798e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.58	0/4699	0.74	1/6387 (0.0%)
1	C	0.61	0/4699	0.76	1/6387 (0.0%)
1	E	0.56	0/4699	0.76	1/6387 (0.0%)
1	G	0.58	0/4699	0.76	2/6387 (0.0%)
1	I	0.59	0/4699	0.76	4/6387 (0.1%)
1	K	0.59	0/4699	0.74	1/6387 (0.0%)
All	All	0.58	0/28194	0.75	10/38322 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	461	LEU	N-CA-C	7.01	125.73	110.80
1	I	460	TRP	CA-C-N	5.61	132.25	121.54
1	I	460	TRP	C-N-CA	5.61	132.25	121.54
1	K	7	LYS	CB-CA-C	-5.39	110.34	116.54
1	C	7	LYS	CB-CA-C	-5.34	110.40	116.54
1	G	284	ASN	N-CA-C	5.33	119.79	113.28
1	A	285	ASN	N-CA-C	5.19	117.09	110.61
1	E	583	ASN	CB-CA-C	-5.14	110.63	116.54
1	G	7	LYS	CB-CA-C	-5.11	110.67	116.54
1	I	460	TRP	N-CA-C	-5.08	104.39	111.30

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	4601	0	4339	26	0
1	C	4601	0	4339	26	2
1	E	4601	0	4339	33	0
1	G	4601	0	4339	29	0
1	I	4601	0	4339	21	0
1	K	4601	0	4339	27	0
2	A	8	0	0	0	0
2	C	8	0	0	0	0
2	E	8	0	0	0	0
2	G	8	0	0	0	0
2	I	8	0	0	0	0
2	K	8	0	0	0	0
3	A	322	0	0	10	0
3	C	360	0	0	13	0
3	E	285	0	0	9	0
3	G	346	0	0	8	0
3	I	305	0	0	4	0
3	K	303	0	0	6	2
All	All	29575	0	26034	160	2

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 (160) 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:C:199:GLU:HG3	3:C:923:HOH:O	1.52	1.10
1:K:424:LYS:HE3	3:K:763:HOH:O	1.53	1.05
1:E:129:SER:O	1:E:130:GLU:HG3	1.59	1.02
1:I:461:LEU:O	1:I:461:LEU:HG	1.53	1.01
1:A:458:THR:HG23	1:A:463:PHE:HA	1.46	0.98
1:C:424:LYS:CE	3:C:839:HOH:O	2.16	0.93
1:I:458:THR:HG23	1:I:461:LEU:HD12	1.54	0.89
1:K:129:SER:O	1:K:130:GLU:HG3	1.73	0.88
1:C:129:SER:O	1:C:130:GLU:HG3	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HE3	3:C:867:HOH:O	1.72	0.88
1:I:458:THR:CG2	1:I:461:LEU:HD12	2.08	0.83
1:E:600:VAL:HG11	1:E:605:ILE:HD11	1.63	0.81
1:K:438:ARG:NH2	1:K:524:THR:OG1	2.15	0.80
1:A:535:LYS:HE2	3:A:874:HOH:O	1.82	0.79
1:G:129:SER:O	1:G:130:GLU:HG3	1.83	0.78
1:K:427:GLU:OE2	1:K:438:ARG:HD2	1.85	0.77
1:G:364:GLU:OE2	3:G:924:HOH:O	2.03	0.76
1:G:458:THR:HG23	1:G:463:PHE:HA	1.67	0.76
1:K:424:LYS:HD2	3:K:825:HOH:O	1.86	0.76
1:K:458:THR:HG21	1:K:461:LEU:O	1.87	0.75
1:E:586:LEU:C	3:E:888:HOH:O	2.30	0.74
1:A:458:THR:CG2	1:A:463:PHE:HA	2.18	0.73
1:K:424:LYS:CE	3:K:825:HOH:O	2.36	0.73
1:E:307:ASN:OD1	1:E:309:PRO:HD2	1.89	0.73
1:A:463:PHE:O	1:A:464:ASN:ND2	2.22	0.72
1:C:424:LYS:CD	3:C:839:HOH:O	2.33	0.72
1:C:169:LYS:HE2	3:C:747:HOH:O	1.88	0.72
1:K:424:LYS:CD	3:K:825:HOH:O	2.38	0.72
1:C:424:LYS:HD2	3:C:839:HOH:O	1.89	0.71
1:C:169:LYS:NZ	3:C:747:HOH:O	2.23	0.70
1:K:129:SER:O	1:K:130:GLU:CG	2.39	0.70
1:G:129:SER:O	1:G:130:GLU:CG	2.38	0.70
1:I:576:ARG:HG2	1:I:602:LEU:HD21	1.73	0.70
1:E:587:VAL:HG23	3:E:888:HOH:O	1.92	0.69
1:G:463:PHE:O	1:G:464:ASN:ND2	2.26	0.69
1:G:307:ASN:OD1	1:G:309:PRO:HD2	1.92	0.68
1:G:129:SER:O	1:G:130:GLU:CB	2.39	0.68
1:I:199:GLU:HG3	3:I:792:HOH:O	1.94	0.68
1:A:458:THR:HG23	1:A:463:PHE:CA	2.22	0.68
1:A:580:THR:HG23	3:A:862:HOH:O	1.93	0.68
1:C:420:GLN:OE1	3:C:899:HOH:O	2.12	0.67
1:C:77:GLU:OE1	1:C:106:ARG:CZ	2.42	0.67
1:C:169:LYS:CE	3:C:747:HOH:O	2.42	0.67
1:C:458:THR:HG21	1:C:461:LEU:O	1.95	0.66
1:K:607:THR:HG23	3:K:852:HOH:O	1.96	0.66
1:E:71:PRO:HD2	1:E:72:TRP:CZ3	2.31	0.65
1:E:77:GLU:HG3	3:E:809:HOH:O	1.95	0.65
1:E:420:GLN:OE1	3:E:853:HOH:O	2.14	0.65
1:A:458:THR:HG22	1:A:459:SER:N	2.12	0.64
1:C:129:SER:O	1:C:130:GLU:CG	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:OE1	1:A:106:ARG:CZ	2.45	0.64
1:C:498:GLN:HG3	3:C:786:HOH:O	1.96	0.64
1:G:498:GLN:CG	3:G:919:HOH:O	2.45	0.64
1:E:586:LEU:CD2	1:E:605:ILE:HG13	2.28	0.62
1:K:129:SER:O	1:K:130:GLU:CB	2.48	0.61
1:E:29:TYR:OH	1:E:206:HIS:HD2	1.83	0.61
1:G:498:GLN:HG3	3:G:919:HOH:O	2.01	0.61
1:G:458:THR:HG22	1:G:459:SER:N	2.17	0.60
1:K:78:GLN:NE2	1:K:82:GLU:OE2	2.31	0.60
1:A:459:SER:N	3:A:907:HOH:O	2.33	0.60
1:K:93:SER:H	1:K:96:GLN:HE21	1.49	0.60
1:A:458:THR:HG22	1:A:459:SER:H	1.66	0.60
1:C:307:ASN:OD1	1:C:309:PRO:HD2	2.03	0.59
1:I:574:ASN:HD21	1:I:576:ARG:NH1	2.00	0.59
1:K:58:ILE:HG22	1:K:67:LEU:HD22	1.84	0.59
1:I:78:GLN:NE2	1:I:82:GLU:OE2	2.34	0.58
1:A:307:ASN:OD1	1:A:309:PRO:HD2	2.02	0.58
1:K:77:GLU:OE1	1:K:106:ARG:CZ	2.50	0.58
1:A:199:GLU:HG3	3:A:872:HOH:O	2.02	0.58
1:G:129:SER:O	1:G:130:GLU:HB2	2.03	0.58
1:I:466:GLU:HG3	3:I:912:HOH:O	2.02	0.58
1:C:498:GLN:CG	3:C:786:HOH:O	2.51	0.58
1:I:77:GLU:OE1	1:I:106:ARG:CZ	2.52	0.57
1:A:458:THR:C	3:A:907:HOH:O	2.46	0.57
1:A:364:GLU:OE2	3:A:942:HOH:O	2.18	0.56
1:I:574:ASN:HD21	1:I:576:ARG:HH11	1.52	0.56
1:K:29:TYR:OH	1:K:206:HIS:HD2	1.89	0.56
1:A:29:TYR:OH	1:A:206:HIS:HD2	1.88	0.56
1:E:580:THR:HG23	3:E:832:HOH:O	2.06	0.56
1:A:462:ILE:HG13	1:A:462:ILE:O	2.06	0.55
1:G:458:THR:HG23	1:G:463:PHE:C	2.31	0.55
1:K:582:GLN:O	1:K:583:ASN:HB2	2.08	0.54
1:C:424:LYS:HE2	3:C:839:HOH:O	1.93	0.54
1:G:458:THR:HG23	1:G:463:PHE:CA	2.35	0.54
1:I:580:THR:HG23	3:I:881:HOH:O	2.07	0.54
1:C:29:TYR:OH	1:C:206:HIS:HD2	1.90	0.54
1:I:58:ILE:HG22	1:I:67:LEU:HD22	1.89	0.54
1:I:29:TYR:OH	1:I:206:HIS:HD2	1.93	0.52
1:A:458:THR:HG23	1:A:463:PHE:C	2.34	0.51
1:G:462:ILE:O	1:G:462:ILE:HG13	2.10	0.51
1:G:458:THR:CG2	1:G:463:PHE:HA	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:498:GLN:HG2	3:G:919:HOH:O	2.05	0.51
1:E:533:ILE:HD12	1:E:533:ILE:N	2.26	0.51
1:A:459:SER:CB	3:A:907:HOH:O	2.59	0.50
1:G:211:LEU:HD23	1:G:211:LEU:C	2.37	0.49
1:E:128:ASP:OD2	1:E:132:ASN:HB2	2.12	0.49
1:A:535:LYS:CE	3:A:874:HOH:O	2.53	0.49
1:I:211:LEU:C	1:I:211:LEU:HD23	2.37	0.49
1:I:459:SER:O	1:I:460:TRP:C	2.54	0.49
1:I:461:LEU:O	1:I:461:LEU:CG	2.37	0.49
1:C:607:THR:HG21	3:I:873:HOH:O	2.12	0.48
1:G:93:SER:OG	1:G:96:GLN:HG3	2.14	0.48
1:E:600:VAL:HG11	1:E:605:ILE:CD1	2.39	0.48
1:K:555:TYR:CZ	1:K:598:ILE:HD12	2.49	0.48
1:E:129:SER:O	1:E:130:GLU:CG	2.48	0.47
1:I:458:THR:HG21	1:I:461:LEU:HD12	1.92	0.47
1:G:461:LEU:HD22	3:G:903:HOH:O	2.14	0.47
1:C:268:THR:OG1	1:C:270:PRO:HD2	2.14	0.47
1:E:186:ASP:OD1	1:G:576:ARG:NH2	2.48	0.47
1:G:424:LYS:HD2	3:G:868:HOH:O	2.15	0.46
1:K:49:LEU:N	1:K:50:PRO:HD2	2.31	0.46
1:E:587:VAL:N	3:E:888:HOH:O	2.46	0.46
1:A:459:SER:HB3	3:A:907:HOH:O	2.17	0.45
1:A:458:THR:CG2	1:A:459:SER:N	2.80	0.45
1:E:460:TRP:O	1:E:461:LEU:HB2	2.17	0.45
1:I:143:THR:O	1:I:144:SER:CB	2.65	0.44
1:E:143:THR:O	1:E:144:SER:CB	2.65	0.44
1:A:608:ASP:OD1	1:A:608:ASP:N	2.51	0.44
1:E:531:ASP:HB3	1:E:551:ARG:O	2.18	0.44
1:C:129:SER:O	1:C:130:GLU:CB	2.65	0.44
1:E:102:LYS:HE3	1:E:110:TYR:CD1	2.53	0.44
1:E:111:GLY:HA3	1:E:116:TYR:O	2.18	0.43
1:K:513:ASP:HB2	1:K:532:ASP:OD1	2.18	0.43
1:A:253:TYR:CG	1:A:288:ASN:HB2	2.53	0.43
1:C:597:LEU:N	1:C:597:LEU:HD12	2.33	0.43
1:E:67:LEU:HD23	1:E:70:LEU:HD11	2.01	0.43
1:G:330:GLU:HG3	3:G:828:HOH:O	2.19	0.43
1:G:554:LEU:C	1:G:554:LEU:HD23	2.44	0.43
1:G:253:TYR:CG	1:G:288:ASN:HB2	2.54	0.43
1:E:211:LEU:C	1:E:211:LEU:HD23	2.44	0.43
1:I:253:TYR:CG	1:I:288:ASN:HB2	2.53	0.43
1:G:128:ASP:C	1:G:128:ASP:OD1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:C	1:A:211:LEU:HD23	2.44	0.42
1:C:253:TYR:CG	1:C:288:ASN:HB2	2.54	0.42
1:K:128:ASP:OD2	1:K:132:ASN:HB2	2.19	0.42
1:K:441:LYS:HB3	1:K:441:LYS:HE2	1.87	0.42
1:K:492:ASP:HA	1:K:510:ALA:HB3	2.01	0.42
1:E:464:ASN:HD22	1:E:464:ASN:N	2.18	0.42
1:E:477:LYS:HG2	1:E:482:LEU:HD13	2.01	0.42
1:C:211:LEU:HD23	1:C:211:LEU:C	2.45	0.42
1:C:533:ILE:HD11	1:G:533:ILE:HD11	2.01	0.42
1:E:586:LEU:N	3:E:888:HOH:O	2.51	0.42
1:E:253:TYR:CG	1:E:288:ASN:HB2	2.55	0.42
1:E:585:ASP:C	3:E:888:HOH:O	2.63	0.42
1:C:424:LYS:NZ	3:C:839:HOH:O	2.35	0.42
1:K:253:TYR:CG	1:K:288:ASN:HB2	2.55	0.42
1:E:128:ASP:OD1	1:E:128:ASP:C	2.63	0.41
1:G:330:GLU:CD	3:G:828:HOH:O	2.63	0.41
1:G:458:THR:CG2	1:G:459:SER:N	2.83	0.41
1:K:597:LEU:N	1:K:597:LEU:HD12	2.35	0.41
1:A:462:ILE:HG13	3:A:907:HOH:O	2.20	0.41
1:A:315:LEU:HA	1:A:316:PRO:HD3	1.99	0.41
1:I:315:LEU:HA	1:I:316:PRO:HD3	1.96	0.41
1:E:551:ARG:HG2	1:E:594:GLN:HG2	2.03	0.40
1:E:583:ASN:HB3	1:E:584:ASP:H	1.65	0.40
1:K:570:GLY:O	3:K:820:HOH:O	2.21	0.40
1:E:587:VAL:CG2	3:E:888:HOH:O	2.61	0.40
1:I:49:LEU:N	1:I:50:PRO:CD	2.85	0.40
1:G:315:LEU:HA	1:G:316:PRO:HD3	1.92	0.40
1:K:129:SER:O	1:K:130:GLU:HB2	2.19	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:LEU:CD1	3:K:768:HOH:O[9_444]	1.05	1.15
1:C:461:LEU:CG	3:K:768:HOH:O[9_444]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	G	66/474 (14%)	66 (100%)	0	100	100
1	I	57/474 (12%)	57 (100%)	0	100	100
1	K	200/474 (42%)	200 (100%)	0	100	100
All	All	323/1422 (23%)	323 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	553	GLN
1	G	582	GLN
1	I	73	ASN
1	K	328	ASN
1	K	498	GLN
1	K	518	HIS
1	K	522	ASN
1	K	553	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	615/615 (100%)	0.53	47 (7%)	2018	14, 22, 31, 43	0
1	C	615/615 (100%)	0.21	18 (2%)	5353	14, 22, 29, 43	0
1	E	615/615 (100%)	0.80	83 (13%)	75	13, 22, 32, 41	0
1	G	615/615 (100%)	0.39	35 (5%)	2928	13, 22, 30, 42	0
1	I	615/615 (100%)	0.37	26 (4%)	4040	16, 22, 30, 44	0
1	K	615/615 (100%)	0.66	68 (11%)	108	15, 22, 30, 44	0
All	All	3690/3690 (100%)	0.49	277 (7%)	2018	13, 22, 30, 44	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	463	PHE	6.7
1	E	584	ASP	5.9
1	E	467	VAL	5.5
1	I	461	LEU	5.4
1	E	462	ILE	5.4
1	I	462	ILE	5.4
1	A	463	PHE	5.2
1	K	462	ILE	5.2
1	E	460	TRP	5.1
1	E	510	ALA	5.1
1	E	471	VAL	5.1
1	E	473	ALA	5.0
1	E	600	VAL	5.0
1	E	491	GLY	4.9
1	E	129	SER	4.9
1	G	460	TRP	4.8
1	G	463	PHE	4.8
1	E	458	THR	4.8
1	I	458	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	463	PHE	4.6
1	E	464	ASN	4.6
1	K	463	PHE	4.6
1	A	462	ILE	4.5
1	A	467	VAL	4.5
1	G	458	THR	4.5
1	G	461	LEU	4.5
1	I	129	SER	4.4
1	G	462	ILE	4.4
1	A	8	ASP	4.3
1	A	458	THR	4.3
1	E	598	ILE	4.3
1	K	458	THR	4.2
1	E	8	ASP	4.2
1	K	-1	SER	4.2
1	E	604	HIS	4.2
1	E	472	THR	4.2
1	K	584	ASP	4.2
1	E	468	ASP	4.1
1	E	530	GLY	4.0
1	E	529	SER	4.0
1	A	584	ASP	3.9
1	E	585	ASP	3.9
1	K	555	TYR	3.8
1	E	-1	SER	3.8
1	C	72	TRP	3.8
1	E	605	ILE	3.8
1	A	461	LEU	3.7
1	E	603	ASP	3.7
1	G	48	GLY	3.6
1	K	129	SER	3.6
1	K	559	ALA	3.6
1	K	496	VAL	3.6
1	E	481	GLY	3.6
1	A	601	SER	3.6
1	E	459	SER	3.6
1	E	478	SER	3.6
1	E	511	GLY	3.5
1	K	580	THR	3.5
1	C	129	SER	3.5
1	E	579	ALA	3.5
1	E	480	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	-1	SER	3.4
1	K	583	ASN	3.4
1	K	467	VAL	3.4
1	I	0	HIS	3.4
1	E	465	LYS	3.4
1	E	550	GLY	3.4
1	E	482	LEU	3.4
1	A	-1	SER	3.4
1	A	583	ASN	3.4
1	G	46	GLY	3.3
1	E	476	LEU	3.3
1	K	604	HIS	3.3
1	C	458	THR	3.3
1	K	497	LEU	3.3
1	E	597	LEU	3.2
1	K	571	ALA	3.2
1	E	477	LYS	3.2
1	E	581	GLN	3.1
1	E	461	LEU	3.1
1	K	599	GLY	3.1
1	E	131	GLY	3.1
1	E	602	LEU	3.1
1	G	433	ASN	3.1
1	G	47	LEU	3.0
1	A	471	VAL	3.0
1	C	131	GLY	3.0
1	K	511	GLY	3.0
1	E	466	GLU	3.0
1	C	-1	SER	3.0
1	E	531	ASP	3.0
1	G	129	SER	3.0
1	A	472	THR	3.0
1	G	39	GLY	3.0
1	I	467	VAL	2.9
1	I	269	LEU	2.9
1	E	492	ASP	2.9
1	K	495	ASP	2.9
1	E	493	GLY	2.9
1	K	534	LEU	2.9
1	E	592	HIS	2.9
1	E	474	ALA	2.9
1	A	480	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	501	SER	2.9
1	I	460	TRP	2.9
1	E	528	GLY	2.9
1	K	611	VAL	2.8
1	E	559	ALA	2.8
1	K	575	ILE	2.8
1	I	8	ASP	2.8
1	K	492	ASP	2.8
1	K	612	LEU	2.8
1	E	72	TRP	2.8
1	K	130	GLU	2.8
1	E	509	ASN	2.8
1	E	470	GLN	2.8
1	K	528	GLY	2.8
1	A	269	LEU	2.8
1	A	460	TRP	2.8
1	K	537	VAL	2.8
1	G	459	SER	2.7
1	C	199	GLU	2.7
1	E	46	GLY	2.7
1	E	580	THR	2.7
1	E	586	LEU	2.7
1	I	608	ASP	2.7
1	C	42	GLN	2.7
1	K	600	VAL	2.7
1	A	465	LYS	2.7
1	E	484	ALA	2.6
1	K	493	GLY	2.6
1	K	508	GLY	2.6
1	A	608	ASP	2.6
1	K	578	TYR	2.6
1	I	576	ARG	2.6
1	E	47	LEU	2.6
1	K	464	ASN	2.6
1	K	602	LEU	2.6
1	A	46	GLY	2.6
1	G	52	THR	2.6
1	K	166	PHE	2.6
1	K	478	SER	2.6
1	A	468	ASP	2.6
1	G	8	ASP	2.6
1	A	481	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	473	ALA	2.6
1	K	587	VAL	2.6
1	K	570	GLY	2.5
1	K	605	ILE	2.5
1	I	433	ASN	2.5
1	K	433	ASN	2.5
1	A	78	GLN	2.5
1	A	130	GLU	2.5
1	A	585	ASP	2.5
1	E	479	ASP	2.5
1	I	10	ASP	2.5
1	C	246	GLY	2.5
1	G	-1	SER	2.5
1	A	222	ALA	2.5
1	K	474	ALA	2.5
1	G	43	THR	2.5
1	A	475	GLY	2.5
1	K	509	ASN	2.5
1	C	244	ALA	2.5
1	K	499	ALA	2.5
1	I	492	ASP	2.5
1	A	459	SER	2.4
1	K	105	ALA	2.4
1	K	607	THR	2.4
1	G	72	TRP	2.4
1	E	557	PHE	2.4
1	C	608	ASP	2.4
1	K	134	THR	2.4
1	G	604	HIS	2.4
1	C	478	SER	2.4
1	G	49	LEU	2.4
1	K	482	LEU	2.4
1	A	40	TYR	2.4
1	E	500	ARG	2.4
1	E	555	TYR	2.3
1	K	510	ALA	2.3
1	G	464	ASN	2.3
1	A	39	GLY	2.3
1	C	8	ASP	2.3
1	C	584	ASP	2.3
1	E	513	ASP	2.3
1	G	42	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	134	THR	2.3
1	C	474	ALA	2.3
1	K	598	ILE	2.3
1	E	508	GLY	2.3
1	G	98	GLY	2.3
1	E	560	SER	2.3
1	K	531	ASP	2.3
1	A	470	GLN	2.3
1	K	519	ALA	2.3
1	K	613	ALA	2.3
1	K	514	THR	2.3
1	E	127	TYR	2.2
1	E	485	TYR	2.2
1	G	510	ALA	2.2
1	I	131	GLY	2.2
1	A	10	ASP	2.2
1	E	608	ASP	2.2
1	K	8	ASP	2.2
1	K	494	ASP	2.2
1	A	607	THR	2.2
1	A	48	GLY	2.2
1	C	78	GLN	2.2
1	K	521	GLY	2.2
1	E	166	PHE	2.2
1	G	40	TYR	2.2
1	G	54	ILE	2.2
1	K	465	LYS	2.2
1	E	158	VAL	2.2
1	E	587	VAL	2.2
1	K	274	VAL	2.2
1	K	595	VAL	2.2
1	A	466	GLU	2.2
1	E	52	THR	2.2
1	E	55	THR	2.2
1	A	47	LEU	2.2
1	K	498	GLN	2.2
1	I	528	GLY	2.2
1	A	72	TRP	2.2
1	G	311	TRP	2.2
1	E	128	ASP	2.2
1	E	50	PRO	2.2
1	A	41	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	548	ASP	2.1
1	A	600	VAL	2.1
1	K	564	VAL	2.1
1	G	44	GLY	2.1
1	A	604	HIS	2.1
1	C	130	GLU	2.1
1	G	130	GLU	2.1
1	K	592	HIS	2.1
1	A	433	ASN	2.1
1	A	510	ALA	2.1
1	E	512	ASN	2.1
1	I	464	ASN	2.1
1	A	603	ASP	2.1
1	G	608	ASP	2.1
1	A	478	SER	2.1
1	I	551	ARG	2.1
1	E	0	HIS	2.1
1	K	586	LEU	2.1
1	G	244	ALA	2.1
1	G	571	ALA	2.1
1	A	54	ILE	2.1
1	C	10	ASP	2.1
1	E	552	ASP	2.1
1	I	584	ASP	2.1
1	K	10	ASP	2.1
1	K	552	ASP	2.1
1	I	459	SER	2.1
1	I	606	SER	2.1
1	I	130	GLU	2.1
1	E	599	GLY	2.1
1	E	433	ASN	2.1
1	G	576	ARG	2.1
1	E	469	HIS	2.0
1	I	493	GLY	2.0
1	K	0	HIS	2.0
1	A	464	ASN	2.0
1	G	71	PRO	2.0
1	A	9	LEU	2.0
1	K	300	LEU	2.0
1	A	244	ALA	2.0
1	E	486	ALA	2.0
1	I	199	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	451	SER	2.0
1	G	41	HIS	2.0
1	C	481	GLY	2.0
1	E	86	ASN	2.0
1	K	573	GLY	2.0
1	A	158	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	CA	E	615	1/1	0.90	0.21	27,27,27,27	0
2	CA	E	616	1/1	0.92	0.17	28,28,28,28	0
2	CA	K	614	1/1	0.92	0.19	28,28,28,28	0
2	CA	I	614	1/1	0.95	0.15	28,28,28,28	0
2	CA	A	614	1/1	0.96	0.14	23,23,23,23	0
2	CA	E	614	1/1	0.96	0.18	28,28,28,28	0
2	CA	K	616	1/1	0.96	0.22	25,25,25,25	0
2	CA	C	619	1/1	0.97	0.10	15,15,15,15	0
2	CA	I	616	1/1	0.97	0.16	25,25,25,25	0
2	CA	G	614	1/1	0.98	0.11	20,20,20,20	0
2	CA	A	615	1/1	0.98	0.12	20,20,20,20	0
2	CA	I	615	1/1	0.98	0.13	24,24,24,24	0
2	CA	A	616	1/1	0.98	0.14	21,21,21,21	0
2	CA	A	619	1/1	0.98	0.10	16,16,16,16	0
2	CA	K	615	1/1	0.98	0.23	25,25,25,25	0
2	CA	A	621	1/1	0.98	0.14	17,17,17,17	0
2	CA	K	617	1/1	0.98	0.12	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	K	619	1/1	0.98	0.11	17,17,17,17	0
2	CA	E	620	1/1	0.99	0.13	14,14,14,14	0
2	CA	E	621	1/1	0.99	0.11	15,15,15,15	0
2	CA	C	618	1/1	0.99	0.09	16,16,16,16	0
2	CA	G	615	1/1	0.99	0.13	17,17,17,17	0
2	CA	G	616	1/1	0.99	0.12	18,18,18,18	0
2	CA	G	618	1/1	0.99	0.10	17,17,17,17	0
2	CA	G	619	1/1	0.99	0.10	16,16,16,16	0
2	CA	G	620	1/1	0.99	0.11	13,13,13,13	0
2	CA	G	621	1/1	0.99	0.14	15,15,15,15	0
2	CA	A	618	1/1	0.99	0.11	16,16,16,16	0
2	CA	C	620	1/1	0.99	0.11	13,13,13,13	0
2	CA	C	614	1/1	0.99	0.12	20,20,20,20	0
2	CA	I	617	1/1	0.99	0.12	16,16,16,16	0
2	CA	I	618	1/1	0.99	0.10	17,17,17,17	0
2	CA	I	619	1/1	0.99	0.09	16,16,16,16	0
2	CA	I	620	1/1	0.99	0.10	15,15,15,15	0
2	CA	I	621	1/1	0.99	0.11	14,14,14,14	0
2	CA	C	615	1/1	0.99	0.14	16,16,16,16	0
2	CA	C	616	1/1	0.99	0.11	18,18,18,18	0
2	CA	E	617	1/1	0.99	0.10	15,15,15,15	0
2	CA	E	618	1/1	0.99	0.13	16,16,16,16	0
2	CA	K	618	1/1	0.99	0.12	19,19,19,19	0
2	CA	E	619	1/1	0.99	0.10	15,15,15,15	0
2	CA	K	620	1/1	0.99	0.13	15,15,15,15	0
2	CA	K	621	1/1	0.99	0.12	15,15,15,15	0
2	CA	C	621	1/1	1.00	0.12	15,15,15,15	0
2	CA	A	617	1/1	1.00	0.11	14,14,14,14	0
2	CA	A	620	1/1	1.00	0.10	14,14,14,14	0
2	CA	C	617	1/1	1.00	0.10	14,14,14,14	0
2	CA	G	617	1/1	1.00	0.11	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.