Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:29 AM GMT

PDB ID	:	2QUB
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
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:

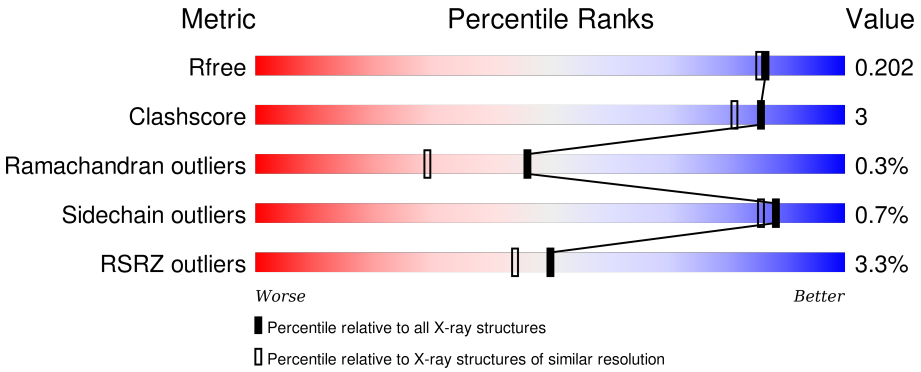
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 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	615	3% 96% .
1	C	615	3% 95% .
1	E	615	3% 93% 7%
1	G	615	3% 95% 5%
1	I	615	3% 95% 5%

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Mol	Chain	Length	Quality of chain
1	K	615	4% 93% 7%

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	CA	K	615	-	-	-	X
2	CA	K	616	-	-	-	X

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

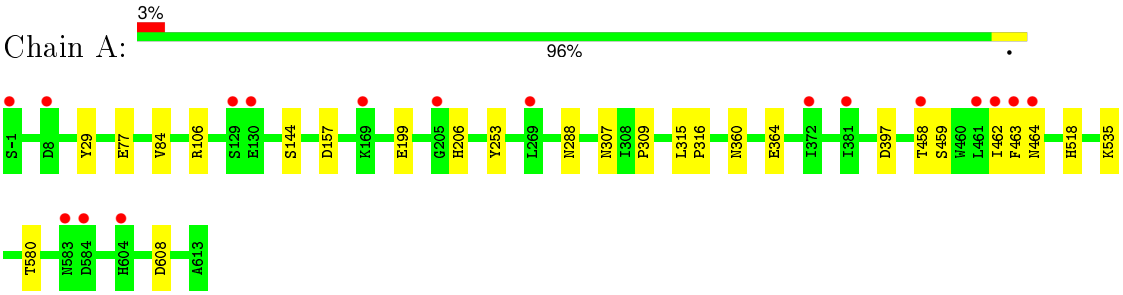
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	322	Total O 322 322	0	0
3	C	360	Total O 360 360	0	0
3	E	285	Total O 285 285	0	0
3	G	346	Total O 346 346	0	0
3	I	305	Total O 305 305	0	0
3	K	303	Total O 303 303	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

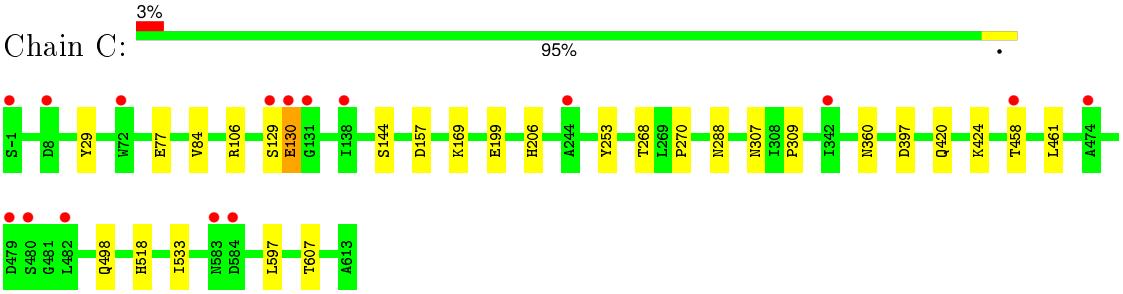
- Molecule 1: Extracellular lipase

Chain A:



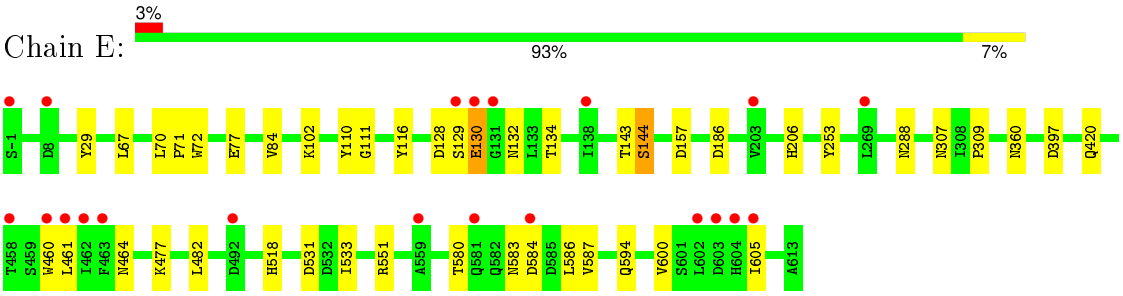
- Molecule 1: Extracellular lipase

Chain C:



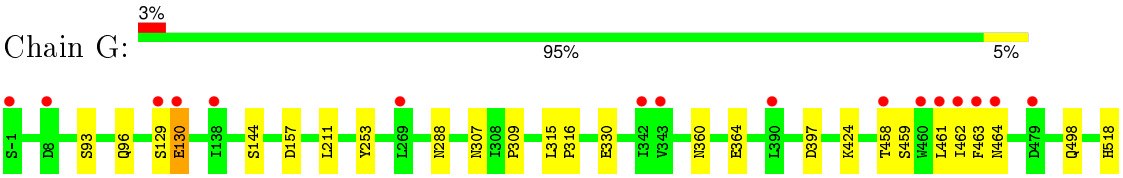
- Molecule 1: Extracellular lipase

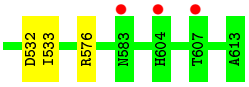
Chain E:



- Molecule 1: Extracellular lipase

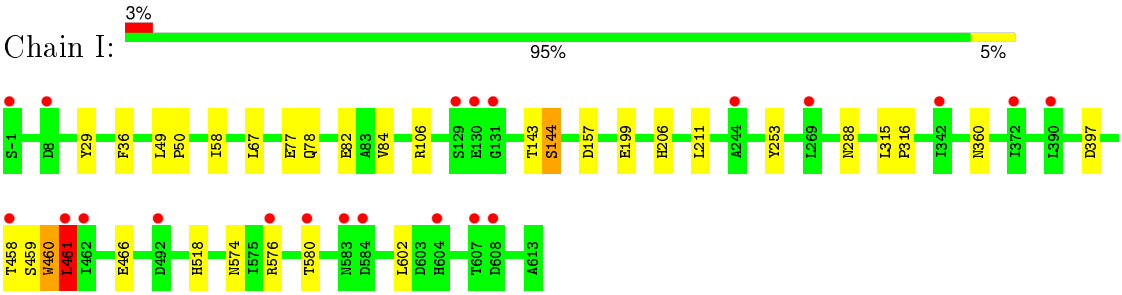
Chain G:





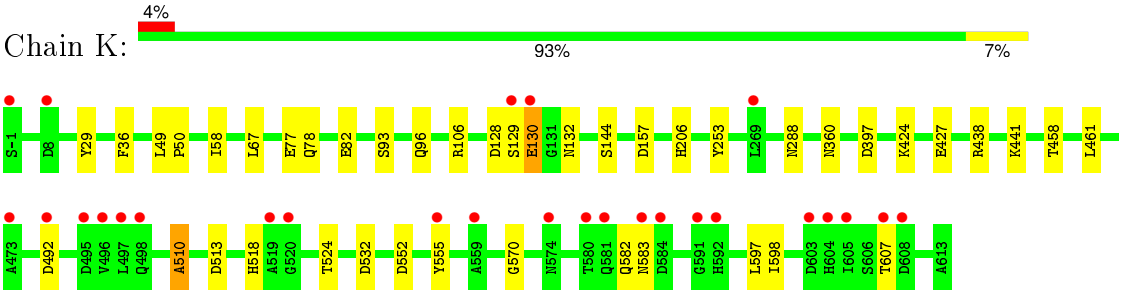
• Molecule 1: Extracellular lipase

Chain I:



• Molecule 1: Extracellular lipase

Chain K:



4 Data and refinement statistics (i)

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 24.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.93-1.80) 95.6 (24.83-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.171 , 0.200 0.174 , 0.202	Depositor DCC
R_{free} test set	1275 reflections (0.30%)	DCC
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 , 51.5	EDS
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 429965 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[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: 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	0.46	0/4699	0.56	2/6387 (0.0%)
1	C	0.50	0/4699	0.57	2/6387 (0.0%)
1	E	0.45	0/4699	0.56	2/6387 (0.0%)
1	G	0.48	0/4699	0.58	3/6387 (0.0%)
1	I	0.48	0/4699	0.57	3/6387 (0.0%)
1	K	0.47	0/4699	0.57	3/6387 (0.0%)
All	All	0.47	0/28194	0.57	15/38322 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	157	ASP	CB-CG-OD1	7.87	125.38	118.30
1	K	157	ASP	CB-CG-OD1	6.96	124.56	118.30
1	G	157	ASP	CB-CG-OD1	6.85	124.46	118.30
1	E	397	ASP	CB-CG-OD2	6.74	124.37	118.30
1	K	397	ASP	CB-CG-OD2	6.62	124.25	118.30
1	E	157	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	157	ASP	CB-CG-OD1	6.48	124.14	118.30
1	C	157	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	397	ASP	CB-CG-OD2	5.58	123.32	118.30
1	G	397	ASP	CB-CG-OD2	5.48	123.23	118.30
1	I	461	LEU	N-CA-C	5.46	125.73	111.00
1	G	532	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	397	ASP	CB-CG-OD2	5.19	122.97	118.30
1	K	552	ASP	CB-CG-OD1	5.15	122.94	118.30
1	I	397	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	25	0
1	C	4601	0	4339	25	2
1	E	4601	0	4339	30	0
1	G	4601	0	4339	26	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	8	0
3	G	346	0	0	7	0
3	I	305	0	0	4	0
3	K	303	0	0	6	2
All	All	29575	0	26034	152	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 (152) 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: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:K:129:SER:O	1:K:130:GLU:CG	2.39	0.70
1:C:169:LYS:NZ	3:C:747:HOH:O	2.23	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:E:586:LEU:C	3:E:888:HOH:O	2.30	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:169:LYS:CE	3:C:747:HOH:O	2.42	0.67
1:C:77:GLU:OE1	1:C:106:ARG:CZ	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:C:498:GLN:HG3	3:C:786:HOH:O	1.96	0.64
1:A:77:GLU:OE1	1:A:106:ARG:CZ	2.45	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: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:364:GLU:OE2	3:A:942:HOH:O	2.18	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: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:A:458:THR:C	3:A:907:HOH:O	2.46	0.53
1:I:29:TYR:OH	1:I:206:HIS:HD2	1.93	0.52
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
1:G:498:GLN:HG2	3:G:919:HOH:O	2.05	0.51
1:E:533:ILE:N	1:E:533:ILE:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:SER:CB	3:A:907:HOH:O	2.59	0.50
1:G:458:THR:HG23	1:G:463:PHE:C	2.31	0.50
1:E:128:ASP:OD2	1:E:132:ASN:HB2	2.12	0.49
1:I:461:LEU:CG	1:I:461:LEU:O	2.37	0.49
1:A:535:LYS:CE	3:A:874:HOH:O	2.53	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:E:587:VAL:N	3:E:888:HOH:O	2.46	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:A:458:THR:HG23	1:A:463:PHE:C	2.34	0.46
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: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:I:459:SER:O	1:I:460:TRP:C	2.54	0.44
1:I:211:LEU:C	1:I:211:LEU:HD23	2.37	0.44
1:A:608:ASP:N	1:A:608:ASP:OD1	2.51	0.44
1:G:211:LEU:HD23	1:G:211:LEU:C	2.37	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:HD12	1:C:597:LEU:N	2.33	0.43
1:G:330:GLU:HG3	3:G:828:HOH:O	2.19	0.43
1:E:67:LEU:HD23	1:E:70:LEU:HD11	2.01	0.43
1:G:253:TYR:CG	1:G:288:ASN:HB2	2.54	0.43
1:I:253:TYR:CG	1:I:288:ASN:HB2	2.53	0.43
1:K:128:ASP:OD2	1:K:132:ASN:HB2	2.19	0.42
1:C:253:TYR:CG	1:C:288:ASN:HB2	2.54	0.42
1:K:492:ASP:HA	1:K:510:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:441:LYS:HE2	1:K:441:LYS:HB3	1.87	0.42
1:K:129:SER:O	1:K:130:GLU:HB2	2.19	0.42
1:E:464:ASN:N	1:E:464:ASN:HD22	2.18	0.42
1:E:477:LYS:HG2	1:E:482:LEU:HD13	2.01	0.42
1:E:586:LEU:N	3:E:888:HOH:O	2.51	0.42
1:C:533:ILE:HD11	1:G:533:ILE:HD11	2.01	0.42
1:E:253:TYR:CG	1:E:288:ASN:HB2	2.55	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: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:K:570:GLY:O	3:K:820:HOH:O	2.21	0.40
1:E:583:ASN:HB3	1:E:584:ASP:H	1.65	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

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)

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	613/615 (100%)	602 (98%)	10 (2%)	1 (0%)	52	35
1	C	613/615 (100%)	599 (98%)	12 (2%)	2 (0%)	46	29
1	E	613/615 (100%)	598 (98%)	13 (2%)	2 (0%)	46	29
1	G	613/615 (100%)	600 (98%)	11 (2%)	2 (0%)	46	29
1	I	613/615 (100%)	601 (98%)	10 (2%)	2 (0%)	46	29
1	K	613/615 (100%)	592 (97%)	18 (3%)	3 (0%)	34	17
All	All	3678/3690 (100%)	3592 (98%)	74 (2%)	12 (0%)	46	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	C	130	GLU
1	C	144	SER
1	E	130	GLU
1	E	144	SER
1	G	130	GLU
1	G	144	SER
1	I	144	SER
1	I	461	LEU
1	K	130	GLU
1	K	144	SER
1	K	510	ALA

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	474/474 (100%)	471 (99%)	3 (1%)	90	88
1	C	474/474 (100%)	471 (99%)	3 (1%)	90	88
1	E	474/474 (100%)	470 (99%)	4 (1%)	86	83
1	G	474/474 (100%)	472 (100%)	2 (0%)	93	92
1	I	474/474 (100%)	469 (99%)	5 (1%)	80	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	474/474 (100%)	471 (99%)	3 (1%)	90 88
All	All	2844/2844 (100%)	2824 (99%)	20 (1%)	88 86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	360	ASN
1	A	518	HIS
1	C	84	VAL
1	C	360	ASN
1	C	518	HIS
1	E	84	VAL
1	E	134	THR
1	E	360	ASN
1	E	518	HIS
1	G	360	ASN
1	G	518	HIS
1	I	36	PHE
1	I	84	VAL
1	I	360	ASN
1	I	460	TRP
1	I	518	HIS
1	K	36	PHE
1	K	360	ASN
1	K	518	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	206	HIS
1	A	275	HIS
1	A	328	ASN
1	A	464	ASN
1	A	498	GLN
1	C	182	ASN
1	C	206	HIS
1	C	420	GLN
1	C	433	ASN
1	C	464	ASN

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Mol	Chain	Res	Type
1	C	522	ASN
1	C	582	GLN
1	C	583	ASN
1	E	85	ASN
1	E	206	HIS
1	E	275	HIS
1	E	420	GLN
1	E	464	ASN
1	E	522	ASN
1	G	275	HIS
1	G	362	ASN
1	G	433	ASN
1	G	464	ASN
1	I	206	HIS
1	I	328	ASN
1	I	433	ASN
1	I	498	GLN
1	I	582	GLN
1	K	62	GLN
1	K	96	GLN
1	K	206	HIS
1	K	498	GLN
1	K	522	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 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

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	615/615 (100%)	0.01	17 (2%) 56 51	14, 22, 31, 43	0
1	C	615/615 (100%)	-0.04	16 (2%) 59 54	14, 22, 29, 43	0
1	E	615/615 (100%)	0.15	21 (3%) 49 43	13, 22, 32, 41	0
1	G	615/615 (100%)	0.00	19 (3%) 52 47	13, 22, 30, 42	0
1	I	615/615 (100%)	0.01	21 (3%) 49 43	16, 22, 30, 44	0
1	K	615/615 (100%)	0.22	27 (4%) 38 32	15, 22, 30, 44	0
All	All	3690/3690 (100%)	0.06	121 (3%) 50 44	13, 22, 30, 44	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	583	ASN	7.5
1	K	584	ASP	6.9
1	E	129	SER	6.6
1	G	463	PHE	6.5
1	E	462	ILE	5.2
1	K	129	SER	4.9
1	I	461	LEU	4.8
1	K	130	GLU	4.6
1	C	129	SER	4.4
1	E	460	TRP	4.3
1	I	269	LEU	4.2
1	I	129	SER	4.1
1	A	583	ASN	4.0
1	E	8	ASP	4.0
1	K	607	THR	4.0
1	G	130	GLU	3.9
1	E	463	PHE	3.8
1	E	130	GLU	3.8
1	K	492	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	-1	SER	3.7
1	G	461	LEU	3.7
1	A	464	ASN	3.6
1	K	496	VAL	3.6
1	K	603	ASP	3.6
1	C	130	GLU	3.4
1	A	130	GLU	3.4
1	E	203	VAL	3.3
1	K	473	ALA	3.3
1	E	584	ASP	3.2
1	I	576	ARG	3.2
1	K	592	HIS	3.2
1	A	129	SER	3.2
1	G	129	SER	3.2
1	I	604	HIS	3.2
1	K	580	THR	3.1
1	A	8	ASP	3.1
1	A	463	PHE	3.1
1	A	462	ILE	3.1
1	K	269	LEU	3.1
1	E	603	ASP	2.9
1	E	269	LEU	2.9
1	C	131	GLY	2.9
1	E	131	GLY	2.9
1	E	604	HIS	2.9
1	G	460	TRP	2.9
1	I	583	ASN	2.8
1	G	458	THR	2.8
1	I	492	ASP	2.8
1	C	583	ASN	2.8
1	A	461	LEU	2.8
1	K	581	GLN	2.8
1	K	604	HIS	2.8
1	C	244	ALA	2.8
1	E	461	LEU	2.7
1	K	591	GLY	2.7
1	K	574	ASN	2.7
1	E	559	ALA	2.7
1	A	584	ASP	2.7
1	K	520	GLY	2.7
1	I	8	ASP	2.7
1	E	605	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	130	GLU	2.6
1	G	342	ILE	2.6
1	C	-1	SER	2.6
1	G	8	ASP	2.6
1	A	458	THR	2.6
1	C	479	ASP	2.6
1	I	462	ILE	2.6
1	I	584	ASP	2.6
1	C	8	ASP	2.5
1	E	-1	SER	2.5
1	I	458	THR	2.5
1	G	479	ASP	2.5
1	A	-1	SER	2.5
1	A	269	LEU	2.5
1	G	604	HIS	2.5
1	K	519	ALA	2.5
1	E	138	ILE	2.5
1	K	555	TYR	2.5
1	C	72	TRP	2.4
1	K	498	GLN	2.4
1	C	584	ASP	2.4
1	K	8	ASP	2.4
1	G	583	ASN	2.4
1	I	342	ILE	2.4
1	A	604	HIS	2.4
1	E	492	ASP	2.4
1	G	269	LEU	2.3
1	I	-1	SER	2.3
1	E	458	THR	2.2
1	C	482	LEU	2.2
1	C	138	ILE	2.2
1	G	390	LEU	2.2
1	K	497	LEU	2.2
1	G	343	VAL	2.2
1	C	474	ALA	2.2
1	G	462	ILE	2.2
1	K	495	ASP	2.2
1	C	480	SER	2.2
1	A	205	GLY	2.2
1	A	381	ILE	2.1
1	C	342	ILE	2.1
1	G	138	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	169	LYS	2.1
1	I	580	THR	2.1
1	G	464	ASN	2.1
1	I	372	ILE	2.1
1	E	581	GLN	2.1
1	K	608	ASP	2.1
1	G	607	THR	2.1
1	E	602	LEU	2.1
1	I	390	LEU	2.1
1	K	559	ALA	2.1
1	I	608	ASP	2.1
1	A	372	ILE	2.1
1	K	605	ILE	2.1
1	I	244	ALA	2.1
1	G	-1	SER	2.1
1	C	458	THR	2.0
1	I	607	THR	2.0
1	I	131	GLY	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
2	CA	K	615	1/1	0.98	0.18	2.75	25,25,25,25	0
2	CA	K	616	1/1	0.97	0.17	2.32	25,25,25,25	0
2	CA	I	616	1/1	0.98	0.12	0.66	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	K	614	1/1	0.96	0.20	0.34	28,28,28,28	0
2	CA	E	614	1/1	0.96	0.13	0.11	28,28,28,28	0
2	CA	E	615	1/1	0.91	0.12	-0.01	27,27,27,27	0
2	CA	E	616	1/1	0.94	0.10	-0.25	28,28,28,28	0
2	CA	A	614	1/1	0.97	0.09	-0.34	23,23,23,23	0
2	CA	I	614	1/1	0.98	0.12	-0.37	28,28,28,28	0
2	CA	C	614	1/1	0.99	0.08	-0.39	20,20,20,20	0
2	CA	G	614	1/1	0.99	0.07	-0.54	20,20,20,20	0
2	CA	I	615	1/1	0.98	0.08	-0.70	24,24,24,24	0
2	CA	A	616	1/1	0.99	0.07	-0.90	21,21,21,21	0
2	CA	A	618	1/1	1.00	0.06	-1.04	16,16,16,16	0
2	CA	A	615	1/1	0.99	0.06	-1.07	20,20,20,20	0
2	CA	K	618	1/1	0.99	0.06	-1.14	19,19,19,19	0
2	CA	I	617	1/1	1.00	0.05	-1.22	16,16,16,16	0
2	CA	E	620	1/1	0.99	0.07	-1.35	14,14,14,14	0
2	CA	K	617	1/1	0.99	0.06	-1.35	18,18,18,18	0
2	CA	G	618	1/1	1.00	0.06	-1.42	17,17,17,17	0
2	CA	C	619	1/1	0.99	0.06	-1.52	15,15,15,15	0
2	CA	E	618	1/1	1.00	0.06	-1.57	16,16,16,16	0
2	CA	K	621	1/1	0.99	0.06	-1.69	15,15,15,15	0
2	CA	G	615	1/1	1.00	0.05	-1.71	17,17,17,17	0
2	CA	G	617	1/1	1.00	0.04	-1.79	15,15,15,15	0
2	CA	K	620	1/1	0.99	0.06	-1.93	15,15,15,15	0
2	CA	G	621	1/1	0.99	0.05	-1.99	15,15,15,15	0
2	CA	E	617	1/1	0.99	0.04	-2.06	15,15,15,15	0
2	CA	A	617	1/1	1.00	0.03	-2.07	14,14,14,14	0
2	CA	C	621	1/1	0.99	0.05	-2.11	15,15,15,15	0
2	CA	I	618	1/1	1.00	0.04	-2.12	17,17,17,17	0
2	CA	K	619	1/1	0.98	0.04	-2.14	17,17,17,17	0
2	CA	A	621	1/1	0.99	0.06	-2.19	17,17,17,17	0
2	CA	C	617	1/1	1.00	0.02	-2.22	14,14,14,14	0
2	CA	C	615	1/1	1.00	0.06	-2.26	16,16,16,16	0
2	CA	E	619	1/1	0.99	0.05	-2.36	15,15,15,15	0
2	CA	C	618	1/1	1.00	0.04	-2.49	16,16,16,16	0
2	CA	A	620	1/1	1.00	0.04	-2.68	14,14,14,14	0
2	CA	A	619	1/1	0.98	0.04	-2.92	16,16,16,16	0
2	CA	G	620	1/1	0.99	0.03	-2.96	13,13,13,13	0
2	CA	C	616	1/1	1.00	0.05	-3.02	18,18,18,18	0
2	CA	I	621	1/1	0.99	0.04	-3.03	14,14,14,14	0
2	CA	I	620	1/1	1.00	0.04	-3.07	15,15,15,15	0
2	CA	C	620	1/1	1.00	0.04	-3.19	13,13,13,13	0
2	CA	G	619	1/1	0.99	0.03	-3.22	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	G	616	1/1	0.99	0.05	-3.24	18,18,18,18	0
2	CA	E	621	1/1	1.00	0.03	-3.50	15,15,15,15	0
2	CA	I	619	1/1	0.99	0.03	-5.40	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.