Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:16 am BST

PDB ID	:	3W6G
Title	:	Structure of peroxiredoxin from anaerobic hyperthermophilic archaeon Pyrococcus horikoshii
Authors	:	Nakamura, T.; Mori, A.; Niiyama, M.; Matsumura, H.; Tokuyama, C.; Morita, J.; Uegaki, K.; Inoue, T.
Deposited on	:	2013-02-14
Resolution	:	2.25 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 following versions of software and data (see references ⓘ) were used in the production of this report:

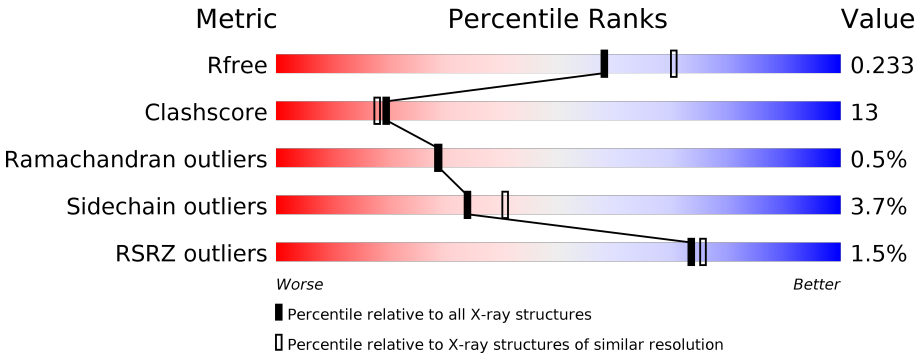
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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 <=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	216	64% 31%
1	B	216	2% 67% 29%
1	C	216	71% 26%
1	D	216	72% 26%
1	E	216	3% 68% 28%
1	F	216	2% 72% 25%

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Mol	Chain	Length	Quality of chain
1	G	216	2% 71% 27%
1	H	216	3% 73% 24%
1	I	216	72% 25%
1	J	216	2% 72% 26%
1	K	216	% 68% 30%
1	L	216	2% 70% 27%
1	M	216	74% 24%
1	N	216	2% 73% 22%
1	O	216	% 75% 22%
1	P	216	2% 73% 23%
1	Q	216	75% 23%
1	R	216	2% 74% 24%
1	S	216	% 77% 19%
1	T	216	75% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35926 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	B	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	C	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	D	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	E	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	F	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	G	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	H	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	I	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	J	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	K	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	L	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	M	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	N	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	O	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	P	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			

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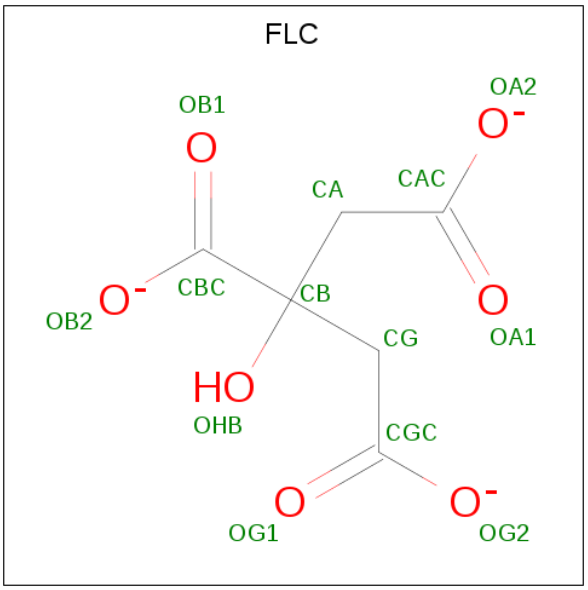
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	R	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	S	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			
1	T	214	Total	C	N	O	S	0	0	0
			1732	1133	282	312	5			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 13 6 7	0	0
2	I	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0
2	K	1	Total C O 13 6 7	0	0
2	L	1	Total C O 13 6 7	0	0
2	M	1	Total C O 13 6 7	0	0
2	N	1	Total C O 13 6 7	0	0
2	O	1	Total C O 13 6 7	0	0
2	P	1	Total C O 13 6 7	0	0
2	Q	1	Total C O 13 6 7	0	0
2	R	1	Total C O 13 6 7	0	0
2	S	1	Total C O 13 6 7	0	0
2	T	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	47	Total O 47 47	0	0
3	C	36	Total O 36 36	0	0
3	D	43	Total O 43 43	0	0
3	E	41	Total O 41 41	0	0
3	F	50	Total O 50 50	0	0

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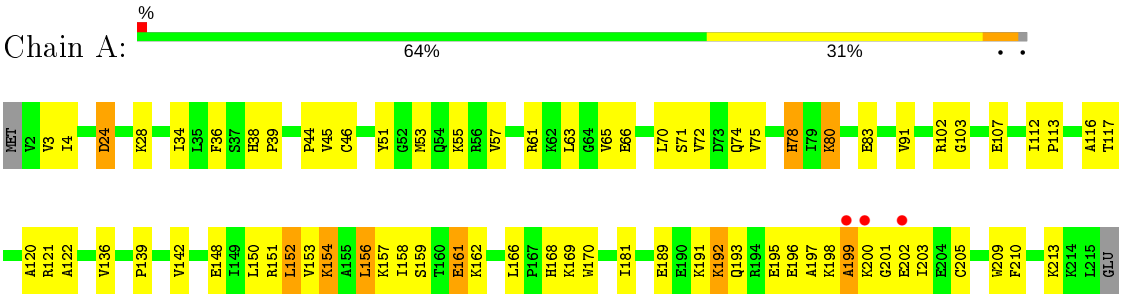
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	53	Total O 53 53	0	0
3	H	40	Total O 40 40	0	0
3	I	42	Total O 42 42	0	0
3	J	46	Total O 46 46	0	0
3	K	42	Total O 42 42	0	0
3	L	52	Total O 52 52	0	0
3	M	62	Total O 62 62	0	0
3	N	64	Total O 64 64	0	0
3	O	60	Total O 60 60	0	0
3	P	60	Total O 60 60	0	0
3	Q	62	Total O 62 62	0	0
3	R	60	Total O 60 60	0	0
3	S	63	Total O 63 63	0	0
3	T	62	Total O 62 62	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 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.

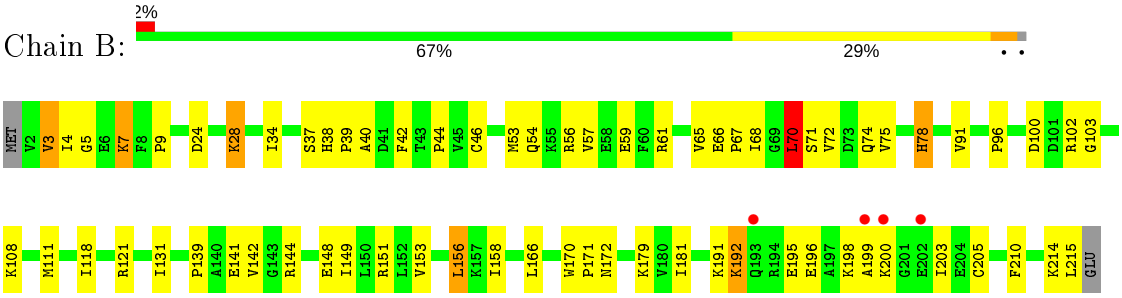
- Molecule 1: Probable peroxiredoxin

Chain A:



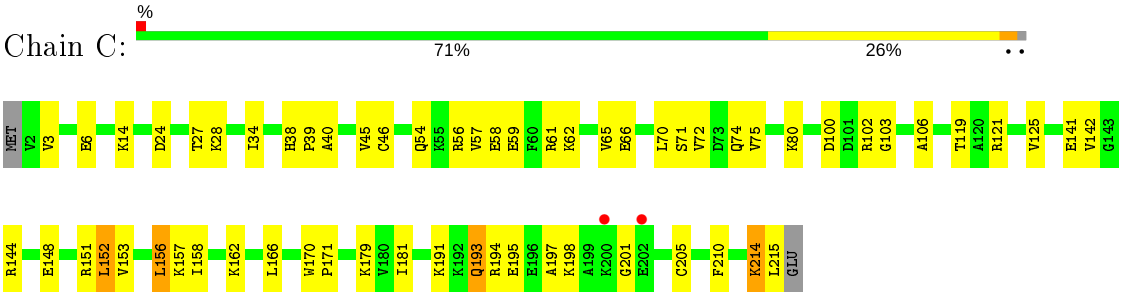
- Molecule 1: Probable peroxiredoxin

Chain B:



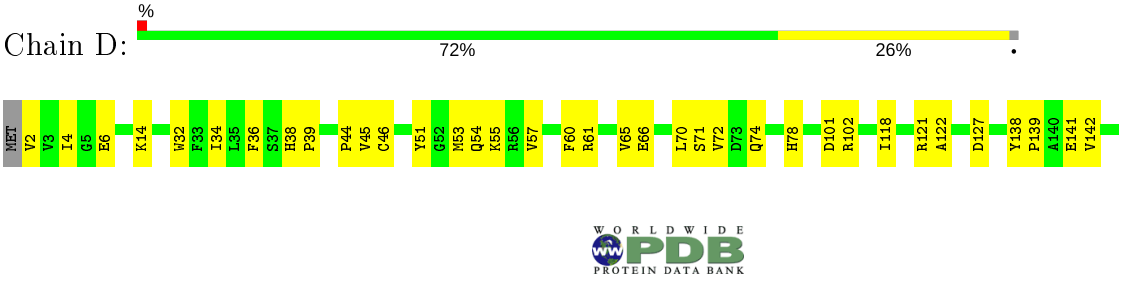
- Molecule 1: Probable peroxiredoxin

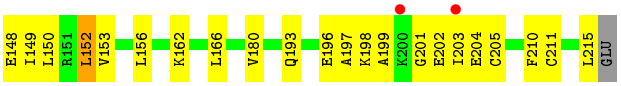
Chain C:



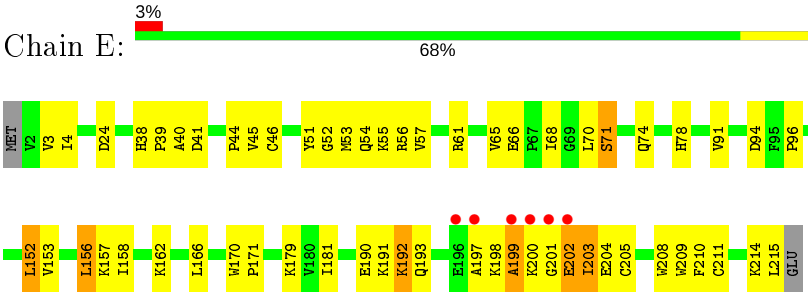
- Molecule 1: Probable peroxiredoxin

Chain D:

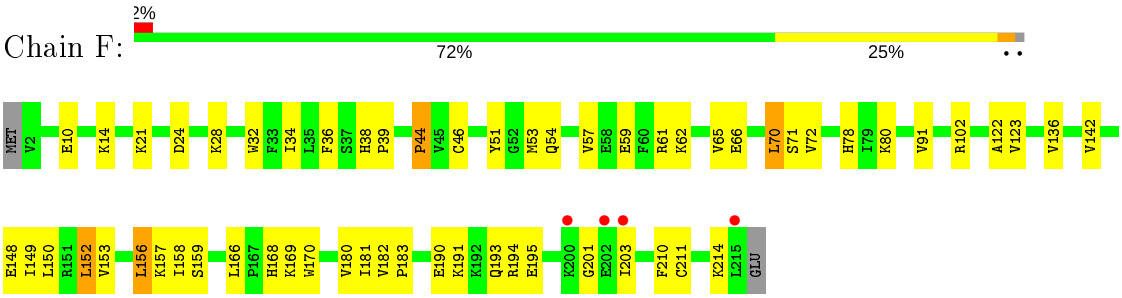




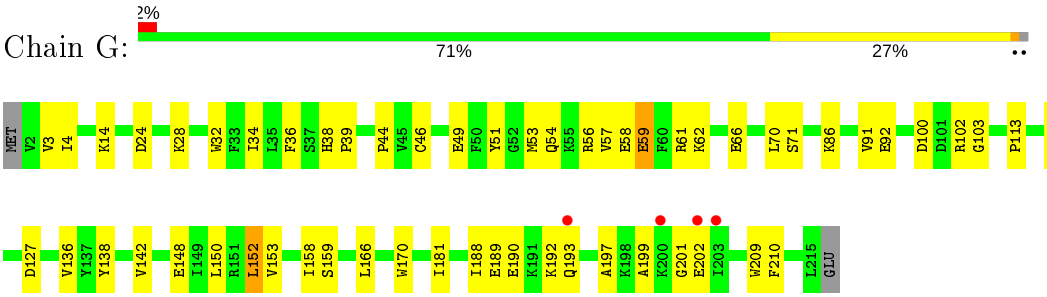
• Molecule 1: Probable peroxiredoxin



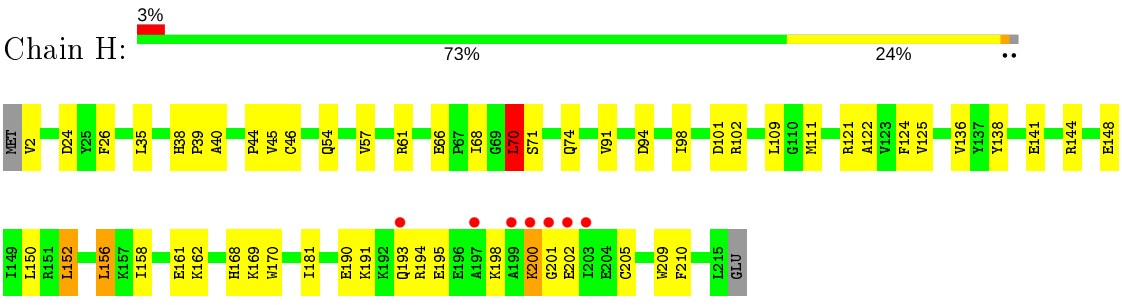
• Molecule 1: Probable peroxiredoxin



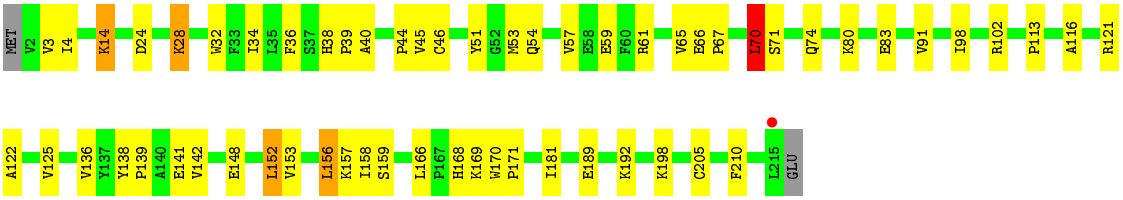
• Molecule 1: Probable peroxiredoxin



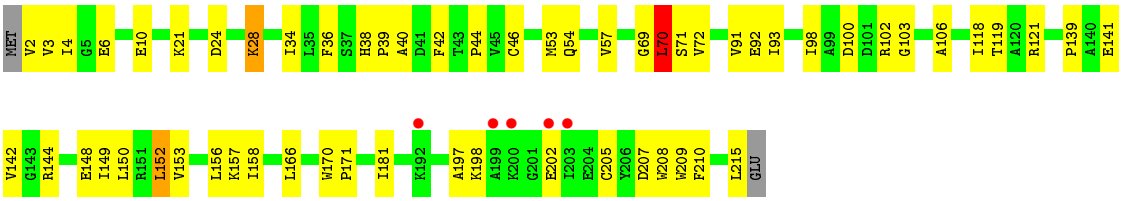
• Molecule 1: Probable peroxiredoxin



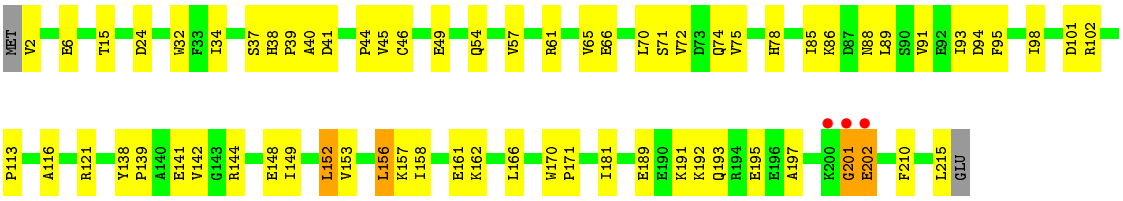
• Molecule 1: Probable peroxiredoxin



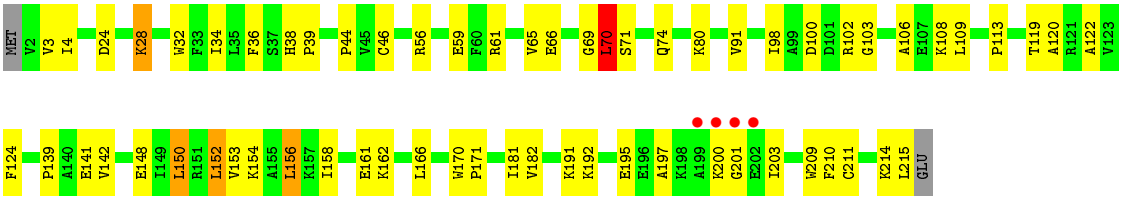
• Molecule 1: Probable peroxiredoxin



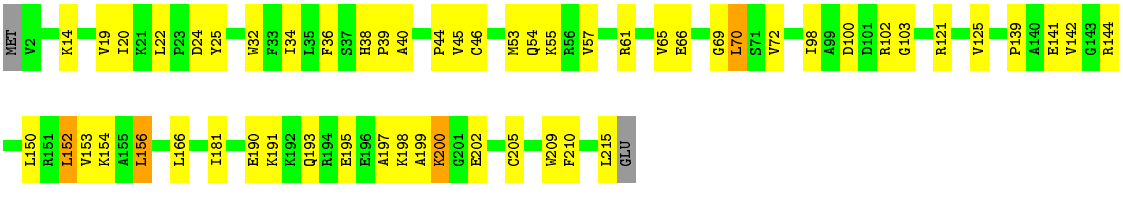
• Molecule 1: Probable peroxiredoxin



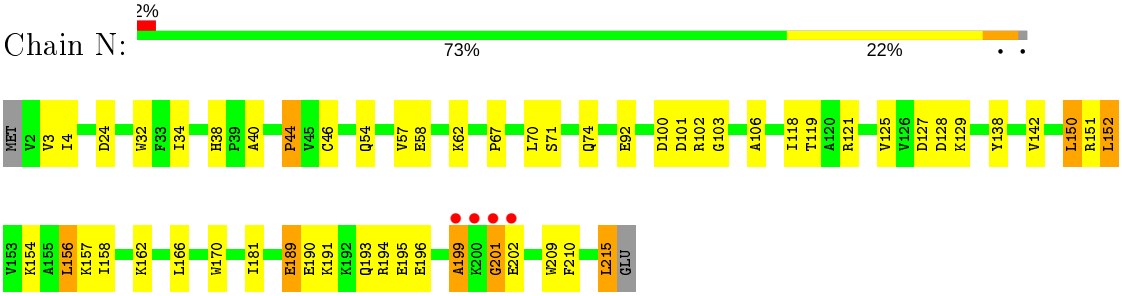
• Molecule 1: Probable peroxiredoxin



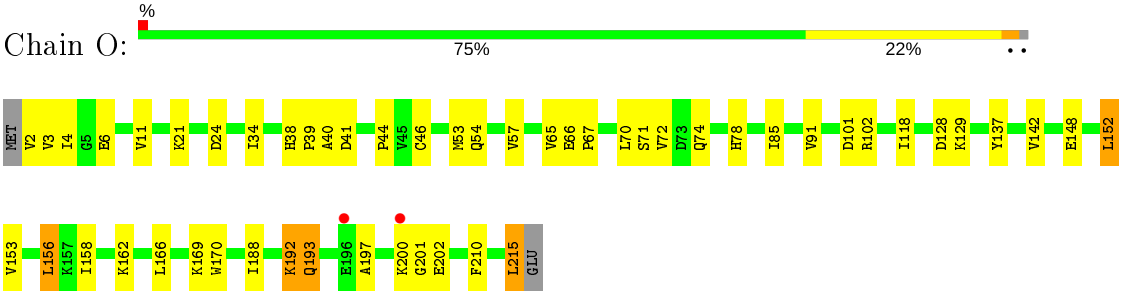
• Molecule 1: Probable peroxiredoxin



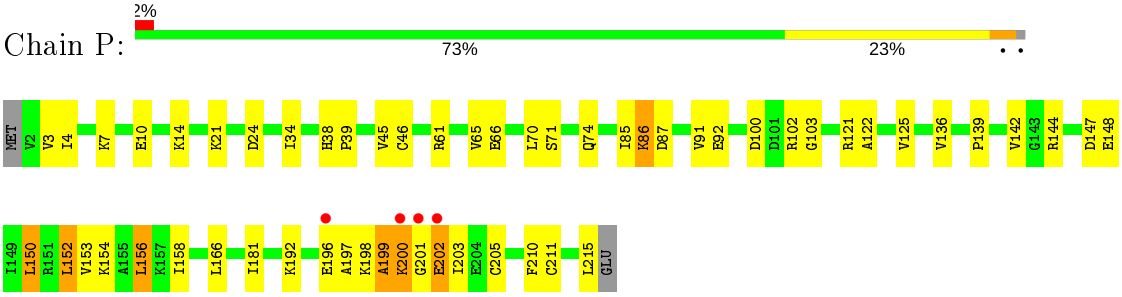
• Molecule 1: Probable peroxiredoxin



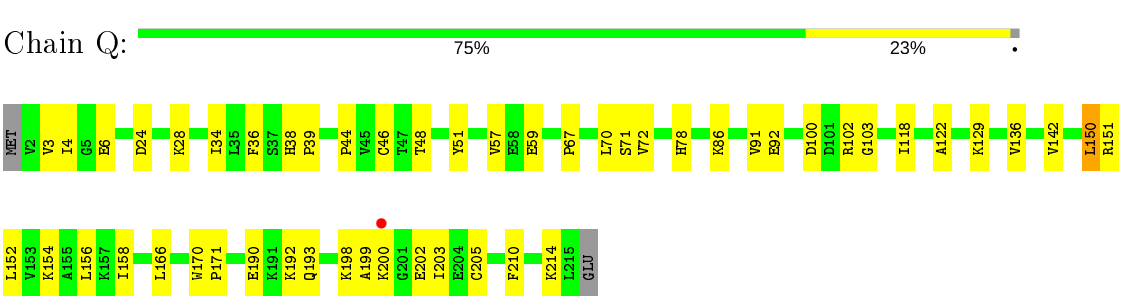
• Molecule 1: Probable peroxiredoxin



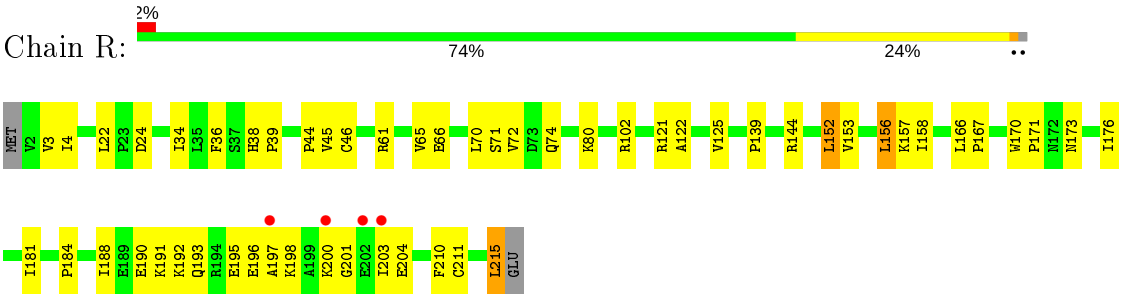
• Molecule 1: Probable peroxiredoxin



• Molecule 1: Probable peroxiredoxin

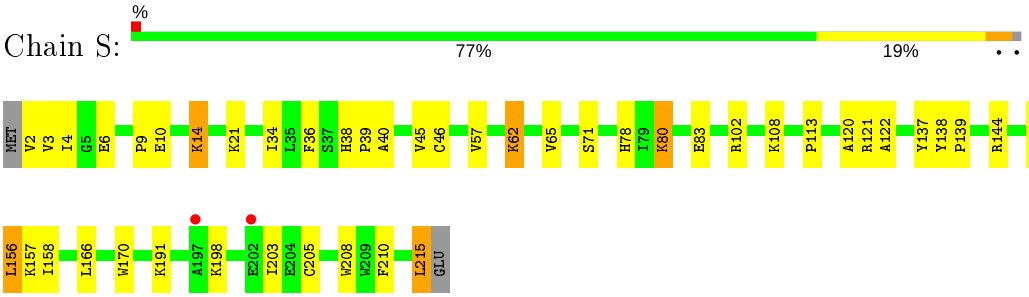


• Molecule 1: Probable peroxiredoxin



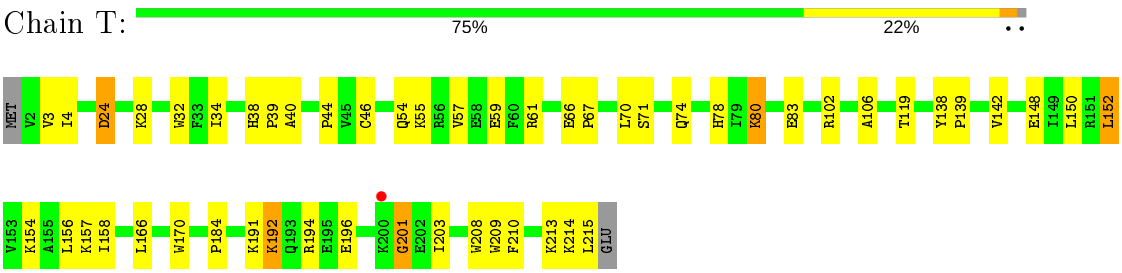
• Molecule 1: Probable peroxiredoxin

Chain S:



• Molecule 1: Probable peroxiredoxin

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.35Å 94.73Å 228.20Å 90.00° 103.31° 90.00°	Depositor
Resolution (Å)	43.57 – 2.25 43.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.57-2.25) 94.8 (43.57-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.05 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.237 0.195 , 0.233	Depositor DCC
R_{free} test set	11674 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	35926	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 39.83 % 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 2.9945e-04. 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, 0.333 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: FLC

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	0.35	0/1778	0.61	0/2410
1	B	0.34	0/1778	0.62	1/2410 (0.0%)
1	C	0.35	0/1778	0.60	0/2410
1	D	0.35	0/1778	0.61	0/2410
1	E	0.35	0/1778	0.61	0/2410
1	F	0.35	0/1778	0.61	0/2410
1	G	0.36	0/1778	0.60	0/2410
1	H	0.36	0/1778	0.61	1/2410 (0.0%)
1	I	0.35	0/1778	0.61	1/2410 (0.0%)
1	J	0.34	0/1778	0.60	1/2410 (0.0%)
1	K	0.33	0/1778	0.58	0/2410
1	L	0.35	0/1778	0.61	1/2410 (0.0%)
1	M	0.35	0/1778	0.62	0/2410
1	N	0.37	0/1778	0.62	0/2410
1	O	0.37	0/1778	0.62	0/2410
1	P	0.37	0/1778	0.63	0/2410
1	Q	0.37	0/1778	0.62	0/2410
1	R	0.35	0/1778	0.62	0/2410
1	S	0.37	0/1778	0.62	0/2410
1	T	0.36	0/1778	0.63	1/2410 (0.0%)
All	All	0.35	0/35560	0.61	6/48200 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	70	LEU	CA-CB-CG	5.53	128.03	115.30
1	B	70	LEU	CA-CB-CG	5.51	127.97	115.30
1	H	70	LEU	CA-CB-CG	5.37	127.66	115.30
1	L	70	LEU	CA-CB-CG	5.36	127.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	201	GLY	N-CA-C	5.21	126.13	113.10
1	I	70	LEU	CA-CB-CG	5.01	126.81	115.30

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	1732	0	1749	68	0
1	B	1732	0	1749	61	0
1	C	1732	0	1749	57	0
1	D	1732	0	1749	49	0
1	E	1732	0	1749	66	0
1	F	1732	0	1749	53	0
1	G	1732	0	1749	47	0
1	H	1732	0	1749	49	0
1	I	1732	0	1749	52	0
1	J	1732	0	1749	49	0
1	K	1732	0	1749	58	0
1	L	1732	0	1749	59	0
1	M	1732	0	1749	52	0
1	N	1732	0	1749	51	0
1	O	1732	0	1749	51	0
1	P	1732	0	1749	43	0
1	Q	1732	0	1749	38	0
1	R	1732	0	1749	44	0
1	S	1732	0	1749	42	0
1	T	1732	0	1749	44	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	1	0
2	F	13	0	5	1	0
2	G	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	13	0	5	0	0
2	I	13	0	5	1	0
2	J	13	0	5	1	0
2	K	13	0	5	1	0
2	L	13	0	5	1	0
2	M	13	0	5	1	0
2	N	13	0	5	1	0
2	O	13	0	5	0	0
2	P	13	0	5	0	0
2	Q	13	0	5	1	0
2	R	13	0	5	2	0
2	S	13	0	5	0	0
2	T	13	0	5	1	0
3	A	41	0	0	2	0
3	B	47	0	0	2	0
3	C	36	0	0	2	0
3	D	43	0	0	3	0
3	E	41	0	0	2	0
3	F	50	0	0	2	0
3	G	53	0	0	2	0
3	H	40	0	0	4	0
3	I	42	0	0	2	0
3	J	46	0	0	2	0
3	K	42	0	0	2	0
3	L	52	0	0	1	0
3	M	62	0	0	3	0
3	N	64	0	0	7	0
3	O	60	0	0	3	0
3	P	60	0	0	3	0
3	Q	62	0	0	6	0
3	R	60	0	0	2	0
3	S	63	0	0	5	0
3	T	62	0	0	7	0
All	All	35926	0	35080	897	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 13.

All (897) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LYS:HD2	1:E:199:ALA:H	1.25	0.98
1:I:24:ASP:HB3	1:I:28:LYS:HE2	1.46	0.97
1:H:61:ARG:HD2	1:H:66:GLU:OE2	1.63	0.96
1:G:44:PRO:HB2	1:H:181:ILE:HD13	1.46	0.93
1:H:200:LYS:HA	1:H:200:LYS:HE3	1.51	0.91
1:G:34:ILE:HD11	1:G:153:VAL:HG11	1.55	0.88
1:T:192:LYS:HE3	1:T:192:LYS:HA	1.57	0.85
1:M:198:LYS:HG2	1:M:199:ALA:H	1.40	0.85
1:P:150:LEU:HD22	1:P:154:LYS:HE3	1.58	0.85
1:R:158:ILE:HD12	1:R:170:TRP:CH2	2.13	0.83
1:B:200:LYS:HE2	1:B:200:LYS:HA	1.63	0.81
1:K:44:PRO:HB2	1:L:181:ILE:HD13	1.63	0.81
1:C:162:LYS:HG3	1:C:215:LEU:HD11	1.64	0.80
1:I:44:PRO:HB2	1:J:181:ILE:HD13	1.62	0.79
1:B:38:HIS:CE1	1:B:71:SER:HB3	2.18	0.79
1:E:198:LYS:HD2	1:E:199:ALA:N	1.98	0.79
1:A:181:ILE:HD13	1:B:44:PRO:HB2	1.65	0.79
1:C:179:LYS:HG2	1:C:214:LYS:HD2	1.63	0.78
1:G:54:GLN:HA	1:G:57:VAL:HG23	1.65	0.78
1:D:203:ILE:HG21	1:D:211:CYS:HB3	1.65	0.78
1:A:112:ILE:HG22	3:A:407:HOH:O	1.81	0.77
1:A:38:HIS:CE1	1:A:71:SER:HB2	2.19	0.77
1:O:101:ASP:HB3	3:O:420:HOH:O	1.83	0.77
1:E:129:LYS:HG3	1:L:28:LYS:HE2	1.67	0.77
1:D:54:GLN:HA	1:D:57:VAL:HG23	1.66	0.76
1:O:152:LEU:HD22	1:O:156:LEU:HD22	1.65	0.76
1:S:34:ILE:HD11	1:S:153:VAL:HG11	1.68	0.76
1:S:152:LEU:HD22	1:S:156:LEU:HD22	1.68	0.76
1:O:54:GLN:HA	1:O:57:VAL:HG23	1.65	0.76
1:O:156:LEU:HD13	1:P:142:VAL:HG21	1.67	0.76
1:Q:38:HIS:CE1	1:Q:71:SER:HB2	2.21	0.75
1:E:162:LYS:HD2	1:E:215:LEU:HD22	1.69	0.75
1:G:56:ARG:O	1:G:59:GLU:HG2	1.86	0.75
1:F:54:GLN:HA	1:F:57:VAL:HG23	1.68	0.74
1:A:152:LEU:HD22	1:A:156:LEU:HD22	1.69	0.74
1:O:44:PRO:HB2	1:P:181:ILE:HD13	1.69	0.74
1:P:34:ILE:HD11	1:P:153:VAL:HG21	1.68	0.74
1:E:44:PRO:HB2	1:F:181:ILE:HD13	1.69	0.73
1:K:38:HIS:CE1	1:K:71:SER:HB3	2.23	0.73
1:L:152:LEU:HD22	1:L:156:LEU:HD22	1.70	0.73
1:A:192:LYS:HE3	1:A:192:LYS:O	1.88	0.73
1:D:61:ARG:HD2	1:D:66:GLU:OE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:LEU:HD22	1:K:156:LEU:HD22	1.70	0.73
1:J:215:LEU:H	1:J:215:LEU:HD23	1.53	0.72
1:C:61:ARG:HD2	1:C:66:GLU:OE2	1.89	0.72
1:H:70:LEU:HB2	1:H:98:ILE:HB	1.71	0.72
1:M:61:ARG:HD2	1:M:66:GLU:OE2	1.89	0.72
1:L:61:ARG:HD2	1:L:66:GLU:OE2	1.89	0.72
1:C:197:ALA:O	1:C:201:GLY:HA3	1.89	0.71
1:C:34:ILE:HD11	1:C:153:VAL:HG11	1.72	0.71
1:Q:59:GLU:HG2	3:Q:441:HOH:O	1.89	0.71
1:T:39:PRO:HD2	1:T:46:CYS:SG	2.31	0.71
1:D:198:LYS:HD2	1:D:205:CYS:SG	2.31	0.70
1:F:38:HIS:CE1	1:F:71:SER:HB2	2.25	0.70
1:L:182:VAL:HG21	1:L:203:ILE:HD11	1.72	0.70
1:O:38:HIS:CE1	1:O:71:SER:HB3	2.25	0.70
1:L:161:GLU:HG3	1:L:162:LYS:HG3	1.72	0.70
1:B:102:ARG:HD2	1:C:102:ARG:O	1.91	0.70
1:Q:86:LYS:HD3	1:Q:92:GLU:HG2	1.72	0.70
1:H:102:ARG:HD2	1:I:102:ARG:O	1.92	0.70
1:K:85:ILE:HG22	1:K:91:VAL:HG13	1.74	0.70
1:A:34:ILE:HD11	1:A:153:VAL:HG11	1.74	0.69
1:P:38:HIS:CE1	1:P:71:SER:HB3	2.28	0.69
1:J:198:LYS:HD2	1:J:205:CYS:SG	2.32	0.69
1:D:39:PRO:HD2	1:D:46:CYS:SG	2.33	0.69
1:F:168:HIS:CE1	1:F:169:LYS:HG3	2.28	0.69
1:H:74:GLN:HE22	1:I:40:ALA:HB2	1.57	0.69
1:T:61:ARG:HD2	1:T:66:GLU:OE2	1.92	0.68
1:K:142:VAL:HG21	1:L:156:LEU:HD13	1.76	0.68
1:O:158:ILE:HD12	1:O:170:TRP:CH2	2.29	0.68
1:S:80:LYS:HE2	1:S:83:GLU:OE1	1.94	0.68
1:C:54:GLN:HA	1:C:57:VAL:CG2	2.24	0.67
1:L:150:LEU:HD22	1:L:154:LYS:HE3	1.75	0.67
1:N:102:ARG:O	1:O:102:ARG:HD2	1.94	0.67
1:L:191:LYS:O	1:L:195:GLU:HG3	1.93	0.67
1:N:189:GLU:HG3	3:N:439:HOH:O	1.93	0.67
1:K:102:ARG:HD2	1:T:102:ARG:O	1.93	0.67
1:C:158:ILE:HD12	1:C:170:TRP:CH2	2.30	0.67
1:O:162:LYS:HE3	1:O:215:LEU:HD23	1.77	0.67
1:I:152:LEU:HD22	1:I:156:LEU:HD22	1.76	0.67
1:N:152:LEU:HD22	1:N:156:LEU:HD22	1.77	0.66
1:N:102:ARG:HD2	1:O:102:ARG:O	1.95	0.66
1:F:61:ARG:HD2	1:F:66:GLU:OE2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:GLN:HA	1:E:57:VAL:HG23	1.76	0.66
1:R:102:ARG:HD2	1:S:102:ARG:O	1.96	0.66
1:C:38:HIS:CE1	1:C:71:SER:HB3	2.31	0.66
1:L:70:LEU:HB2	1:L:98:ILE:HB	1.77	0.66
1:T:150:LEU:HD22	1:T:154:LYS:HE3	1.78	0.66
1:E:198:LYS:CD	1:E:199:ALA:H	2.03	0.66
1:M:156:LEU:HD13	1:N:142:VAL:HG21	1.78	0.66
3:E:419:HOH:O	1:F:169:LYS:HE2	1.96	0.65
1:I:54:GLN:HA	1:I:57:VAL:HG23	1.76	0.65
1:E:70:LEU:HD21	1:E:100:ASP:HB2	1.78	0.65
1:G:54:GLN:HA	1:G:57:VAL:CG2	2.26	0.65
1:N:40:ALA:HB2	1:O:74:GLN:NE2	2.11	0.65
1:A:39:PRO:HD2	1:A:46:CYS:SG	2.36	0.65
1:E:152:LEU:HD22	1:E:156:LEU:HD22	1.78	0.65
1:E:190:GLU:O	1:E:193:GLN:HG2	1.95	0.65
1:F:14:LYS:HD3	3:F:435:HOH:O	1.97	0.65
1:N:54:GLN:HA	1:N:57:VAL:HG13	1.79	0.65
1:O:54:GLN:HA	1:O:57:VAL:CG2	2.27	0.65
1:P:61:ARG:HD2	1:P:66:GLU:OE2	1.97	0.65
1:B:198:LYS:HD2	1:B:205:CYS:SG	2.36	0.65
1:E:179:LYS:HG2	1:E:214:LYS:HG2	1.79	0.65
1:E:70:LEU:HD13	1:E:71:SER:N	2.12	0.65
1:I:70:LEU:HD12	1:I:70:LEU:C	2.17	0.65
1:R:34:ILE:CD1	1:R:125:VAL:HG22	2.27	0.65
1:R:203:ILE:HG21	1:R:211:CYS:HB3	1.78	0.65
1:S:156:LEU:HD13	1:T:142:VAL:HG21	1.79	0.65
1:M:39:PRO:HD2	1:M:46:CYS:SG	2.37	0.65
1:M:54:GLN:HA	1:M:57:VAL:HG23	1.78	0.65
1:A:63:LEU:HD11	1:A:154:LYS:HD3	1.79	0.64
1:I:181:ILE:HD13	1:J:44:PRO:HB2	1.78	0.64
1:O:39:PRO:HD2	1:O:46:CYS:SG	2.37	0.64
1:A:44:PRO:HB2	1:B:181:ILE:HD13	1.80	0.64
1:T:54:GLN:O	1:T:57:VAL:HG22	1.98	0.64
1:D:4:ILE:HG13	3:D:415:HOH:O	1.97	0.64
1:I:70:LEU:HB2	1:I:98:ILE:HB	1.80	0.64
1:A:156:LEU:HD13	1:B:142:VAL:HG21	1.79	0.64
1:A:197:ALA:O	1:A:201:GLY:HA3	1.98	0.63
1:I:61:ARG:HD2	1:I:66:GLU:OE2	1.98	0.63
1:K:72:VAL:HG12	3:T:416:HOH:O	1.98	0.63
1:B:70:LEU:HD13	1:B:71:SER:N	2.13	0.63
1:N:40:ALA:HB2	1:O:74:GLN:HE22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ASP:O	1:J:28:LYS:HG3	1.99	0.63
1:A:102:ARG:HD2	1:J:102:ARG:O	1.98	0.63
1:K:156:LEU:HD13	1:L:142:VAL:HG21	1.80	0.63
1:H:161:GLU:HG3	1:H:162:LYS:HG3	1.81	0.63
1:M:53:MET:O	1:M:57:VAL:HG23	1.98	0.63
1:G:86:LYS:HD3	1:G:92:GLU:HG2	1.80	0.63
1:P:201:GLY:O	1:P:202:GLU:HB2	1.98	0.63
1:Q:190:GLU:HA	1:Q:193:GLN:HG2	1.79	0.63
1:D:102:ARG:HD2	1:E:102:ARG:O	1.99	0.62
1:F:102:ARG:HD2	1:G:102:ARG:O	1.99	0.62
1:A:107:GLU:HB2	1:J:102:ARG:HH12	1.64	0.62
1:I:158:ILE:HD12	1:I:170:TRP:CH2	2.35	0.62
1:N:191:LYS:HE3	3:N:442:HOH:O	1.99	0.62
1:Q:39:PRO:HD2	1:Q:46:CYS:SG	2.39	0.62
1:C:70:LEU:HD23	1:C:71:SER:N	2.15	0.62
1:F:152:LEU:HD22	1:F:156:LEU:HD22	1.82	0.61
1:M:44:PRO:HB2	1:N:181:ILE:HD13	1.82	0.61
1:I:125:VAL:HG11	1:I:156:LEU:HD23	1.83	0.61
1:L:102:ARG:O	1:M:102:ARG:HD2	1.99	0.61
1:M:14:LYS:HD3	1:M:19:VAL:HG22	1.82	0.61
1:E:158:ILE:HD12	1:E:170:TRP:CH2	2.36	0.61
1:L:197:ALA:O	1:L:201:GLY:HA3	2.00	0.61
1:B:24:ASP:O	1:B:28:LYS:HG2	2.00	0.61
1:D:162:LYS:HD2	1:D:215:LEU:HD11	1.80	0.61
1:D:70:LEU:C	1:D:70:LEU:HD23	2.21	0.61
1:K:40:ALA:HB2	1:T:74:GLN:HE22	1.64	0.61
1:D:72:VAL:HG12	1:D:72:VAL:O	2.00	0.61
1:H:74:GLN:NE2	1:I:40:ALA:HB2	2.16	0.61
1:J:70:LEU:C	1:J:70:LEU:HD12	2.22	0.61
1:K:45:VAL:HB	1:K:121:ARG:NH1	2.14	0.61
1:H:102:ARG:O	1:I:102:ARG:HD2	2.01	0.60
1:K:158:ILE:HD12	1:K:170:TRP:CH2	2.36	0.60
1:R:158:ILE:HD12	1:R:170:TRP:HH2	1.63	0.60
1:E:142:VAL:HG21	1:F:156:LEU:HD13	1.84	0.60
1:G:181:ILE:HD13	1:H:44:PRO:HB2	1.83	0.60
1:B:102:ARG:O	1:C:102:ARG:HD2	2.01	0.60
1:E:39:PRO:HD2	1:E:46:CYS:SG	2.41	0.60
1:H:39:PRO:HD2	1:H:46:CYS:SG	2.41	0.60
1:K:40:ALA:HB2	1:T:74:GLN:NE2	2.16	0.60
1:T:38:HIS:CE1	1:T:71:SER:HB3	2.37	0.60
1:L:182:VAL:HG21	1:L:203:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:VAL:HG22	1:R:4:ILE:N	2.16	0.60
1:O:137:TYR:O	1:P:4:ILE:HD11	2.02	0.60
1:C:39:PRO:HD2	1:C:46:CYS:SG	2.42	0.60
1:D:102:ARG:O	1:E:102:ARG:HD2	2.02	0.60
1:P:85:ILE:HG22	1:P:91:VAL:HG13	1.83	0.60
1:R:152:LEU:HD22	1:R:156:LEU:HD22	1.83	0.60
1:F:59:GLU:HG2	1:F:150:LEU:HD11	1.84	0.60
1:B:192:LYS:HA	1:B:192:LYS:HE3	1.83	0.59
1:D:54:GLN:HA	1:D:57:VAL:CG2	2.31	0.59
1:E:65:VAL:HG21	1:E:153:VAL:HG21	1.85	0.59
1:A:3:VAL:HG12	1:A:4:ILE:N	2.16	0.59
1:F:102:ARG:O	1:G:102:ARG:HD2	2.02	0.59
1:G:61:ARG:HD2	1:G:66:GLU:OE2	2.02	0.59
3:K:442:HOH:O	1:L:3:VAL:HG13	2.02	0.59
1:C:58:GLU:O	1:C:62:LYS:HG3	2.02	0.59
1:F:34:ILE:HG13	1:F:65:VAL:CG1	2.33	0.59
1:G:148:GLU:HG2	1:H:148:GLU:HG2	1.85	0.59
1:T:184:PRO:HA	3:T:445:HOH:O	2.02	0.59
1:D:72:VAL:HG12	3:E:425:HOH:O	2.02	0.59
1:G:190:GLU:HA	1:G:193:GLN:HE21	1.66	0.59
1:L:70:LEU:HD12	1:L:70:LEU:C	2.23	0.59
1:A:158:ILE:HD12	1:A:170:TRP:CH2	2.38	0.59
1:R:3:VAL:HG22	1:R:4:ILE:H	1.68	0.59
1:A:142:VAL:HG21	1:B:156:LEU:HD13	1.85	0.58
1:I:198:LYS:HD2	1:I:205:CYS:SG	2.42	0.58
1:M:198:LYS:HD2	1:M:205:CYS:SG	2.42	0.58
1:S:39:PRO:HD2	1:S:46:CYS:SG	2.43	0.58
1:R:38:HIS:CE1	1:R:71:SER:HB3	2.39	0.58
1:R:72:VAL:O	3:R:441:HOH:O	2.17	0.58
1:H:125:VAL:HG11	1:H:156:LEU:HD23	1.86	0.58
1:L:34:ILE:HD11	1:L:153:VAL:HG21	1.84	0.58
1:C:158:ILE:HD12	1:C:170:TRP:HH2	1.69	0.58
1:M:70:LEU:C	1:M:70:LEU:HD12	2.24	0.58
1:J:166:LEU:N	1:J:166:LEU:HD22	2.18	0.58
1:K:54:GLN:O	1:K:57:VAL:HG22	2.04	0.58
1:O:128:ASP:OD1	1:O:129:LYS:HD2	2.03	0.58
1:F:70:LEU:HD13	1:F:71:SER:N	2.18	0.58
1:C:125:VAL:HG11	1:C:156:LEU:HD23	1.85	0.58
1:K:201:GLY:O	1:K:202:GLU:HB3	2.04	0.58
1:Q:192:LYS:HG3	3:Q:414:HOH:O	2.03	0.58
1:B:192:LYS:O	1:B:196:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:PRO:HD2	1:G:46:CYS:SG	2.44	0.58
1:T:3:VAL:HG12	1:T:4:ILE:N	2.19	0.58
1:K:32:TRP:HB2	1:K:65:VAL:HG22	1.84	0.57
1:N:70:LEU:C	1:N:70:LEU:HD23	2.25	0.57
1:D:199:ALA:HA	3:D:412:HOH:O	2.03	0.57
1:H:170:TRP:HD1	3:H:433:HOH:O	1.86	0.57
1:L:158:ILE:HD12	1:L:170:TRP:HH2	1.69	0.57
1:F:10:GLU:OE1	1:F:21:LYS:HE2	2.04	0.57
1:L:158:ILE:HD12	1:L:170:TRP:CH2	2.39	0.57
1:Q:129:LYS:HE2	3:Q:418:HOH:O	2.03	0.57
1:Q:214:LYS:HD2	3:Q:433:HOH:O	2.03	0.57
1:I:153:VAL:O	1:I:157:LYS:HG2	2.05	0.57
1:P:102:ARG:HD2	1:Q:102:ARG:O	2.04	0.57
1:R:80:LYS:HE2	1:T:209:TRP:HE1	1.69	0.57
1:H:158:ILE:HD12	1:H:170:TRP:CH2	2.39	0.57
1:F:54:GLN:HA	1:F:57:VAL:CG2	2.33	0.57
1:A:74:GLN:NE2	1:J:40:ALA:HB2	2.20	0.57
1:L:214:LYS:HD2	3:L:410:HOH:O	2.04	0.57
1:P:70:LEU:HD23	1:P:71:SER:N	2.20	0.57
1:C:193:GLN:HE21	1:C:194:ARG:HD3	1.69	0.57
1:I:158:ILE:HD12	1:I:170:TRP:HH2	1.68	0.57
1:R:34:ILE:HD12	1:R:125:VAL:HG22	1.85	0.57
1:D:118:ILE:HG21	1:E:74:GLN:NE2	2.20	0.57
1:M:142:VAL:HG21	1:N:156:LEU:HD13	1.87	0.57
1:L:38:HIS:CE1	1:L:71:SER:HB3	2.39	0.56
1:Q:142:VAL:HG21	1:R:156:LEU:HD13	1.86	0.56
1:D:34:ILE:HG13	1:D:65:VAL:CG1	2.35	0.56
1:F:34:ILE:HD11	1:F:153:VAL:HG21	1.87	0.56
1:H:70:LEU:C	1:H:70:LEU:HD12	2.25	0.56
1:L:141:GLU:HG2	1:L:142:VAL:HG23	1.86	0.56
1:A:61:ARG:HD2	1:A:66:GLU:OE2	2.05	0.56
1:D:38:HIS:CE1	1:D:71:SER:HB3	2.41	0.56
1:J:10:GLU:OE1	1:J:21:LYS:HE2	2.06	0.56
1:R:102:ARG:O	1:S:102:ARG:HD2	2.06	0.56
1:E:197:ALA:O	1:E:201:GLY:HA3	2.05	0.56
1:P:152:LEU:HD22	1:P:156:LEU:HD22	1.86	0.56
1:O:72:VAL:HG12	1:O:72:VAL:O	2.05	0.56
1:B:100:ASP:OD2	1:B:103:GLY:HA2	2.06	0.56
1:B:28:LYS:NZ	1:B:28:LYS:HB3	2.20	0.56
1:I:14:LYS:HB3	1:I:14:LYS:NZ	2.19	0.56
1:K:70:LEU:HD23	1:K:70:LEU:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:TRP:HB2	1:L:65:VAL:HG22	1.88	0.56
1:A:113:PRO:HG3	1:A:120:ALA:HB2	1.87	0.56
1:A:53:MET:O	1:A:57:VAL:HG23	2.06	0.56
1:C:3:VAL:HG23	3:C:425:HOH:O	2.05	0.56
1:D:65:VAL:HG21	1:D:153:VAL:HG11	1.87	0.56
1:B:39:PRO:HD2	1:B:46:CYS:SG	2.45	0.56
1:H:2:VAL:HG11	1:H:109:LEU:HD23	1.88	0.56
1:K:44:PRO:HG2	2:K:301:FLC:OB2	2.06	0.56
1:Q:44:PRO:HB2	1:R:181:ILE:HD13	1.87	0.56
1:R:39:PRO:HD2	1:R:46:CYS:SG	2.46	0.56
1:S:158:ILE:HD12	1:S:170:TRP:CH2	2.41	0.56
1:C:181:ILE:HD13	1:D:44:PRO:HB2	1.87	0.55
1:P:39:PRO:HD2	1:P:46:CYS:SG	2.46	0.55
1:D:51:TYR:O	1:D:55:LYS:HG2	2.06	0.55
1:G:54:GLN:CA	1:G:57:VAL:HG23	2.36	0.55
1:O:188:ILE:O	1:O:192:LYS:HE2	2.06	0.55
1:O:53:MET:O	1:O:57:VAL:HG23	2.06	0.55
1:R:34:ILE:HG12	1:R:65:VAL:CG1	2.36	0.55
1:L:70:LEU:CB	1:L:98:ILE:HB	2.36	0.55
1:L:102:ARG:HD2	1:M:102:ARG:O	2.06	0.55
1:O:70:LEU:HD23	1:O:70:LEU:C	2.27	0.55
3:N:440:HOH:O	1:O:72:VAL:HG12	2.07	0.55
1:T:71:SER:OG	1:T:78:HIS:HE1	1.87	0.55
1:F:194:ARG:NH1	3:F:445:HOH:O	2.38	0.55
1:T:158:ILE:HD12	1:T:170:TRP:CH2	2.42	0.55
1:A:199:ALA:O	1:A:200:LYS:HB2	2.06	0.55
1:M:198:LYS:HG2	1:M:199:ALA:N	2.14	0.55
1:O:158:ILE:HD12	1:O:170:TRP:HH2	1.69	0.55
1:R:197:ALA:O	1:R:201:GLY:O	2.24	0.55
1:E:156:LEU:HD13	1:F:142:VAL:HG21	1.88	0.55
1:J:121:ARG:HB3	1:J:144:ARG:CZ	2.37	0.55
1:K:158:ILE:HD12	1:K:170:TRP:HH2	1.72	0.55
1:A:151:ARG:HD2	1:A:170:TRP:O	2.07	0.54
1:B:158:ILE:HD13	1:B:215:LEU:HD11	1.89	0.54
1:B:61:ARG:HD2	1:B:66:GLU:OE2	2.06	0.54
1:F:71:SER:HB3	1:F:78:HIS:HE1	1.72	0.54
1:P:45:VAL:HB	1:P:121:ARG:NH1	2.22	0.54
1:C:54:GLN:HA	1:C:57:VAL:HG23	1.88	0.54
3:B:432:HOH:O	1:C:72:VAL:HG22	2.07	0.54
1:D:166:LEU:N	1:D:166:LEU:HD22	2.21	0.54
1:E:129:LYS:HG3	1:L:28:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:190:GLU:O	1:M:193:GLN:HG2	2.07	0.54
1:O:70:LEU:HD23	1:O:71:SER:N	2.22	0.54
1:R:125:VAL:HG11	1:R:156:LEU:HD23	1.88	0.54
1:G:100:ASP:OD2	1:G:103:GLY:HA2	2.07	0.54
1:I:53:MET:O	1:I:57:VAL:HG23	2.07	0.54
1:P:70:LEU:C	1:P:70:LEU:HD23	2.27	0.54
1:F:166:LEU:N	1:F:166:LEU:HD22	2.22	0.54
1:K:72:VAL:HG12	1:K:72:VAL:O	2.06	0.54
1:O:197:ALA:O	1:O:201:GLY:O	2.26	0.54
1:P:14:LYS:HD2	3:P:428:HOH:O	2.07	0.54
1:A:198:LYS:O	1:A:199:ALA:O	2.26	0.54
1:D:152:LEU:HD22	1:D:156:LEU:HD22	1.88	0.54
1:F:191:LYS:O	1:F:195:GLU:HG3	2.07	0.54
1:K:39:PRO:HD2	1:K:46:CYS:SG	2.47	0.54
1:O:215:LEU:HD22	1:O:215:LEU:C	2.27	0.54
1:R:61:ARG:HD2	1:R:66:GLU:OE2	2.07	0.54
1:B:151:ARG:HD2	1:B:170:TRP:O	2.08	0.54
1:G:113:PRO:HG3	1:G:120:ALA:HB2	1.89	0.54
1:M:191:LYS:O	1:M:195:GLU:HG3	2.07	0.54
1:S:3:VAL:HG12	1:S:4:ILE:N	2.22	0.54
1:B:200:LYS:HE2	1:B:200:LYS:CA	2.37	0.54
1:O:142:VAL:HG21	1:P:156:LEU:HD13	1.89	0.54
1:B:40:ALA:HB2	1:C:74:GLN:NE2	2.23	0.54
1:E:192:LYS:O	1:E:192:LYS:HE3	2.07	0.54
1:S:156:LEU:HD11	1:T:139:PRO:HG3	1.89	0.54
1:B:65:VAL:HG21	1:B:153:VAL:HG21	1.89	0.54
1:E:54:GLN:HA	1:E:57:VAL:CG2	2.38	0.54
1:B:191:LYS:O	1:B:195:GLU:HG3	2.08	0.54
1:S:38:HIS:CE1	1:S:71:SER:HB3	2.43	0.54
1:Q:150:LEU:HD22	1:Q:154:LYS:HE3	1.90	0.53
1:J:149:ILE:O	1:J:153:VAL:HG13	2.08	0.53
1:K:156:LEU:HD11	1:L:139:PRO:HG3	1.90	0.53
1:S:34:ILE:HG13	1:S:65:VAL:CG1	2.38	0.53
1:B:118:ILE:HG21	1:C:74:GLN:NE2	2.24	0.53
1:D:65:VAL:HG21	1:D:153:VAL:CG1	2.39	0.53
1:O:201:GLY:O	1:O:202:GLU:HB3	2.08	0.53
3:O:433:HOH:O	1:P:3:VAL:HG23	2.06	0.53
1:S:2:VAL:HA	1:S:6:GLU:OE2	2.09	0.53
1:K:139:PRO:HG3	1:L:156:LEU:HD11	1.90	0.53
1:K:85:ILE:CG2	1:K:91:VAL:HG13	2.37	0.53
1:L:39:PRO:HD2	1:L:46:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HB	1:A:121:ARG:NH1	2.24	0.53
1:L:214:LYS:HG3	1:L:215:LEU:H	1.73	0.53
1:S:148:GLU:HG2	1:T:148:GLU:HG2	1.89	0.53
1:C:156:LEU:HD11	1:D:139:PRO:HG3	1.90	0.53
1:E:181:ILE:HD13	1:F:44:PRO:HB2	1.91	0.53
1:H:54:GLN:HA	1:H:57:VAL:HG13	1.90	0.53
1:E:129:LYS:HZ3	1:L:28:LYS:HG2	1.73	0.53
1:T:38:HIS:HB2	1:T:46:CYS:SG	2.49	0.53
1:G:14:LYS:HD3	3:G:416:HOH:O	2.09	0.53
1:H:38:HIS:CE1	1:H:71:SER:HB3	2.44	0.53
1:J:39:PRO:HD2	1:J:46:CYS:SG	2.48	0.53
1:M:34:ILE:HG13	1:M:65:VAL:CG1	2.37	0.53
1:A:158:ILE:HD12	1:A:170:TRP:HH2	1.73	0.53
1:C:141:GLU:HG2	1:C:142:VAL:HG23	1.90	0.53
1:Q:156:LEU:HD21	1:R:139:PRO:HG3	1.91	0.52
1:T:80:LYS:HE2	1:T:83:GLU:OE1	2.09	0.52
1:E:41:ASP:OD1	1:E:78:HIS:ND1	2.42	0.52
1:I:148:GLU:HG2	1:J:148:GLU:HG2	1.90	0.52
1:O:85:ILE:CG2	1:O:91:VAL:HG13	2.38	0.52
1:S:9:PRO:CB	1:S:108:LYS:HE3	2.40	0.52
1:C:151:ARG:HD2	1:C:170:TRP:O	2.10	0.52
1:D:74:GLN:NE2	1:E:40:ALA:HB2	2.24	0.52
1:G:142:VAL:HG21	1:H:156:LEU:CD1	2.39	0.52
1:L:166:LEU:N	1:L:166:LEU:HD22	2.24	0.52
1:O:85:ILE:HG22	1:O:91:VAL:HG13	1.92	0.52
1:S:45:VAL:HB	1:S:121:ARG:NH1	2.24	0.52
1:N:128:ASP:OD2	1:N:129:LYS:HE2	2.09	0.52
1:T:192:LYS:O	1:T:196:GLU:HG3	2.09	0.52
1:H:26:PHE:HE2	1:H:66:GLU:HG2	1.73	0.52
1:O:166:LEU:HD22	1:O:166:LEU:N	2.24	0.52
1:T:24:ASP:O	1:T:28:LYS:HG2	2.09	0.52
1:M:70:LEU:HB2	1:M:98:ILE:HB	1.90	0.52
1:A:112:ILE:HD11	1:A:116:ALA:O	2.09	0.52
1:A:112:ILE:HD11	1:A:117:THR:HA	1.92	0.52
1:A:70:LEU:HD23	1:A:70:LEU:C	2.30	0.52
1:C:54:GLN:O	1:C:57:VAL:HG23	2.10	0.52
1:G:3:VAL:HG12	1:G:4:ILE:N	2.25	0.52
1:J:70:LEU:HB2	1:J:98:ILE:HB	1.91	0.52
1:M:54:GLN:HA	1:M:57:VAL:CG2	2.39	0.52
1:C:156:LEU:HD13	1:D:142:VAL:HG21	1.92	0.52
1:E:203:ILE:HD12	1:E:211:CYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:3:VAL:HG22	1:O:4:ILE:N	2.25	0.52
1:B:7:LYS:HG2	1:B:131:ILE:HD13	1.90	0.52
1:G:38:HIS:HB2	1:G:46:CYS:SG	2.49	0.52
1:K:61:ARG:NH2	1:K:94:ASP:OD1	2.38	0.52
1:P:158:ILE:HD13	1:P:215:LEU:HD11	1.92	0.52
1:D:203:ILE:HG22	1:D:204:GLU:O	2.10	0.52
1:I:156:LEU:HD13	1:J:142:VAL:HG21	1.92	0.51
1:E:191:LYS:HE2	1:E:208:TRP:CD1	2.45	0.51
1:G:70:LEU:C	1:G:70:LEU:HD23	2.31	0.51
1:S:198:LYS:HD2	1:S:205:CYS:SG	2.51	0.51
1:T:192:LYS:CE	1:T:192:LYS:HA	2.34	0.51
1:F:32:TRP:CE2	1:F:157:LYS:HE3	2.45	0.51
1:Q:199:ALA:HA	3:Q:425:HOH:O	2.10	0.51
1:E:158:ILE:HD12	1:E:170:TRP:HH2	1.73	0.51
1:E:70:LEU:CD2	1:E:100:ASP:HB2	2.40	0.51
1:G:122:ALA:HA	1:G:136:VAL:O	2.11	0.51
1:M:198:LYS:CG	1:M:199:ALA:H	2.18	0.51
1:G:142:VAL:HG21	1:H:156:LEU:HD13	1.92	0.51
1:H:198:LYS:HE2	3:H:412:HOH:O	2.11	0.51
1:K:41:ASP:OD1	1:K:78:HIS:ND1	2.38	0.51
1:N:125:VAL:HG11	1:N:156:LEU:HD23	1.93	0.51
1:O:41:ASP:OD1	1:O:78:HIS:ND1	2.42	0.51
1:Q:3:VAL:HG12	1:Q:4:ILE:N	2.26	0.51
1:D:197:ALA:O	1:D:201:GLY:O	2.28	0.51
1:E:53:MET:O	1:E:57:VAL:HG23	2.11	0.51
1:I:113:PRO:HG2	1:I:116:ALA:HB3	1.93	0.51
1:G:197:ALA:O	1:G:201:GLY:HA3	2.11	0.51
1:Q:34:ILE:HG23	1:Q:67:PRO:HA	1.93	0.51
1:A:148:GLU:HG2	1:B:148:GLU:HG2	1.92	0.51
1:E:38:HIS:CE1	1:E:71:SER:HB3	2.46	0.51
1:Q:71:SER:HB3	1:Q:78:HIS:HE1	1.76	0.51
1:I:39:PRO:HD2	1:I:46:CYS:SG	2.50	0.50
1:J:44:PRO:HG2	2:J:301:FLC:OB2	2.11	0.50
1:N:158:ILE:HD12	1:N:170:TRP:CH2	2.46	0.50
1:B:40:ALA:HB2	1:C:74:GLN:HE22	1.77	0.50
1:C:70:LEU:C	1:C:70:LEU:HD23	2.31	0.50
1:K:161:GLU:HG3	1:K:162:LYS:HG3	1.94	0.50
1:L:74:GLN:OE1	1:M:40:ALA:HB2	2.10	0.50
1:M:20:ILE:HG23	1:M:25:TYR:HB2	1.93	0.50
1:P:198:LYS:HD3	1:P:205:CYS:SG	2.51	0.50
1:A:3:VAL:CG1	1:A:4:ILE:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:LYS:O	1:K:195:GLU:HG3	2.11	0.50
1:M:197:ALA:O	1:M:202:GLU:HB3	2.11	0.50
1:O:54:GLN:CA	1:O:57:VAL:HG23	2.40	0.50
1:R:34:ILE:HD13	1:R:125:VAL:HA	1.93	0.50
1:R:196:GLU:C	1:R:198:LYS:H	2.14	0.50
1:D:36:PHE:HA	1:D:122:ALA:O	2.12	0.50
1:P:85:ILE:CG2	1:P:91:VAL:HG13	2.42	0.50
1:M:150:LEU:HD22	1:M:154:LYS:HE3	1.93	0.50
1:D:54:GLN:CA	1:D:57:VAL:HG23	2.38	0.50
1:E:166:LEU:HD22	1:E:166:LEU:N	2.25	0.50
1:I:181:ILE:HG21	1:J:44:PRO:HB2	1.94	0.50
1:K:181:ILE:HD13	1:L:44:PRO:HB2	1.94	0.50
1:O:11:VAL:O	1:O:21:LYS:HD2	2.12	0.50
1:A:34:ILE:HG13	1:A:65:VAL:CG1	2.42	0.50
1:M:34:ILE:HD11	1:M:153:VAL:HG11	1.94	0.50
1:O:156:LEU:HD11	1:P:139:PRO:HG3	1.92	0.50
1:S:191:LYS:HB3	3:S:434:HOH:O	2.11	0.50
1:A:192:LYS:HE2	1:A:196:GLU:HG3	1.93	0.50
1:F:53:MET:O	1:F:57:VAL:HG23	2.11	0.50
1:J:207:ASP:OD1	1:J:208:TRP:N	2.38	0.50
1:J:3:VAL:HG22	1:J:4:ILE:N	2.27	0.50
1:J:36:PHE:O	1:J:69:GLY:HA2	2.12	0.50
1:K:113:PRO:HG2	1:K:116:ALA:HB3	1.93	0.50
1:M:70:LEU:CB	1:M:98:ILE:HB	2.42	0.49
1:B:179:LYS:HG2	1:B:214:LYS:HD2	1.93	0.49
1:F:59:GLU:O	1:F:62:LYS:HG2	2.12	0.49
1:H:194:ARG:NH1	3:H:402:HOH:O	2.42	0.49
1:L:182:VAL:CG2	1:L:203:ILE:HD11	2.42	0.49
1:M:44:PRO:HG2	2:M:301:FLC:OB2	2.12	0.49
1:T:34:ILE:HG23	1:T:67:PRO:HA	1.94	0.49
1:A:44:PRO:HG2	2:A:301:FLC:OB2	2.12	0.49
1:J:92:GLU:HA	3:J:406:HOH:O	2.10	0.49
1:Q:44:PRO:HG2	2:Q:301:FLC:OB1	2.11	0.49
1:S:14:LYS:HG2	3:S:420:HOH:O	2.10	0.49
1:E:100:ASP:OD2	1:E:103:GLY:HA2	2.12	0.49
1:E:44:PRO:HG2	2:E:301:FLC:OB2	2.12	0.49
1:A:80:LYS:HG2	1:J:42:PHE:CE2	2.47	0.49
1:N:191:LYS:O	1:N:195:GLU:HG3	2.13	0.49
1:A:202:GLU:O	1:A:202:GLU:HG2	2.12	0.49
1:E:129:LYS:NZ	1:L:28:LYS:HG2	2.27	0.49
3:M:408:HOH:O	1:N:3:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:VAL:HB	1:E:121:ARG:NH1	2.27	0.49
1:D:14:LYS:HE3	1:D:101:ASP:OD2	2.12	0.49
1:Q:200:LYS:HE3	1:Q:202:GLU:CD	2.33	0.49
1:R:166:LEU:N	1:R:166:LEU:HD22	2.27	0.49
1:E:54:GLN:NE2	1:E:94:ASP:OD1	2.45	0.49
1:M:34:ILE:HG13	1:M:65:VAL:HG11	1.94	0.49
1:M:72:VAL:O	3:M:439:HOH:O	2.19	0.49
1:E:162:LYS:CD	1:E:215:LEU:HD22	2.42	0.49
1:G:166:LEU:HD22	1:G:166:LEU:N	2.28	0.49
1:K:34:ILE:O	1:K:34:ILE:HG23	2.11	0.49
1:N:44:PRO:HG2	2:N:301:FLC:OB2	2.13	0.49
1:B:121:ARG:HB3	1:B:144:ARG:CZ	2.43	0.48
1:E:209:TRP:O	1:F:44:PRO:HD3	2.12	0.48
1:I:38:HIS:HB2	1:I:46:CYS:SG	2.52	0.48
1:P:197:ALA:O	1:P:201:GLY:O	2.31	0.48
1:I:36:PHE:HA	1:I:122:ALA:O	2.14	0.48
1:I:4:ILE:HG13	3:I:432:HOH:O	2.12	0.48
1:A:161:GLU:HG3	1:A:162:LYS:HG2	1.95	0.48
1:C:191:LYS:O	1:C:195:GLU:HG3	2.13	0.48
1:D:71:SER:OG	1:D:78:HIS:HE1	1.96	0.48
1:E:141:GLU:HG3	1:F:159:SER:OG	2.13	0.48
1:G:53:MET:O	1:G:57:VAL:HG23	2.12	0.48
1:S:152:LEU:HD22	1:S:156:LEU:CD2	2.40	0.48
1:S:57:VAL:HG12	3:S:411:HOH:O	2.13	0.48
1:T:191:LYS:HE2	1:T:208:TRP:CD1	2.49	0.48
1:A:166:LEU:HD22	1:A:166:LEU:N	2.28	0.48
1:E:141:GLU:HG2	1:E:142:VAL:HG23	1.95	0.48
1:M:100:ASP:OD2	1:M:103:GLY:HA2	2.14	0.48
1:R:36:PHE:HA	1:R:122:ALA:O	2.14	0.48
1:G:24:ASP:O	1:G:28:LYS:HG2	2.14	0.48
1:Q:166:LEU:HD22	1:Q:166:LEU:N	2.28	0.48
1:K:74:GLN:HE22	1:T:40:ALA:HB2	1.78	0.48
1:N:190:GLU:HA	1:N:193:GLN:HG2	1.94	0.48
1:A:159:SER:OG	1:B:141:GLU:HG3	2.14	0.48
1:B:68:ILE:HG13	1:B:96:PRO:HG2	1.96	0.48
1:D:72:VAL:HG23	3:D:405:HOH:O	2.13	0.48
1:E:170:TRP:CD1	1:E:171:PRO:HA	2.48	0.48
1:K:93:ILE:HG23	1:K:95:PHE:CE2	2.48	0.48
1:K:138:TYR:CZ	1:L:152:LEU:HG	2.48	0.48
1:Q:100:ASP:OD2	1:Q:103:GLY:HA2	2.14	0.48
1:S:139:PRO:HG3	1:T:156:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:PRO:HD2	1:F:46:CYS:SG	2.53	0.48
1:G:51:TYR:CE2	1:G:91:VAL:HG21	2.48	0.48
1:J:170:TRP:CD1	1:J:171:PRO:HA	2.49	0.48
1:N:74:GLN:NE2	1:O:118:ILE:HG21	2.28	0.48
1:C:106:ALA:HB1	1:C:119:THR:HG22	1.96	0.48
1:K:141:GLU:HG2	1:K:142:VAL:HG23	1.95	0.48
1:N:70:LEU:HD23	1:N:71:SER:N	2.29	0.48
1:O:2:VAL:HA	1:O:6:GLU:OE1	2.14	0.48
1:B:171:PRO:C	1:B:172:ASN:HD22	2.16	0.47
1:B:42:PHE:CD2	1:C:80:LYS:HG3	2.48	0.47
1:C:45:VAL:HB	1:C:121:ARG:NH1	2.29	0.47
1:K:113:PRO:HA	1:L:3:VAL:HG12	1.96	0.47
1:Q:200:LYS:HE3	1:Q:202:GLU:OE2	2.14	0.47
1:Q:198:LYS:HD2	1:Q:205:CYS:SG	2.54	0.47
1:A:197:ALA:C	1:A:201:GLY:HA3	2.35	0.47
1:G:3:VAL:HG13	3:G:411:HOH:O	2.13	0.47
1:P:86:LYS:HG3	1:P:87:ASP:N	2.27	0.47
1:R:203:ILE:HG22	1:R:204:GLU:O	2.13	0.47
1:S:10:GLU:OE1	1:S:21:LYS:HE2	2.14	0.47
1:D:60:PHE:CZ	1:D:150:LEU:HG	2.49	0.47
1:F:71:SER:HB3	1:F:78:HIS:CE1	2.49	0.47
1:L:24:ASP:O	1:L:28:LYS:HB3	2.14	0.47
1:K:74:GLN:NE2	1:T:40:ALA:HB2	2.28	0.47
1:B:74:GLN:NE2	1:C:40:ALA:HB2	2.29	0.47
1:C:193:GLN:HE21	1:C:194:ARG:CD	2.26	0.47
1:K:2:VAL:HA	1:K:6:GLU:OE1	2.14	0.47
1:M:152:LEU:HD22	1:M:156:LEU:HD22	1.95	0.47
1:M:36:PHE:O	1:M:69:GLY:HA2	2.14	0.47
1:N:201:GLY:O	1:N:202:GLU:HB3	2.14	0.47
1:S:203:ILE:HG13	3:S:437:HOH:O	2.14	0.47
1:F:158:ILE:HD12	1:F:170:TRP:CH2	2.49	0.47
1:M:166:LEU:HD22	1:M:166:LEU:N	2.29	0.47
1:G:58:GLU:O	1:G:62:LYS:HG3	2.15	0.47
1:I:38:HIS:CE1	1:I:71:SER:HB3	2.49	0.47
1:I:3:VAL:HG22	1:I:4:ILE:H	1.79	0.47
1:N:166:LEU:HD22	1:N:166:LEU:N	2.29	0.47
1:S:9:PRO:HB3	1:S:108:LYS:HE3	1.96	0.47
1:A:198:LYS:HG2	1:A:199:ALA:H	1.79	0.47
1:E:61:ARG:HD2	1:E:66:GLU:OE2	2.14	0.47
1:Q:203:ILE:HD12	1:Q:203:ILE:O	2.15	0.47
1:E:38:HIS:HB2	1:E:46:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:ILE:O	1:F:153:VAL:HG23	2.15	0.47
1:I:166:LEU:N	1:I:166:LEU:HD22	2.30	0.47
1:I:3:VAL:HG22	1:I:4:ILE:N	2.29	0.47
1:I:80:LYS:HE2	1:I:83:GLU:OE1	2.14	0.47
1:P:166:LEU:HD22	1:P:166:LEU:N	2.29	0.47
1:P:74:GLN:NE2	1:Q:118:ILE:HG21	2.29	0.47
1:S:191:LYS:HE2	1:S:208:TRP:CG	2.49	0.47
1:T:166:LEU:N	1:T:166:LEU:HD22	2.30	0.47
1:D:141:GLU:HG2	1:D:142:VAL:HG23	1.95	0.47
1:H:66:GLU:HG3	3:H:410:HOH:O	2.15	0.47
1:K:15:THR:HG22	1:K:98:ILE:HG12	1.97	0.47
1:N:194:ARG:NH1	3:N:453:HOH:O	2.47	0.47
1:P:125:VAL:HG11	1:P:156:LEU:HD23	1.97	0.47
1:Q:158:ILE:HD12	1:Q:170:TRP:CH2	2.50	0.47
1:R:45:VAL:HB	1:R:121:ARG:NH1	2.30	0.47
1:R:153:VAL:O	1:R:157:LYS:HG2	2.15	0.47
3:S:429:HOH:O	1:T:3:VAL:HG13	2.14	0.47
1:A:198:LYS:HG2	1:A:199:ALA:N	2.30	0.47
1:E:148:GLU:HG2	1:F:148:GLU:HG2	1.95	0.47
1:G:38:HIS:CE1	1:G:71:SER:HB3	2.49	0.47
1:I:113:PRO:HG2	1:I:116:ALA:CB	2.45	0.47
1:N:150:LEU:HD22	1:N:154:LYS:HE3	1.97	0.47
1:A:3:VAL:HG13	3:A:430:HOH:O	2.14	0.47
1:D:149:ILE:O	1:D:153:VAL:HG23	2.15	0.47
1:C:142:VAL:HG21	1:D:156:LEU:HD13	1.98	0.47
1:J:28:LYS:HD2	3:J:429:HOH:O	2.15	0.47
1:J:54:GLN:OE1	1:J:93:ILE:HA	2.15	0.47
1:K:49:GLU:OE1	1:K:121:ARG:NH2	2.48	0.47
1:P:10:GLU:OE1	1:P:21:LYS:HE3	2.15	0.47
1:R:191:LYS:O	1:R:195:GLU:HG3	2.14	0.47
1:A:112:ILE:O	1:A:112:ILE:HG23	2.15	0.46
1:A:168:HIS:CE1	1:A:169:LYS:HB2	2.50	0.46
1:D:203:ILE:HG22	1:D:204:GLU:N	2.30	0.46
1:J:153:VAL:O	1:J:157:LYS:HG2	2.14	0.46
1:K:34:ILE:CD1	1:K:149:ILE:HG21	2.45	0.46
1:P:121:ARG:HB3	1:P:144:ARG:CZ	2.45	0.46
1:T:194:ARG:NH1	3:T:445:HOH:O	2.43	0.46
1:A:80:LYS:HE2	1:A:83:GLU:OE1	2.14	0.46
1:L:170:TRP:CD1	1:L:171:PRO:HA	2.50	0.46
1:S:62:LYS:NZ	1:S:62:LYS:CB	2.78	0.46
1:F:123:VAL:HB	1:F:136:VAL:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:PRO:HA	1:L:3:VAL:CG1	2.45	0.46
1:K:34:ILE:HD11	1:K:149:ILE:HG21	1.96	0.46
1:R:44:PRO:HG2	2:R:301:FLC:OB1	2.15	0.46
1:R:70:LEU:C	1:R:70:LEU:HD23	2.34	0.46
1:A:74:GLN:NE2	1:J:118:ILE:HG21	2.31	0.46
1:C:152:LEU:HG	1:D:138:TYR:CZ	2.51	0.46
1:F:38:HIS:HB2	1:F:46:CYS:SG	2.55	0.46
1:O:74:GLN:HG2	3:O:420:HOH:O	2.15	0.46
1:S:3:VAL:CG1	1:S:4:ILE:N	2.78	0.46
1:G:123:VAL:HB	1:G:136:VAL:HB	1.97	0.46
1:H:111:MET:HE2	1:H:124:PHE:HE1	1.81	0.46
1:K:148:GLU:HG2	1:L:148:GLU:HG2	1.97	0.46
1:K:162:LYS:HD2	1:K:215:LEU:HD22	1.97	0.46
1:M:198:LYS:O	1:M:199:ALA:C	2.54	0.46
1:N:38:HIS:CE1	1:N:71:SER:HB3	2.51	0.46
1:F:54:GLN:CA	1:F:57:VAL:HG23	2.42	0.46
1:R:34:ILE:HG12	1:R:65:VAL:HG11	1.98	0.46
1:E:192:LYS:HE3	1:E:192:LYS:HA	1.98	0.46
1:M:139:PRO:HG3	1:N:156:LEU:HD11	1.97	0.46
1:P:203:ILE:HD12	1:P:211:CYS:SG	2.56	0.46
1:A:71:SER:HB3	1:A:78:HIS:HE1	1.81	0.46
1:G:32:TRP:CD2	1:G:127:ASP:HA	2.51	0.46
1:G:158:ILE:HD12	1:G:170:TRP:HH2	1.81	0.46
1:K:75:VAL:O	1:K:78:HIS:HB2	2.16	0.46
1:Q:51:TYR:CE2	1:Q:91:VAL:HG21	2.50	0.46
1:B:54:GLN:HA	1:B:57:VAL:HG23	1.97	0.45
1:I:14:LYS:HG2	3:I:420:HOH:O	2.15	0.45
1:N:103:GLY:HA3	1:O:102:ARG:HD3	1.97	0.45
1:F:65:VAL:HG21	1:F:153:VAL:HG11	1.98	0.45
1:H:200:LYS:CE	1:H:200:LYS:HA	2.36	0.45
1:J:158:ILE:HD12	1:J:170:TRP:CH2	2.51	0.45
1:G:36:PHE:HA	1:G:122:ALA:O	2.16	0.45
1:H:202:GLU:HG2	1:H:202:GLU:O	2.16	0.45
1:H:61:ARG:NH2	1:H:94:ASP:OD1	2.47	0.45
1:I:34:ILE:HG23	1:I:67:PRO:HA	1.98	0.45
1:J:106:ALA:HB1	1:J:119:THR:HG22	1.98	0.45
1:N:34:ILE:HG23	1:N:67:PRO:HA	1.98	0.45
1:N:62:LYS:HG3	3:N:458:HOH:O	2.16	0.45
1:R:45:VAL:HG23	2:R:301:FLC:OB1	2.16	0.45
1:E:198:LYS:HE2	1:E:205:CYS:SG	2.56	0.45
1:H:70:LEU:HD12	1:H:71:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:53:MET:O	1:J:57:VAL:HG23	2.16	0.45
1:D:202:GLU:O	1:D:203:ILE:HD13	2.17	0.45
1:G:34:ILE:HD11	1:G:153:VAL:CG1	2.36	0.45
1:M:152:LEU:HG	1:N:138:TYR:CZ	2.52	0.45
1:P:92:GLU:HG3	3:P:424:HOH:O	2.16	0.45
1:R:74:GLN:OE1	1:S:40:ALA:HB2	2.16	0.45
1:T:106:ALA:HB1	1:T:119:THR:HG22	1.99	0.45
1:A:192:LYS:CE	1:A:196:GLU:HG3	2.47	0.45
1:A:75:VAL:O	1:A:78:HIS:HB2	2.17	0.45
1:E:198:LYS:O	1:E:199:ALA:C	2.54	0.45
1:H:54:GLN:HG2	1:H:91:VAL:HG22	1.99	0.45
1:O:162:LYS:CE	1:O:215:LEU:HD23	2.45	0.45
1:A:191:LYS:O	1:A:195:GLU:HG3	2.17	0.45
1:C:152:LEU:HD22	1:C:156:LEU:HD22	1.99	0.45
1:E:156:LEU:CD1	1:F:142:VAL:HG21	2.46	0.45
1:G:150:LEU:HA	1:G:153:VAL:HG22	1.99	0.45
1:L:203:ILE:HD13	1:L:211:CYS:HB3	1.99	0.45
1:P:192:LYS:O	1:P:196:GLU:HG3	2.16	0.45
1:E:190:GLU:HA	1:E:193:GLN:HG2	1.98	0.45
1:G:189:GLU:O	1:G:193:GLN:HG3	2.16	0.45
1:J:100:ASP:OD2	1:J:103:GLY:HA2	2.17	0.45
1:P:199:ALA:O	1:P:200:LYS:CB	2.65	0.45
1:C:121:ARG:HB3	1:C:144:ARG:CZ	2.47	0.45
1:I:141:GLU:HG2	1:I:142:VAL:HG23	1.98	0.45
1:P:7:LYS:HE2	3:P:415:HOH:O	2.17	0.45
1:R:215:LEU:HD12	1:R:215:LEU:H	1.82	0.45
1:B:192:LYS:HG2	3:B:428:HOH:O	2.17	0.45
1:E:203:ILE:HD13	1:E:204:GLU:H	1.82	0.45
1:F:190:GLU:O	1:F:194:ARG:HG2	2.17	0.45
1:G:158:ILE:HD12	1:G:170:TRP:CH2	2.52	0.45
1:K:88:ASN:O	1:K:89:LEU:HD23	2.17	0.45
1:E:3:VAL:HG22	1:E:4:ILE:N	2.33	0.44
1:N:100:ASP:OD2	1:N:103:GLY:HA2	2.17	0.44
1:Q:170:TRP:CD1	1:Q:171:PRO:HA	2.52	0.44
1:Q:70:LEU:C	1:Q:70:LEU:HD23	2.37	0.44
1:F:65:VAL:HG21	1:F:153:VAL:CG1	2.47	0.44
1:O:34:ILE:HG23	1:O:67:PRO:HA	1.98	0.44
1:P:199:ALA:O	1:P:200:LYS:HB2	2.17	0.44
1:S:137:TYR:O	1:T:4:ILE:HD11	2.17	0.44
1:S:71:SER:OG	1:S:78:HIS:HE1	1.99	0.44
1:D:2:VAL:HG12	1:D:6:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLN:HE22	1:J:40:ALA:HB2	1.81	0.44
1:K:170:TRP:CD1	1:K:171:PRO:HA	2.53	0.44
1:R:121:ARG:HB3	1:R:144:ARG:CZ	2.47	0.44
1:Q:48:THR:HB	1:R:173:ASN:HD21	1.82	0.44
1:C:170:TRP:CD1	1:C:171:PRO:HA	2.52	0.44
1:D:193:GLN:HA	1:D:196:GLU:OE2	2.17	0.44
1:F:182:VAL:O	1:F:183:PRO:C	2.54	0.44
1:L:100:ASP:OD2	1:L:103:GLY:HA2	2.18	0.44
1:R:196:GLU:C	1:R:198:LYS:N	2.71	0.44
1:A:122:ALA:HA	1:A:136:VAL:O	2.17	0.44
1:F:203:ILE:CG2	1:F:211:CYS:HB3	2.48	0.44
1:G:138:TYR:CZ	1:H:152:LEU:HG	2.52	0.44
1:N:196:GLU:O	1:N:199:ALA:HB3	2.18	0.44
1:T:214:LYS:HD3	3:T:440:HOH:O	2.17	0.44
1:C:27:THR:HG22	3:C:417:HOH:O	2.18	0.44
1:A:203:ILE:CD1	1:A:213:LYS:HB3	2.48	0.44
1:A:209:TRP:O	1:B:44:PRO:HD3	2.18	0.44
1:D:180:VAL:HG11	1:D:215:LEU:HD13	2.00	0.44
1:H:158:ILE:HD12	1:H:170:TRP:HH2	1.83	0.44
1:J:54:GLN:HG2	1:J:91:VAL:HG22	1.99	0.44
1:M:44:PRO:HD3	1:N:209:TRP:O	2.18	0.44
1:P:34:ILE:HG13	1:P:65:VAL:CG1	2.48	0.44
1:R:167:PRO:HG3	1:R:176:ILE:HD11	2.00	0.44
1:B:166:LEU:N	1:B:166:LEU:HD22	2.33	0.44
1:B:28:LYS:HZ3	1:B:28:LYS:HB3	1.81	0.44
1:D:53:MET:O	1:D:57:VAL:HG23	2.18	0.44
1:F:36:PHE:HA	1:F:122:ALA:O	2.18	0.44
1:J:38:HIS:HB2	1:J:46:CYS:SG	2.58	0.44
1:B:198:LYS:HA	1:B:203:ILE:HG22	2.00	0.44
1:C:72:VAL:O	1:C:72:VAL:HG22	2.17	0.44
1:I:51:TYR:CE2	1:I:91:VAL:HG21	2.53	0.44
1:I:70:LEU:CD1	1:I:70:LEU:C	2.85	0.44
1:M:45:VAL:HB	1:M:121:ARG:NH1	2.33	0.44
1:N:121:ARG:HH21	1:N:121:ARG:HG2	1.83	0.44
1:S:113:PRO:HG3	1:S:120:ALA:HB2	1.99	0.44
1:S:166:LEU:N	1:S:166:LEU:HD22	2.33	0.44
1:C:100:ASP:OD2	1:C:103:GLY:HA2	2.17	0.43
1:L:36:PHE:HA	1:L:122:ALA:O	2.18	0.43
1:M:61:ARG:HG2	3:M:430:HOH:O	2.17	0.43
1:N:54:GLN:O	1:N:57:VAL:HG22	2.18	0.43
1:S:138:TYR:CZ	1:T:152:LEU:HG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HG22	1:B:5:GLY:N	2.33	0.43
1:D:45:VAL:HB	1:D:121:ARG:NH1	2.33	0.43
1:E:55:LYS:HD2	1:E:56:ARG:NH1	2.32	0.43
1:S:36:PHE:HA	1:S:122:ALA:O	2.18	0.43
1:H:121:ARG:HB3	1:H:144:ARG:CZ	2.48	0.43
1:K:153:VAL:O	1:K:157:LYS:HG2	2.18	0.43
1:K:166:LEU:N	1:K:166:LEU:HD22	2.33	0.43
1:K:61:ARG:HD3	1:K:66:GLU:OE2	2.18	0.43
1:M:190:GLU:HA	1:M:193:GLN:HG2	2.00	0.43
1:N:57:VAL:HG23	1:N:58:GLU:N	2.33	0.43
1:A:38:HIS:NE2	1:A:71:SER:HB2	2.32	0.43
1:B:65:VAL:HG21	1:B:153:VAL:CG2	2.47	0.43
1:B:158:ILE:HD12	1:B:170:TRP:CH2	2.53	0.43
1:D:32:TRP:CD2	1:D:127:ASP:HA	2.53	0.43
1:J:34:ILE:HG23	1:J:34:ILE:O	2.18	0.43
1:K:113:PRO:HG2	1:K:116:ALA:CB	2.49	0.43
1:E:52:GLY:O	1:E:55:LYS:HG3	2.18	0.43
1:F:72:VAL:HG13	1:F:72:VAL:O	2.18	0.43
1:K:86:LYS:HD3	3:K:428:HOH:O	2.18	0.43
1:O:3:VAL:HG22	1:O:4:ILE:H	1.82	0.43
1:R:190:GLU:HA	1:R:193:GLN:HG2	1.99	0.43
1:C:166:LEU:HD22	1:C:166:LEU:N	2.32	0.43
1:J:2:VAL:HA	1:J:6:GLU:OE2	2.18	0.43
1:J:70:LEU:C	1:J:70:LEU:CD1	2.87	0.43
1:K:201:GLY:O	1:K:202:GLU:CB	2.67	0.43
1:L:214:LYS:HG3	1:L:215:LEU:N	2.34	0.43
1:O:169:LYS:NZ	1:P:147:ASP:OD2	2.39	0.43
1:B:9:PRO:HB3	1:B:108:LYS:HE3	2.00	0.43
1:B:3:VAL:HG12	1:B:4:ILE:O	2.19	0.43
1:B:75:VAL:O	1:B:78:HIS:HB2	2.18	0.43
1:D:38:HIS:HB2	1:D:46:CYS:SG	2.58	0.43
1:E:198:LYS:O	1:E:199:ALA:O	2.36	0.43
1:H:198:LYS:HD3	1:H:205:CYS:SG	2.59	0.43
1:O:65:VAL:HG21	1:O:153:VAL:HG11	2.01	0.43
1:P:122:ALA:HA	1:P:136:VAL:O	2.18	0.43
1:Q:158:ILE:HD12	1:Q:170:TRP:HH2	1.83	0.43
1:C:56:ARG:O	1:C:59:GLU:HB2	2.18	0.43
1:F:166:LEU:CD1	1:F:180:VAL:HG12	2.49	0.43
1:S:191:LYS:HE2	1:S:208:TRP:CD1	2.53	0.43
1:I:70:LEU:CB	1:I:98:ILE:HB	2.46	0.43
1:I:159:SER:OG	1:J:141:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:LEU:HB3	1:L:124:PHE:CZ	2.54	0.43
1:M:209:TRP:O	1:N:44:PRO:HD3	2.19	0.43
1:O:193:GLN:HG2	1:O:193:GLN:H	1.57	0.43
1:F:72:VAL:CG1	1:F:72:VAL:O	2.67	0.43
1:I:39:PRO:HB2	2:I:301:FLC:HA2	2.00	0.43
1:R:188:ILE:O	1:R:192:LYS:HG2	2.19	0.43
1:S:152:LEU:HG	1:T:138:TYR:CZ	2.54	0.43
1:B:74:GLN:HE22	1:C:40:ALA:HB2	1.84	0.42
1:E:51:TYR:CE2	1:E:91:VAL:HG21	2.54	0.42
1:K:37:SER:HA	1:K:70:LEU:O	2.18	0.42
1:L:74:GLN:CD	1:M:40:ALA:HB2	2.38	0.42
1:Q:36:PHE:HA	1:Q:122:ALA:O	2.18	0.42
1:R:170:TRP:CD1	1:R:171:PRO:HA	2.54	0.42
1:A:71:SER:HB3	1:A:78:HIS:CE1	2.55	0.42
1:G:56:ARG:HA	1:G:59:GLU:CD	2.40	0.42
1:I:170:TRP:CD1	1:I:171:PRO:HA	2.54	0.42
1:K:44:PRO:HD3	1:L:209:TRP:O	2.19	0.42
1:N:106:ALA:HB1	1:N:119:THR:HG22	2.01	0.42
1:P:100:ASP:OD2	1:P:103:GLY:HA2	2.19	0.42
1:I:44:PRO:HD3	1:J:209:TRP:O	2.19	0.42
1:J:72:VAL:HG22	1:J:72:VAL:O	2.19	0.42
1:L:113:PRO:HG3	1:L:120:ALA:HB2	2.01	0.42
1:O:148:GLU:HG2	1:P:148:GLU:HG2	2.00	0.42
1:Q:203:ILE:C	1:Q:203:ILE:HD12	2.39	0.42
1:E:122:ALA:HA	1:E:136:VAL:O	2.19	0.42
1:E:199:ALA:O	1:E:200:LYS:HB2	2.18	0.42
1:E:202:GLU:H	1:E:202:GLU:CD	2.23	0.42
1:G:188:ILE:O	1:G:192:LYS:HG2	2.19	0.42
1:G:159:SER:OG	1:H:141:GLU:HG3	2.19	0.42
1:S:3:VAL:HG13	3:T:411:HOH:O	2.19	0.42
1:C:54:GLN:CA	1:C:57:VAL:HG23	2.49	0.42
1:D:34:ILE:HG13	1:D:65:VAL:HG12	2.01	0.42
1:G:44:PRO:HD3	1:H:209:TRP:O	2.20	0.42
1:G:209:TRP:O	1:H:44:PRO:HD3	2.19	0.42
1:H:191:LYS:O	1:H:195:GLU:HG3	2.19	0.42
1:I:139:PRO:HG3	1:J:156:LEU:HD21	2.02	0.42
1:A:24:ASP:O	1:A:28:LYS:HG2	2.19	0.42
1:B:111:MET:HE2	1:B:111:MET:HB2	1.82	0.42
1:B:54:GLN:HG2	1:B:91:VAL:HG13	2.01	0.42
1:H:122:ALA:HA	1:H:136:VAL:O	2.19	0.42
1:K:189:GLU:O	1:K:193:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:PRO:CG	1:P:181:ILE:HG21	2.49	0.42
1:T:214:LYS:HD2	3:T:420:HOH:O	2.19	0.42
1:C:24:ASP:N	1:C:24:ASP:OD2	2.52	0.42
1:F:44:PRO:HG2	2:F:301:FLC:OB2	2.20	0.42
1:H:168:HIS:CE1	1:H:169:LYS:HB2	2.53	0.42
1:I:122:ALA:HA	1:I:136:VAL:O	2.20	0.42
1:L:59:GLU:HB3	1:L:150:LEU:HD11	2.01	0.42
1:T:32:TRP:CZ2	1:T:157:LYS:HE3	2.54	0.42
1:B:28:LYS:NZ	1:B:28:LYS:CB	2.83	0.42
1:N:74:GLN:NE2	3:N:432:HOH:O	2.46	0.42
1:Q:24:ASP:HB3	1:Q:28:LYS:HD2	2.02	0.42
1:Q:3:VAL:O	1:Q:6:GLU:HB2	2.19	0.42
1:R:203:ILE:CG2	1:R:211:CYS:HB3	2.46	0.42
1:A:103:GLY:O	1:J:102:ARG:NH1	2.53	0.42
1:A:156:LEU:HD11	1:B:139:PRO:HG3	2.02	0.42
1:C:170:TRP:CG	1:C:171:PRO:HA	2.55	0.42
1:E:192:LYS:CA	1:E:192:LYS:HE3	2.50	0.42
1:H:45:VAL:HB	1:H:121:ARG:NH1	2.35	0.42
1:H:40:ALA:HB2	1:I:74:GLN:NE2	2.35	0.42
1:L:106:ALA:HB1	1:L:119:THR:HG22	2.01	0.42
1:L:56:ARG:O	1:L:59:GLU:HB2	2.19	0.42
1:L:80:LYS:HD2	1:L:80:LYS:HA	1.84	0.42
1:B:34:ILE:CD1	1:B:149:ILE:HG21	2.49	0.41
1:C:3:VAL:HG12	1:C:6:GLU:HG3	2.02	0.41
1:M:32:TRP:HB2	1:M:65:VAL:HG22	2.02	0.41
1:S:2:VAL:HG12	1:S:6:GLU:OE1	2.20	0.41
1:T:70:LEU:C	1:T:70:LEU:HD23	2.41	0.41
1:A:102:ARG:O	1:J:102:ARG:HD2	2.20	0.41
1:B:121:ARG:HG2	1:B:121:ARG:HH21	1.84	0.41
1:H:190:GLU:HA	1:H:193:GLN:HG2	2.01	0.41
1:K:197:ALA:O	1:K:201:GLY:O	2.38	0.41
1:L:3:VAL:HG12	1:L:4:ILE:N	2.35	0.41
1:B:171:PRO:C	1:B:172:ASN:ND2	2.73	0.41
1:C:193:GLN:NE2	1:C:194:ARG:HD3	2.33	0.41
1:C:34:ILE:HG13	1:C:65:VAL:CG1	2.50	0.41
1:H:74:GLN:HG2	1:H:101:ASP:OD1	2.21	0.41
1:H:35:LEU:HA	1:H:68:ILE:O	2.19	0.41
1:I:156:LEU:HD11	1:J:139:PRO:HG3	2.02	0.41
1:A:153:VAL:O	1:A:157:LYS:HG3	2.21	0.41
1:A:198:LYS:O	1:A:199:ALA:C	2.58	0.41
1:E:68:ILE:HG13	1:E:96:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:HIS:HB2	1:M:46:CYS:SG	2.60	0.41
1:N:3:VAL:HG22	1:N:4:ILE:N	2.35	0.41
1:P:197:ALA:O	1:P:202:GLU:HB2	2.20	0.41
1:T:194:ARG:HA	1:T:194:ARG:HD3	1.95	0.41
1:B:56:ARG:O	1:B:59:GLU:HB2	2.20	0.41
1:F:203:ILE:HG21	1:F:211:CYS:HB3	2.02	0.41
1:F:59:GLU:HG2	1:F:150:LEU:CD1	2.49	0.41
1:S:153:VAL:O	1:S:157:LYS:HG2	2.20	0.41
1:T:170:TRP:HD1	3:T:458:HOH:O	2.04	0.41
1:F:70:LEU:HD13	1:F:70:LEU:C	2.41	0.41
1:I:138:TYR:CZ	1:J:152:LEU:HG	2.55	0.41
1:K:121:ARG:HB3	1:K:144:ARG:CZ	2.51	0.41
1:M:141:GLU:HG2	1:M:142:VAL:HG23	2.02	0.41
1:M:54:GLN:CA	1:M:57:VAL:HG23	2.48	0.41
1:A:51:TYR:CD1	1:A:91:VAL:HG21	2.55	0.41
1:G:49:GLU:OE1	1:G:121:ARG:NH2	2.53	0.41
1:H:111:MET:HE2	1:H:124:PHE:CE1	2.56	0.41
1:I:54:GLN:HA	1:I:57:VAL:CG2	2.44	0.41
1:M:125:VAL:HG11	1:M:156:LEU:HD23	2.03	0.41
1:N:74:GLN:NE2	1:O:40:ALA:HB2	2.36	0.41
1:T:3:VAL:CG1	1:T:4:ILE:N	2.84	0.41
1:A:36:PHE:HA	1:A:122:ALA:O	2.21	0.41
1:B:66:GLU:HA	1:B:67:PRO:HD3	1.96	0.41
1:E:153:VAL:O	1:E:157:LYS:HG3	2.21	0.41
1:E:203:ILE:HD13	1:E:204:GLU:N	2.36	0.41
1:F:190:GLU:HA	1:F:193:GLN:HG2	2.01	0.41
1:I:32:TRP:HB2	1:I:65:VAL:HG22	2.02	0.41
1:M:57:VAL:HG11	1:M:61:ARG:NH2	2.35	0.41
1:C:148:GLU:HG2	1:D:148:GLU:HG2	2.03	0.41
1:H:152:LEU:HD22	1:H:156:LEU:HD22	2.01	0.41
1:J:197:ALA:O	1:J:202:GLU:HB2	2.21	0.41
1:L:28:LYS:O	1:L:28:LYS:HD2	2.21	0.41
1:N:118:ILE:HG21	1:O:74:GLN:NE2	2.36	0.41
1:N:151:ARG:HD2	1:N:170:TRP:O	2.21	0.41
1:Q:122:ALA:HA	1:Q:136:VAL:O	2.21	0.41
1:C:153:VAL:O	1:C:157:LYS:HG3	2.21	0.41
1:J:38:HIS:CE1	1:J:71:SER:HB3	2.56	0.41
1:L:69:GLY:O	1:L:70:LEU:HB3	2.21	0.41
1:N:157:LYS:HE3	1:N:157:LYS:HB3	1.91	0.41
1:N:38:HIS:HB2	1:N:46:CYS:SG	2.61	0.41
1:R:184:PRO:HA	3:R:454:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:O	1:A:193:GLN:HG3	2.21	0.41
1:B:37:SER:HA	1:B:70:LEU:O	2.20	0.41
1:B:72:VAL:HG22	1:B:72:VAL:O	2.21	0.41
1:C:14:LYS:HE3	1:C:75:VAL:CG1	2.51	0.41
1:G:152:LEU:HG	1:H:138:TYR:CZ	2.56	0.41
1:I:168:HIS:CE1	1:I:169:LYS:HB2	2.56	0.41
1:L:197:ALA:C	1:L:201:GLY:HA3	2.40	0.41
1:M:121:ARG:HB3	1:M:144:ARG:CZ	2.51	0.41
1:N:32:TRP:CD2	1:N:127:ASP:HA	2.56	0.41
1:Q:151:ARG:HD2	1:Q:170:TRP:O	2.21	0.41
1:T:32:TRP:CE2	1:T:157:LYS:HE3	2.56	0.41
1:P:201:GLY:O	1:P:202:GLU:CB	2.68	0.40
1:S:158:ILE:HD13	1:S:215:LEU:HD11	2.02	0.40
1:T:44:PRO:HG2	2:T:301:FLC:OB1	2.21	0.40
1:I:45:VAL:HB	1:I:121:ARG:NH1	2.36	0.40
1:L:44:PRO:HG2	2:L:301:FLC:OB2	2.21	0.40
1:M:198:LYS:C	1:M:200:LYS:N	2.72	0.40
1:Q:57:VAL:HG12	3:Q:428:HOH:O	2.21	0.40
1:C:54:GLN:C	1:C:57:VAL:HG23	2.41	0.40
1:N:162:LYS:HG3	1:N:215:LEU:HD21	2.04	0.40
1:S:121:ARG:HB3	1:S:144:ARG:CZ	2.52	0.40
1:A:198:LYS:HD2	1:A:205:CYS:SG	2.61	0.40
1:B:34:ILE:HG23	1:B:67:PRO:HA	2.04	0.40
1:F:122:ALA:HA	1:F:136:VAL:O	2.22	0.40
1:F:51:TYR:CE2	1:F:91:VAL:HG21	2.57	0.40
1:M:181:ILE:HD13	1:N:44:PRO:HB2	2.03	0.40
1:M:181:ILE:HG21	1:N:44:PRO:HB2	2.02	0.40
1:N:92:GLU:HG3	3:N:428:HOH:O	2.22	0.40
1:T:203:ILE:HD11	1:T:213:LYS:HD3	2.03	0.40
1:A:139:PRO:HG3	1:B:156:LEU:HD11	2.04	0.40
1:A:38:HIS:HB2	1:A:46:CYS:SG	2.61	0.40
1:B:53:MET:O	1:B:57:VAL:HG23	2.21	0.40
1:C:198:LYS:HD3	1:C:205:CYS:SG	2.61	0.40
1:O:3:VAL:O	1:O:6:GLU:HB2	2.21	0.40
1:O:66:GLU:HA	1:O:67:PRO:HD3	1.88	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	212/216 (98%)	204 (96%)	7 (3%)	1 (0%)	29	29
1	B	212/216 (98%)	200 (94%)	10 (5%)	2 (1%)	17	14
1	C	212/216 (98%)	196 (92%)	16 (8%)	0	100	100
1	D	212/216 (98%)	197 (93%)	15 (7%)	0	100	100
1	E	212/216 (98%)	198 (93%)	13 (6%)	1 (0%)	29	29
1	F	212/216 (98%)	202 (95%)	8 (4%)	2 (1%)	17	14
1	G	212/216 (98%)	198 (93%)	13 (6%)	1 (0%)	29	29
1	H	212/216 (98%)	198 (93%)	13 (6%)	1 (0%)	29	29
1	I	212/216 (98%)	201 (95%)	11 (5%)	0	100	100
1	J	212/216 (98%)	196 (92%)	16 (8%)	0	100	100
1	K	212/216 (98%)	202 (95%)	7 (3%)	3 (1%)	11	7
1	L	212/216 (98%)	200 (94%)	12 (6%)	0	100	100
1	M	212/216 (98%)	199 (94%)	12 (6%)	1 (0%)	29	29
1	N	212/216 (98%)	196 (92%)	12 (6%)	4 (2%)	8	4
1	O	212/216 (98%)	200 (94%)	12 (6%)	0	100	100
1	P	212/216 (98%)	198 (93%)	11 (5%)	3 (1%)	11	7
1	Q	212/216 (98%)	205 (97%)	7 (3%)	0	100	100
1	R	212/216 (98%)	201 (95%)	11 (5%)	0	100	100
1	S	212/216 (98%)	204 (96%)	8 (4%)	0	100	100
1	T	212/216 (98%)	202 (95%)	9 (4%)	1 (0%)	29	29
All	All	4240/4320 (98%)	3997 (94%)	223 (5%)	20 (0%)	29	29

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	200	LYS

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Mol	Chain	Res	Type
1	A	199	ALA
1	B	3	VAL
1	B	199	ALA
1	E	199	ALA
1	F	201	GLY
1	N	201	GLY
1	P	200	LYS
1	P	202	GLU
1	T	201	GLY
1	N	199	ALA
1	G	199	ALA
1	K	101	ASP
1	N	101	ASP
1	P	199	ALA
1	K	201	GLY
1	K	202	GLU
1	N	44	PRO
1	H	201	GLY
1	F	44	PRO

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	187/189 (99%)	175 (94%)	12 (6%)	17	16
1	B	187/189 (99%)	180 (96%)	7 (4%)	34	40
1	C	187/189 (99%)	181 (97%)	6 (3%)	39	47
1	D	187/189 (99%)	185 (99%)	2 (1%)	73	82
1	E	187/189 (99%)	179 (96%)	8 (4%)	29	33
1	F	187/189 (99%)	179 (96%)	8 (4%)	29	33
1	G	187/189 (99%)	183 (98%)	4 (2%)	53	62
1	H	187/189 (99%)	180 (96%)	7 (4%)	34	40
1	I	187/189 (99%)	178 (95%)	9 (5%)	25	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	187/189 (99%)	182 (97%)	5 (3%)	44 54
1	K	187/189 (99%)	182 (97%)	5 (3%)	44 54
1	L	187/189 (99%)	177 (95%)	10 (5%)	22 23
1	M	187/189 (99%)	179 (96%)	8 (4%)	29 33
1	N	187/189 (99%)	180 (96%)	7 (4%)	34 40
1	O	187/189 (99%)	179 (96%)	8 (4%)	29 33
1	P	187/189 (99%)	181 (97%)	6 (3%)	39 47
1	Q	187/189 (99%)	183 (98%)	4 (2%)	53 62
1	R	187/189 (99%)	180 (96%)	7 (4%)	34 40
1	S	187/189 (99%)	180 (96%)	7 (4%)	34 40
1	T	187/189 (99%)	179 (96%)	8 (4%)	29 33
All	All	3740/3780 (99%)	3602 (96%)	138 (4%)	34 40

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	55	LYS
1	A	72	VAL
1	A	78	HIS
1	A	80	LYS
1	A	150	LEU
1	A	152	LEU
1	A	154	LYS
1	A	156	LEU
1	A	161	GLU
1	A	192	LYS
1	A	210	PHE
1	B	7	LYS
1	B	28	LYS
1	B	70	LEU
1	B	78	HIS
1	B	156	LEU
1	B	192	LYS
1	B	210	PHE
1	C	28	LYS
1	C	152	LEU
1	C	156	LEU

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Mol	Chain	Res	Type
1	C	193	GLN
1	C	210	PHE
1	C	214	LYS
1	D	152	LEU
1	D	210	PHE
1	E	24	ASP
1	E	71	SER
1	E	152	LEU
1	E	156	LEU
1	E	192	LYS
1	E	202	GLU
1	E	203	ILE
1	E	210	PHE
1	F	24	ASP
1	F	28	LYS
1	F	70	LEU
1	F	80	LYS
1	F	152	LEU
1	F	156	LEU
1	F	210	PHE
1	F	214	LYS
1	G	59	GLU
1	G	152	LEU
1	G	202	GLU
1	G	210	PHE
1	H	24	ASP
1	H	70	LEU
1	H	150	LEU
1	H	152	LEU
1	H	156	LEU
1	H	200	LYS
1	H	210	PHE
1	I	14	LYS
1	I	28	LYS
1	I	59	GLU
1	I	70	LEU
1	I	152	LEU
1	I	156	LEU
1	I	189	GLU
1	I	192	LYS
1	I	210	PHE
1	J	28	LYS

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Mol	Chain	Res	Type
1	J	70	LEU
1	J	150	LEU
1	J	152	LEU
1	J	210	PHE
1	K	24	ASP
1	K	152	LEU
1	K	156	LEU
1	K	192	LYS
1	K	210	PHE
1	L	28	LYS
1	L	70	LEU
1	L	91	VAL
1	L	108	LYS
1	L	150	LEU
1	L	152	LEU
1	L	156	LEU
1	L	192	LYS
1	L	200	LYS
1	L	210	PHE
1	M	22	LEU
1	M	24	ASP
1	M	55	LYS
1	M	70	LEU
1	M	152	LEU
1	M	156	LEU
1	M	210	PHE
1	M	215	LEU
1	N	24	ASP
1	N	150	LEU
1	N	152	LEU
1	N	156	LEU
1	N	189	GLU
1	N	210	PHE
1	N	215	LEU
1	O	24	ASP
1	O	152	LEU
1	O	156	LEU
1	O	192	LYS
1	O	193	GLN
1	O	200	LYS
1	O	210	PHE
1	O	215	LEU

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Mol	Chain	Res	Type
1	P	24	ASP
1	P	86	LYS
1	P	150	LEU
1	P	152	LEU
1	P	156	LEU
1	P	210	PHE
1	Q	72	VAL
1	Q	150	LEU
1	Q	152	LEU
1	Q	210	PHE
1	R	22	LEU
1	R	24	ASP
1	R	152	LEU
1	R	156	LEU
1	R	200	LYS
1	R	210	PHE
1	R	215	LEU
1	S	14	LYS
1	S	62	LYS
1	S	80	LYS
1	S	152	LEU
1	S	156	LEU
1	S	210	PHE
1	S	215	LEU
1	T	24	ASP
1	T	55	LYS
1	T	59	GLU
1	T	80	LYS
1	T	152	LEU
1	T	192	LYS
1	T	210	PHE
1	T	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	193	GLN
1	B	74	GLN
1	B	88	ASN
1	B	172	ASN
1	C	29	GLN

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Mol	Chain	Res	Type
1	C	74	GLN
1	C	88	ASN
1	C	193	GLN
1	D	74	GLN
1	E	74	GLN
1	G	74	GLN
1	G	193	GLN
1	H	74	GLN
1	H	88	ASN
1	I	74	GLN
1	I	193	GLN
1	J	74	GLN
1	K	54	GLN
1	K	74	GLN
1	K	193	GLN
1	M	74	GLN
1	M	88	ASN
1	N	74	GLN
1	O	74	GLN
1	P	74	GLN
1	T	74	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	FLC	B	301	-	3,12,12	0.99	0	3,17,17	1.31	0
2	FLC	G	301	-	3,12,12	2.94	1 (33%)	3,17,17	2.62	2 (66%)
2	FLC	D	301	-	3,12,12	0.71	0	3,17,17	1.53	0
2	FLC	A	301	-	3,12,12	0.94	0	3,17,17	1.18	0
2	FLC	F	301	-	3,12,12	0.71	0	3,17,17	1.40	0
2	FLC	S	301	-	3,12,12	1.08	0	3,17,17	1.02	0
2	FLC	P	301	-	3,12,12	2.98	1 (33%)	3,17,17	2.85	2 (66%)
2	FLC	M	301	-	3,12,12	1.40	0	3,17,17	0.95	0
2	FLC	R	301	-	3,12,12	3.00	1 (33%)	3,17,17	2.74	2 (66%)
2	FLC	T	301	-	3,12,12	1.59	1 (33%)	3,17,17	1.09	0
2	FLC	Q	301	-	3,12,12	1.26	0	3,17,17	0.72	0
2	FLC	K	301	-	3,12,12	0.95	0	3,17,17	1.56	1 (33%)
2	FLC	H	301	-	3,12,12	1.38	0	3,17,17	0.92	0
2	FLC	E	301	-	3,12,12	0.86	0	3,17,17	1.32	0
2	FLC	J	301	-	3,12,12	1.58	0	3,17,17	0.69	0
2	FLC	O	301	-	3,12,12	0.79	0	3,17,17	1.27	0
2	FLC	L	301	-	3,12,12	0.72	0	3,17,17	1.33	0
2	FLC	I	301	-	3,12,12	3.02	1 (33%)	3,17,17	2.65	2 (66%)
2	FLC	N	301	-	3,12,12	0.81	0	3,17,17	1.45	1 (33%)
2	FLC	C	301	-	3,12,12	0.81	0	3,17,17	1.47	1 (33%)

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
2	FLC	B	301	-	-	3/6/16/16	-
2	FLC	G	301	-	-	4/6/16/16	-
2	FLC	D	301	-	-	4/6/16/16	-
2	FLC	A	301	-	-	3/6/16/16	-
2	FLC	F	301	-	-	4/6/16/16	-
2	FLC	S	301	-	-	3/6/16/16	-
2	FLC	P	301	-	-	4/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	M	301	-	-	6/6/16/16	-
2	FLC	R	301	-	-	4/6/16/16	-
2	FLC	T	301	-	-	3/6/16/16	-
2	FLC	Q	301	-	-	4/6/16/16	-
2	FLC	K	301	-	-	3/6/16/16	-
2	FLC	H	301	-	-	6/6/16/16	-
2	FLC	E	301	-	-	3/6/16/16	-
2	FLC	J	301	-	-	6/6/16/16	-
2	FLC	O	301	-	-	3/6/16/16	-
2	FLC	L	301	-	-	4/6/16/16	-
2	FLC	I	301	-	-	4/6/16/16	-
2	FLC	N	301	-	-	6/6/16/16	-
2	FLC	C	301	-	-	4/6/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	301	FLC	CG-CB	5.04	1.62	1.54
2	P	301	FLC	CG-CB	4.99	1.61	1.54
2	I	301	FLC	CG-CB	4.95	1.61	1.54
2	G	301	FLC	CG-CB	4.94	1.61	1.54
2	T	301	FLC	CG-CB	2.39	1.58	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	301	FLC	CG-CB-CA	3.67	119.14	109.33
2	P	301	FLC	CG-CB-CA	3.63	119.03	109.33
2	P	301	FLC	CB-CG-CGC	3.35	120.35	114.98
2	G	301	FLC	CG-CB-CA	3.31	118.17	109.33
2	I	301	FLC	CG-CB-CA	3.25	118.02	109.33
2	I	301	FLC	CB-CG-CGC	3.22	120.14	114.98
2	G	301	FLC	CB-CG-CGC	2.98	119.75	114.98
2	R	301	FLC	CB-CG-CGC	2.95	119.70	114.98
2	K	301	FLC	CB-CG-CGC	-2.09	111.63	114.98
2	N	301	FLC	CB-CA-CAC	-2.08	111.66	114.98
2	C	301	FLC	CB-CG-CGC	-2.04	111.72	114.98

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FLC	CAC-CA-CB-CBC
2	G	301	FLC	CAC-CA-CB-CG
2	G	301	FLC	CA-CB-CG-CGC
2	D	301	FLC	CAC-CA-CB-CBC
2	A	301	FLC	CAC-CA-CB-CBC
2	A	301	FLC	CAC-CA-CB-CG
2	A	301	FLC	CAC-CA-CB-OHB
2	F	301	FLC	CAC-CA-CB-CBC
2	S	301	FLC	CAC-CA-CB-CBC
2	S	301	FLC	CAC-CA-CB-CG
2	S	301	FLC	CAC-CA-CB-OHB
2	P	301	FLC	CAC-CA-CB-CG
2	P	301	FLC	CA-CB-CG-CGC
2	R	301	FLC	CAC-CA-CB-CG
2	R	301	FLC	OHB-CB-CG-CGC
2	Q	301	FLC	CAC-CA-CB-CG
2	K	301	FLC	CAC-CA-CB-CBC
2	H	301	FLC	CAC-CA-CB-CBC
2	H	301	FLC	CAC-CA-CB-CG
2	E	301	FLC	CAC-CA-CB-CBC
2	O	301	FLC	CAC-CA-CB-CBC
2	L	301	FLC	CAC-CA-CB-CBC
2	L	301	FLC	CAC-CA-CB-OHB
2	I	301	FLC	CAC-CA-CB-CG
2	I	301	FLC	CA-CB-CG-CGC
2	N	301	FLC	CAC-CA-CB-CBC
2	N	301	FLC	CAC-CA-CB-CG
2	N	301	FLC	CAC-CA-CB-OHB
2	C	301	FLC	CAC-CA-CB-CBC
2	G	301	FLC	CAC-CA-CB-OHB
2	P	301	FLC	CAC-CA-CB-OHB
2	R	301	FLC	CAC-CA-CB-OHB
2	R	301	FLC	CA-CB-CG-CGC
2	K	301	FLC	CAC-CA-CB-OHB
2	N	301	FLC	CA-CB-CG-CGC
2	C	301	FLC	CAC-CA-CB-OHB
2	B	301	FLC	CAC-CA-CB-OHB
2	G	301	FLC	OHB-CB-CG-CGC
2	D	301	FLC	CAC-CA-CB-OHB
2	F	301	FLC	CAC-CA-CB-OHB
2	M	301	FLC	CAC-CA-CB-CG
2	H	301	FLC	CAC-CA-CB-OHB

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Mol	Chain	Res	Type	Atoms
2	H	301	FLC	CA-CB-CG-CGC
2	H	301	FLC	OHB-CB-CG-CGC
2	E	301	FLC	CAC-CA-CB-OHB
2	J	301	FLC	CAC-CA-CB-CG
2	J	301	FLC	CA-CB-CG-CGC
2	J	301	FLC	OHB-CB-CG-CGC
2	L	301	FLC	CAC-CA-CB-CG
2	B	301	FLC	CAC-CA-CB-CG
2	F	301	FLC	CAC-CA-CB-CG
2	P	301	FLC	OHB-CB-CG-CGC
2	M	301	FLC	CA-CB-CG-CGC
2	M	301	FLC	OHB-CB-CG-CGC
2	T	301	FLC	CA-CB-CG-CGC
2	T	301	FLC	OHB-CB-CG-CGC
2	K	301	FLC	CAC-CA-CB-CG
2	E	301	FLC	CAC-CA-CB-CG
2	C	301	FLC	CAC-CA-CB-CG
2	D	301	FLC	CAC-CA-CB-CG
2	Q	301	FLC	CAC-CA-CB-OHB
2	O	301	FLC	CAC-CA-CB-CG
2	O	301	FLC	CAC-CA-CB-OHB
2	I	301	FLC	OHB-CB-CG-CGC
2	M	301	FLC	CAC-CA-CB-CBC
2	M	301	FLC	CBC-CB-CG-CGC
2	T	301	FLC	CBC-CB-CG-CGC
2	Q	301	FLC	CAC-CA-CB-CBC
2	H	301	FLC	CBC-CB-CG-CGC
2	J	301	FLC	CAC-CA-CB-CBC
2	J	301	FLC	CBC-CB-CG-CGC
2	I	301	FLC	CAC-CA-CB-CBC
2	N	301	FLC	CBC-CB-CG-CGC
2	F	301	FLC	CA-CB-CG-CGC
2	M	301	FLC	CAC-CA-CB-OHB
2	Q	301	FLC	CA-CB-CG-CGC
2	N	301	FLC	OHB-CB-CG-CGC
2	J	301	FLC	CAC-CA-CB-OHB
2	L	301	FLC	CA-CB-CG-CGC
2	C	301	FLC	CA-CB-CG-CGC
2	D	301	FLC	CA-CB-CG-CGC

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FLC	1	0
2	F	301	FLC	1	0
2	M	301	FLC	1	0
2	R	301	FLC	2	0
2	T	301	FLC	1	0
2	Q	301	FLC	1	0
2	K	301	FLC	1	0
2	E	301	FLC	1	0
2	J	301	FLC	1	0
2	L	301	FLC	1	0
2	I	301	FLC	1	0
2	N	301	FLC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	214/216 (99%)	-0.11	3 (1%)	75	77	15, 25, 44, 70	0
1	B	214/216 (99%)	-0.25	4 (1%)	66	69	16, 25, 46, 69	0
1	C	214/216 (99%)	-0.30	2 (0%)	84	85	17, 25, 45, 68	0
1	D	214/216 (99%)	-0.33	2 (0%)	84	85	14, 25, 41, 66	0
1	E	214/216 (99%)	-0.30	6 (2%)	53	55	14, 24, 42, 66	0
1	F	214/216 (99%)	-0.36	4 (1%)	66	69	14, 24, 47, 59	0
1	G	214/216 (99%)	-0.34	4 (1%)	66	69	13, 22, 46, 71	0
1	H	214/216 (99%)	-0.26	7 (3%)	46	48	13, 24, 42, 61	0
1	I	214/216 (99%)	-0.31	1 (0%)	91	91	14, 25, 40, 46	0
1	J	214/216 (99%)	-0.28	5 (2%)	60	63	16, 26, 45, 71	0
1	K	214/216 (99%)	-0.28	3 (1%)	75	77	16, 25, 42, 62	0
1	L	214/216 (99%)	-0.31	4 (1%)	66	69	12, 24, 45, 74	0
1	M	214/216 (99%)	-0.45	0	100	100	13, 21, 39, 57	0
1	N	214/216 (99%)	-0.47	4 (1%)	66	69	11, 20, 40, 71	0
1	O	214/216 (99%)	-0.43	2 (0%)	84	85	10, 20, 37, 53	0
1	P	214/216 (99%)	-0.45	4 (1%)	66	69	11, 20, 37, 62	0
1	Q	214/216 (99%)	-0.43	1 (0%)	91	91	11, 20, 36, 50	0
1	R	214/216 (99%)	-0.42	4 (1%)	66	69	11, 21, 40, 59	0
1	S	214/216 (99%)	-0.38	2 (0%)	84	85	11, 21, 41, 55	0
1	T	214/216 (99%)	-0.39	1 (0%)	91	91	14, 22, 36, 53	0
All	All	4280/4320 (99%)	-0.34	63 (1%)	73	75	10, 23, 42, 74	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	199	ALA	6.2
1	K	200	LYS	6.0
1	G	200	LYS	5.7
1	N	200	LYS	5.2
1	E	200	LYS	4.9
1	A	202	GLU	4.9
1	L	200	LYS	4.7
1	D	203	ILE	4.6
1	P	200	LYS	4.6
1	E	202	GLU	4.4
1	L	201	GLY	4.3
1	B	200	LYS	4.3
1	J	199	ALA	4.0
1	G	202	GLU	4.0
1	C	202	GLU	3.8
1	F	215	LEU	3.8
1	K	201	GLY	3.7
1	A	200	LYS	3.6
1	B	199	ALA	3.5
1	F	203	ILE	3.4
1	B	202	GLU	3.2
1	H	197	ALA	3.1
1	E	196	GLU	3.1
1	H	202	GLU	3.0
1	P	202	GLU	3.0
1	J	200	LYS	2.9
1	Q	200	LYS	2.8
1	H	200	LYS	2.8
1	T	200	LYS	2.7
1	L	199	ALA	2.7
1	C	200	LYS	2.7
1	A	199	ALA	2.6
1	F	200	LYS	2.6
1	N	199	ALA	2.6
1	L	202	GLU	2.6
1	N	201	GLY	2.5
1	R	200	LYS	2.5
1	E	201	GLY	2.5
1	B	193	GLN	2.5
1	S	197	ALA	2.5
1	E	197	ALA	2.4
1	S	202	GLU	2.4
1	H	201	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	203	ILE	2.4
1	H	199	ALA	2.4
1	F	202	GLU	2.3
1	P	196	GLU	2.3
1	H	193	GLN	2.3
1	R	197	ALA	2.3
1	D	200	LYS	2.3
1	J	202	GLU	2.3
1	R	203	ILE	2.3
1	K	202	GLU	2.2
1	H	203	ILE	2.1
1	R	202	GLU	2.1
1	O	200	LYS	2.1
1	I	215	LEU	2.1
1	J	192	LYS	2.1
1	P	201	GLY	2.1
1	G	193	GLN	2.0
1	J	203	ILE	2.0
1	N	202	GLU	2.0
1	O	196	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. 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	B-factors(Å^2)	Q<0.9
2	FLC	Q	301	13/13	0.77	0.24	53,59,62,63	0
2	FLC	K	301	13/13	0.78	0.23	38,43,46,48	0
2	FLC	I	301	13/13	0.78	0.19	56,57,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FLC	A	301	13/13	0.80	0.22	61,64,65,65	0
2	FLC	R	301	13/13	0.83	0.20	37,44,47,48	0
2	FLC	D	301	13/13	0.83	0.20	49,52,57,57	0
2	FLC	G	301	13/13	0.85	0.18	29,41,48,48	0
2	FLC	N	301	13/13	0.85	0.22	38,42,48,49	0
2	FLC	S	301	13/13	0.86	0.20	52,57,58,58	0
2	FLC	T	301	13/13	0.86	0.19	44,49,51,52	0
2	FLC	F	301	13/13	0.88	0.18	44,47,49,49	0
2	FLC	B	301	13/13	0.88	0.18	42,46,48,49	0
2	FLC	E	301	13/13	0.89	0.18	44,49,51,51	0
2	FLC	P	301	13/13	0.89	0.16	35,41,48,49	0
2	FLC	M	301	13/13	0.89	0.19	43,46,51,51	0
2	FLC	C	301	13/13	0.89	0.19	46,48,52,53	0
2	FLC	H	301	13/13	0.90	0.18	42,48,50,50	0
2	FLC	J	301	13/13	0.91	0.15	38,42,45,46	0
2	FLC	O	301	13/13	0.91	0.19	40,44,47,48	0
2	FLC	L	301	13/13	0.91	0.18	43,46,48,49	0

6.5 Other polymers

There are no such residues in this entry.