wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:48 AM GMT

PDB ID	:	3PVO
Title	:	Monoclinic form of Human C-Reactive Protein
Authors	:	Guillon, C.; Mavoungou Bigouagou, U.; Jeannin, P.; Delneste, Y.; Gouet, P.
Deposited on	:	2010-12-07
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

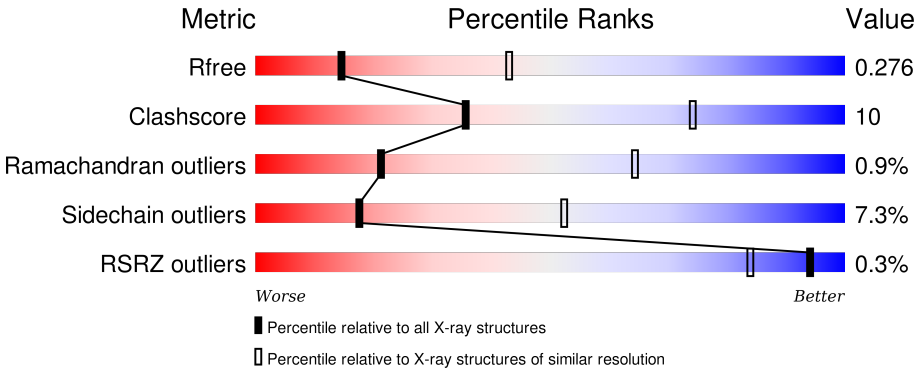
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	206	% 76% 19% 5%
1	B	206	67% 27%
1	C	206	76% 20%
1	D	206	77% 20%
1	E	206	73% 25%

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Mol	Chain	Length	Quality of chain
1	F	206	76% 23%
1	G	206	73% 24%
1	H	206	74% 19% 7%
1	I	206	80% 18%
1	J	206	74% 22%
1	K	206	69% 24% 6%
1	L	206	68% 26% 5%
1	M	206	71% 22% 5%
1	N	206	70% 27%
1	O	206	78% 18%
1	P	206	% 74% 21%
1	Q	206	69% 25% 5%
1	R	206	% 73% 20% 7%
1	S	206	76% 21%
1	T	206	% 78% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	5002	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33077 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 C-Reactive Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	B	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	C	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	D	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	E	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	F	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	G	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	H	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	I	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	J	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	K	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	L	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	M	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	N	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	O	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	P	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	R	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	S	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	T	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total	Ca	0	0
			2	2		
2	G	2	Total	Ca	0	0
			2	2		
2	J	2	Total	Ca	0	0
			2	2		
2	Q	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	K	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		
2	H	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	I	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	T	2	Total	Ca	0	0
			2	2		
2	N	2	Total	Ca	0	0
			2	2		
2	O	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	2	Total Ca 2 2	0	0
2	L	2	Total Ca 2 2	0	0
2	S	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0
2	M	2	Total Ca 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	12	Total O 12 12	0	0
3	B	20	Total O 20 20	0	0
3	C	20	Total O 20 20	0	0
3	D	14	Total O 14 14	0	0
3	E	10	Total O 10 10	0	0
3	F	20	Total O 20 20	0	0
3	G	15	Total O 15 15	0	0
3	H	16	Total O 16 16	0	0
3	I	14	Total O 14 14	0	0
3	J	30	Total O 30 30	0	0
3	K	24	Total O 24 24	0	0
3	L	24	Total O 24 24	0	0
3	M	19	Total O 19 19	0	0
3	N	19	Total O 19 19	0	0

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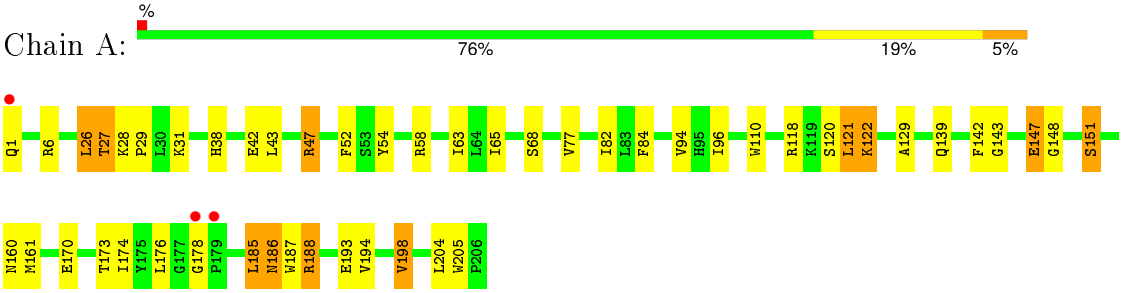
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	25	Total O 25 25	0	0
3	P	19	Total O 19 19	0	0
3	Q	28	Total O 28 28	0	0
3	R	30	Total O 30 30	0	0
3	S	21	Total O 21 21	0	0
3	T	17	Total O 17 17	0	0

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.

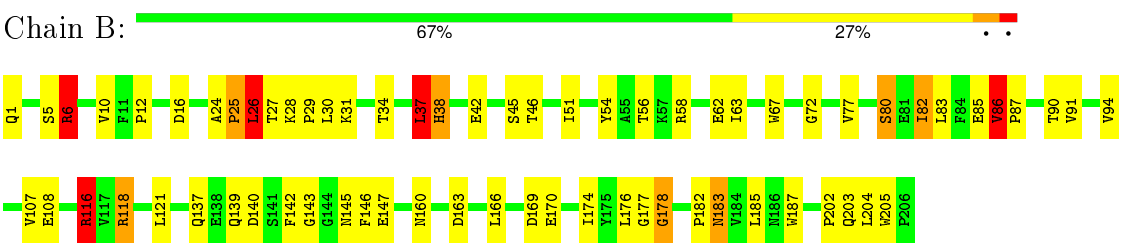
- Molecule 1: C-Reactive Protein

Chain A:



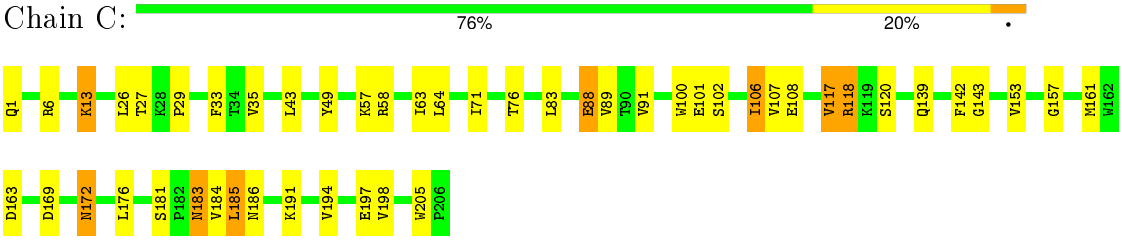
- Molecule 1: C-Reactive Protein

Chain B:



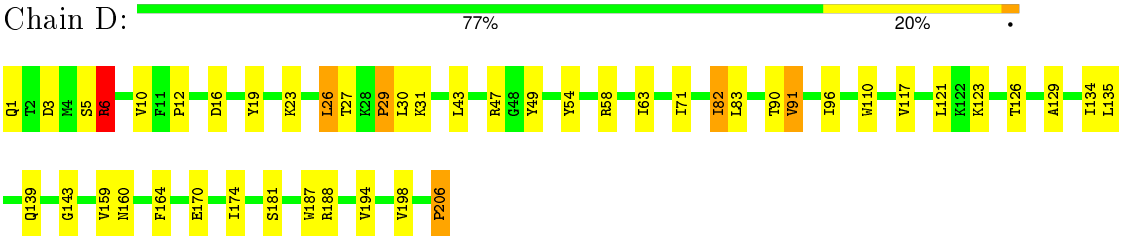
- Molecule 1: C-Reactive Protein

Chain C:



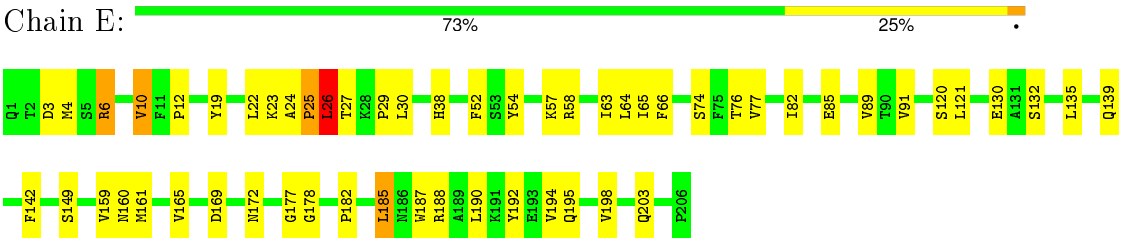
- Molecule 1: C-Reactive Protein

Chain D:



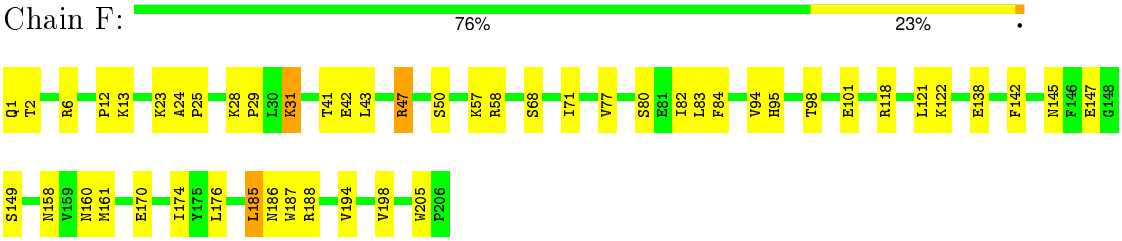
- Molecule 1: C-Reactive Protein

Chain E:



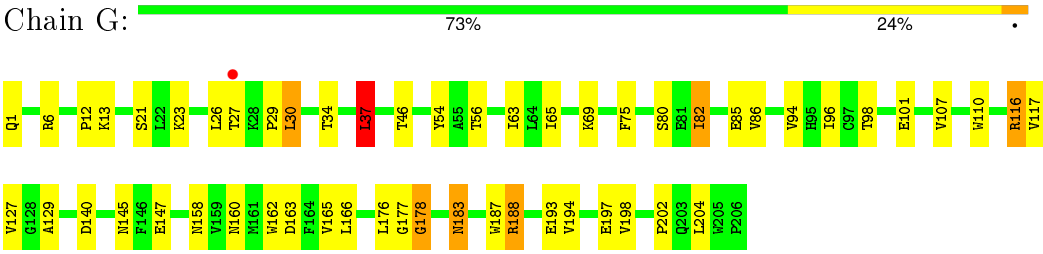
- Molecule 1: C-Reactive Protein

Chain F:



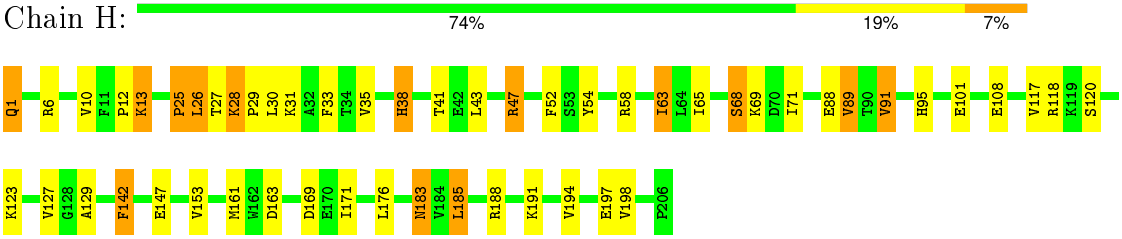
- Molecule 1: C-Reactive Protein

Chain G:



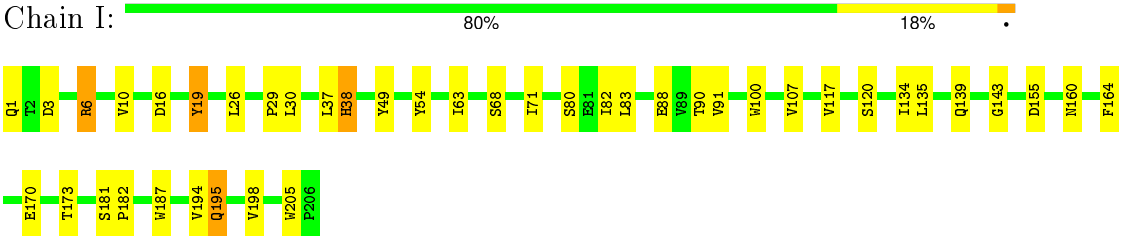
- Molecule 1: C-Reactive Protein

Chain H:



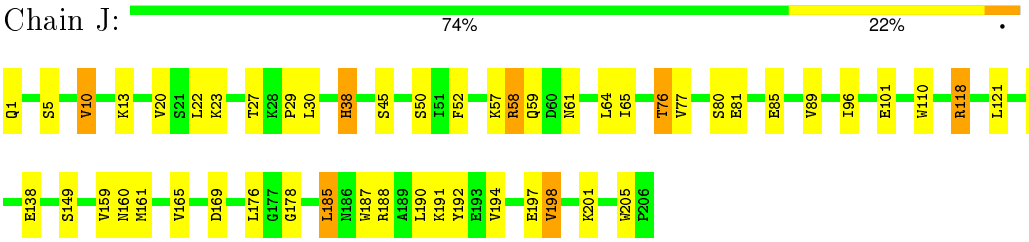
- Molecule 1: C-Reactive Protein

Chain I:



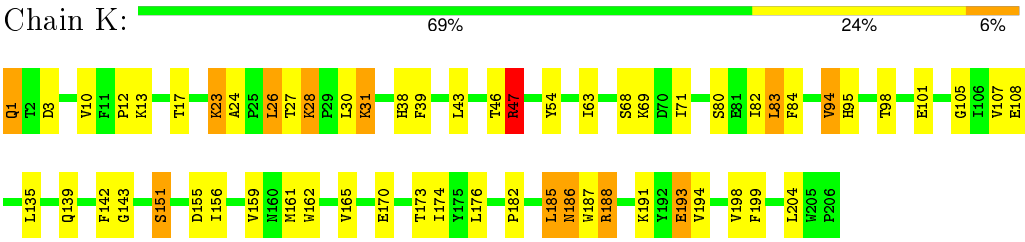
- Molecule 1: C-Reactive Protein

Chain J:



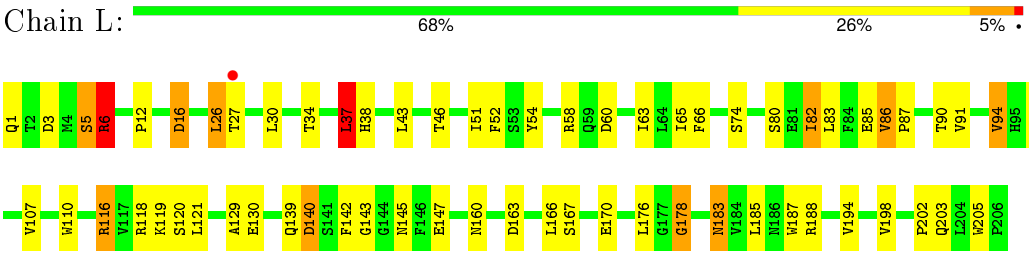
• Molecule 1: C-Reactive Protein

Chain K:



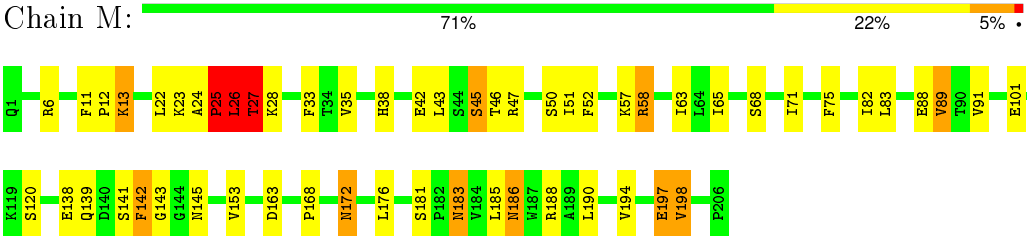
• Molecule 1: C-Reactive Protein

Chain L:



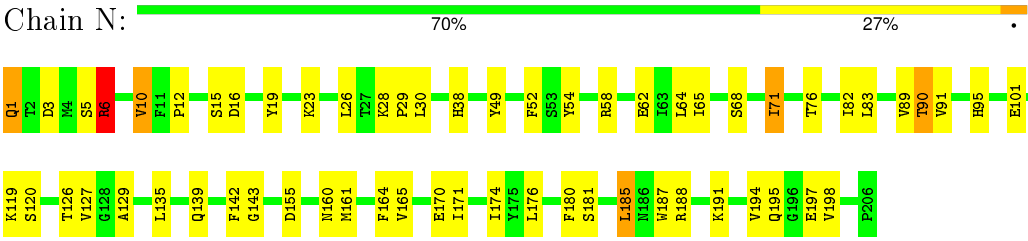
• Molecule 1: C-Reactive Protein

Chain M:



• Molecule 1: C-Reactive Protein

Chain N:

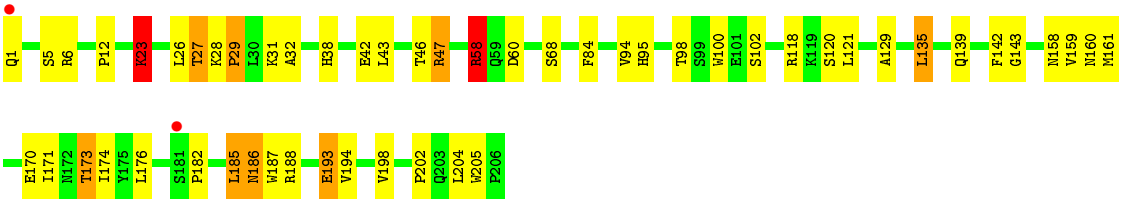


• Molecule 1: C-Reactive Protein

Chain O:

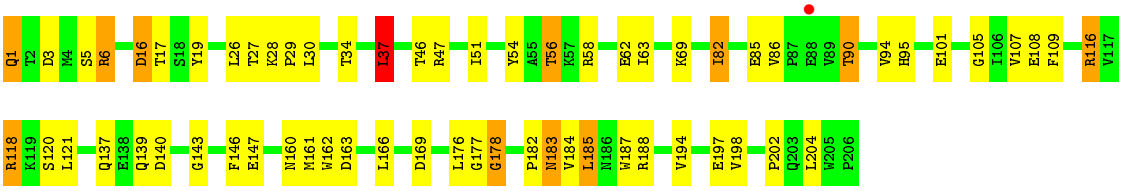
• Molecule 1: C-Reactive Protein

Chain P:



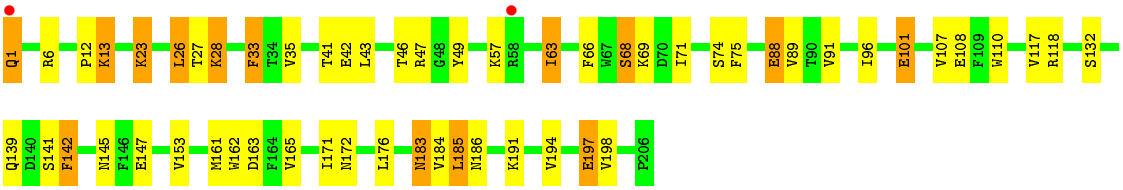
• Molecule 1: C-Reactive Protein

Chain Q:



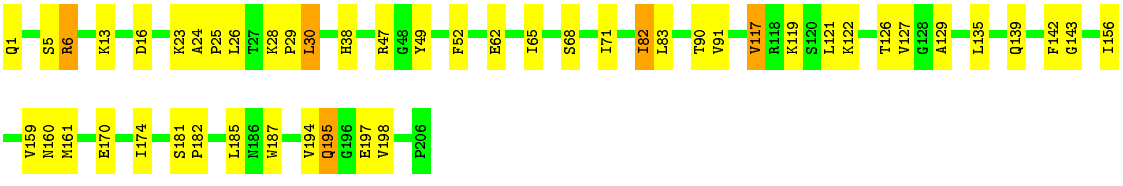
• Molecule 1: C-Reactive Protein

Chain R:



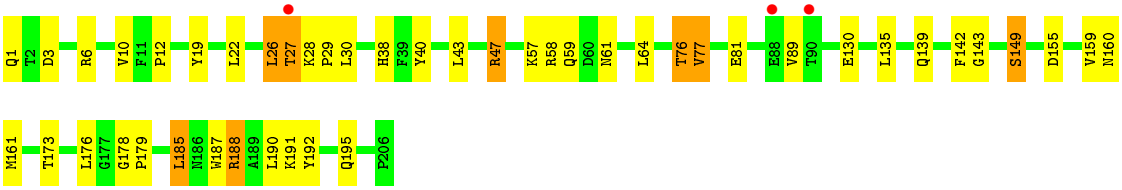
• Molecule 1: C-Reactive Protein

Chain S:



• Molecule 1: C-Reactive Protein

Chain T:


Q1
T2
D3
R6
V10
F11
P12
Y19
L22
L26
T27
K28
P29
L30
H38
F39
Y40
L43
R47
K57
R58
Q59
D60
N61
L64
T76
V77
E81
E88
V89
T90
E130
L135
Q139
F142
G143
S149
D155
V159
N160
M161
T173
L176
G177
G178
P179
L185
N186
W187
R188
A189
L190
K191
Y192
Q195
P206

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.60Å 143.20Å 161.20Å 90.00° 89.70° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.00-3.00) 97.8 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.285 0.222 , 0.276	Depositor DCC
R_{free} test set	4380 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 11.9	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 86415 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	33077	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.99	8/1678 (0.5%)	0.91	7/2279 (0.3%)
1	B	1.03	7/1678 (0.4%)	1.06	14/2279 (0.6%)
1	C	1.13	22/1678 (1.3%)	0.96	7/2279 (0.3%)
1	D	1.07	13/1678 (0.8%)	0.95	9/2279 (0.4%)
1	E	0.95	9/1678 (0.5%)	0.88	5/2279 (0.2%)
1	F	0.94	6/1678 (0.4%)	0.91	7/2279 (0.3%)
1	G	0.99	3/1678 (0.2%)	1.00	9/2279 (0.4%)
1	H	1.10	13/1678 (0.8%)	0.97	8/2279 (0.4%)
1	I	1.06	17/1678 (1.0%)	0.94	10/2279 (0.4%)
1	J	0.99	9/1678 (0.5%)	0.87	6/2279 (0.3%)
1	K	0.95	8/1678 (0.5%)	0.90	4/2279 (0.2%)
1	L	1.02	8/1678 (0.5%)	1.07	15/2279 (0.7%)
1	M	1.13	18/1678 (1.1%)	0.98	10/2279 (0.4%)
1	N	1.07	14/1678 (0.8%)	0.92	6/2279 (0.3%)
1	O	0.97	7/1678 (0.4%)	0.86	3/2279 (0.1%)
1	P	0.94	6/1678 (0.4%)	0.87	5/2279 (0.2%)
1	Q	1.04	8/1678 (0.5%)	1.05	16/2279 (0.7%)
1	R	1.13	20/1678 (1.2%)	0.96	8/2279 (0.4%)
1	S	0.99	7/1678 (0.4%)	0.95	10/2279 (0.4%)
1	T	0.96	7/1678 (0.4%)	0.86	3/2279 (0.1%)
All	All	1.02	210/33560 (0.6%)	0.95	162/45580 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	M	0	1
1	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

The worst 5 of 210 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	23	LYS	C-N	10.72	1.58	1.34
1	M	35	VAL	CB-CG2	-8.90	1.34	1.52
1	R	198	VAL	CB-CG2	-8.09	1.35	1.52
1	M	35	VAL	CB-CG1	-7.71	1.36	1.52
1	N	117	VAL	CB-CG1	-7.68	1.36	1.52

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	116	ARG	NE-CZ-NH2	13.32	126.96	120.30
1	Q	116	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	B	116	ARG	NE-CZ-NH2	11.83	126.22	120.30
1	G	116	ARG	NE-CZ-NH1	-11.70	114.45	120.30
1	L	116	ARG	NE-CZ-NH2	11.57	126.09	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	26	LEU	Peptide
1	M	26	LEU	Peptide
1	R	23	LYS	Mainchain

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	1632	0	1593	27	0
1	B	1632	0	1593	52	0
1	C	1632	0	1593	23	1
1	D	1632	0	1592	24	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1632	0	1593	30	0
1	F	1632	0	1592	22	1
1	G	1632	0	1593	38	0
1	H	1632	0	1593	44	1
1	I	1632	0	1593	17	3
1	J	1632	0	1593	31	1
1	K	1632	0	1593	43	0
1	L	1632	0	1593	47	1
1	M	1632	0	1593	46	0
1	N	1632	0	1593	39	5
1	O	1632	0	1593	27	0
1	P	1632	0	1593	29	1
1	Q	1632	0	1593	41	0
1	R	1632	0	1593	30	0
1	S	1632	0	1593	33	0
1	T	1632	0	1593	25	3
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
3	A	12	0	0	2	0
3	B	20	0	0	8	0
3	C	20	0	0	0	0
3	D	14	0	0	5	0
3	E	10	0	0	6	0
3	F	20	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	15	0	0	6	0
3	H	16	0	0	8	0
3	I	14	0	0	1	0
3	J	30	0	0	4	0
3	K	24	0	0	5	0
3	L	24	0	0	8	0
3	M	19	0	0	8	0
3	N	19	0	0	10	0
3	O	25	0	0	6	0
3	P	19	0	0	5	0
3	Q	28	0	0	3	0
3	R	30	0	0	3	0
3	S	21	0	0	7	0
3	T	17	0	0	2	0
All	All	33077	0	31858	624	11

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 10.

The worst 5 of 624 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:D:31:LYS:HB2	3:D:208:HOH:O	1.30	1.24
1:S:30:LEU:N	1:S:30:LEU:HD12	1.57	1.18
1:J:58:ARG:HG2	1:J:58:ARG:HH11	1.07	1.15
1:F:13:LYS:HE2	3:F:221:HOH:O	1.47	1.11
1:L:130:GLU:HB3	3:L:392:HOH:O	1.49	1.09

The worst 5 of 11 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:N:58:ARG:NH1	1:T:143:GLY:CA[2_656]	1.49	0.71
1:D:123:LYS:NZ	1:I:195:GLN:OE1[2_645]	1.55	0.65
1:D:6:ARG:CD	1:N:188:ARG:NH2[2_646]	1.83	0.37
1:F:145:ASN:ND2	1:L:147:GLU:OE2[2_546]	1.98	0.22
1:D:123:LYS:CE	1:I:195:GLN:OE1[2_645]	2.06	0.14

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	204/206 (99%)	192 (94%)	10 (5%)	2 (1%)	19	61
1	B	204/206 (99%)	191 (94%)	8 (4%)	5 (2%)	7	34
1	C	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	19	61
1	D	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
1	E	204/206 (99%)	191 (94%)	9 (4%)	4 (2%)	9	41
1	F	204/206 (99%)	197 (97%)	6 (3%)	1 (0%)	34	76
1	G	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
1	H	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	61
1	I	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
1	J	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
1	K	204/206 (99%)	192 (94%)	10 (5%)	2 (1%)	19	61
1	L	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	61
1	M	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	19	61
1	N	204/206 (99%)	196 (96%)	7 (3%)	1 (0%)	34	76
1	O	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
1	P	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	13	50
1	Q	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	34	76
1	R	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	19	61
1	S	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
1	T	204/206 (99%)	192 (94%)	9 (4%)	3 (2%)	13	50
All	All	4080/4120 (99%)	3851 (94%)	194 (5%)	35 (1%)	21	64

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	GLY

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Mol	Chain	Res	Type
1	E	26	LEU
1	G	178	GLY
1	L	178	GLY
1	Q	178	GLY

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	180/180 (100%)	166 (92%)	14 (8%)	16 49
1	B	180/180 (100%)	163 (91%)	17 (9%)	11 39
1	C	180/180 (100%)	169 (94%)	11 (6%)	23 61
1	D	180/180 (100%)	173 (96%)	7 (4%)	39 77
1	E	180/180 (100%)	173 (96%)	7 (4%)	39 77
1	F	180/180 (100%)	168 (93%)	12 (7%)	20 57
1	G	180/180 (100%)	170 (94%)	10 (6%)	26 65
1	H	180/180 (100%)	165 (92%)	15 (8%)	14 46
1	I	180/180 (100%)	168 (93%)	12 (7%)	20 57
1	J	180/180 (100%)	170 (94%)	10 (6%)	26 65
1	K	180/180 (100%)	161 (89%)	19 (11%)	8 31
1	L	180/180 (100%)	162 (90%)	18 (10%)	9 34
1	M	180/180 (100%)	162 (90%)	18 (10%)	9 34
1	N	180/180 (100%)	165 (92%)	15 (8%)	14 46
1	O	180/180 (100%)	168 (93%)	12 (7%)	20 57
1	P	180/180 (100%)	164 (91%)	16 (9%)	12 42
1	Q	180/180 (100%)	166 (92%)	14 (8%)	16 49
1	R	180/180 (100%)	165 (92%)	15 (8%)	14 46
1	S	180/180 (100%)	172 (96%)	8 (4%)	35 74
1	T	180/180 (100%)	168 (93%)	12 (7%)	20 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3600/3600 (100%)	3338 (93%)	262 (7%)	17 52

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	28	LYS
1	L	87	PRO
1	S	1	GLN
1	K	47	ARG
1	K	186	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	139	GLN
1	L	38	HIS
1	R	186	ASN
1	I	160	ASN
1	K	38	HIS

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 40 ligands modelled in this entry, 40 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	206/206 (100%)	-0.36	3 (1%) 76 49	6, 16, 27, 32	0
1	B	206/206 (100%)	-0.48	0 100 100	4, 14, 25, 31	0
1	C	206/206 (100%)	-0.52	0 100 100	4, 13, 22, 34	0
1	D	206/206 (100%)	-0.40	0 100 100	4, 16, 28, 33	0
1	E	206/206 (100%)	-0.38	0 100 100	7, 17, 28, 33	0
1	F	206/206 (100%)	-0.38	0 100 100	5, 16, 28, 34	0
1	G	206/206 (100%)	-0.36	1 (0%) 91 76	8, 17, 28, 32	0
1	H	206/206 (100%)	-0.34	0 100 100	9, 18, 29, 35	0
1	I	206/206 (100%)	-0.34	0 100 100	9, 17, 29, 35	0
1	J	206/206 (100%)	-0.44	0 100 100	6, 15, 25, 33	0
1	K	206/206 (100%)	-0.34	0 100 100	7, 16, 27, 36	0
1	L	206/206 (100%)	-0.42	1 (0%) 91 76	6, 15, 27, 38	0
1	M	206/206 (100%)	-0.40	0 100 100	6, 15, 27, 36	0
1	N	206/206 (100%)	-0.37	0 100 100	6, 17, 28, 34	0
1	O	206/206 (100%)	-0.33	0 100 100	7, 16, 27, 36	0
1	P	206/206 (100%)	-0.10	2 (0%) 84 60	8, 20, 32, 44	0
1	Q	206/206 (100%)	-0.38	1 (0%) 91 76	7, 15, 26, 35	0
1	R	206/206 (100%)	-0.44	2 (0%) 84 60	5, 14, 26, 35	0
1	S	206/206 (100%)	-0.37	0 100 100	7, 17, 29, 34	0
1	T	206/206 (100%)	-0.18	3 (1%) 76 49	10, 20, 32, 43	0
All	All	4120/4120 (100%)	-0.37	13 (0%) 94 84	4, 16, 29, 44	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLN	3.8
1	G	27	THR	3.0
1	R	1	GLN	2.5
1	A	179	PRO	2.4
1	P	181	SER	2.4

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	A	5002	1/1	0.93	0.49	7.13	62,62,62,62	0
2	CA	I	5018	1/1	0.80	0.25	1.29	65,65,65,65	0
2	CA	D	5008	1/1	0.91	0.23	0.86	49,49,49,49	0
2	CA	K	5022	1/1	0.89	0.16	-0.99	40,40,40,40	0
2	CA	F	5012	1/1	0.92	0.14	-1.32	68,68,68,68	0
2	CA	M	5026	1/1	0.83	0.15	-1.62	59,59,59,59	0
2	CA	G	5014	1/1	0.92	0.09	-2.17	51,51,51,51	0
2	CA	S	5038	1/1	0.86	0.12	-2.25	29,29,29,29	0
2	CA	T	5040	1/1	0.87	0.11	-2.26	50,50,50,50	0
2	CA	C	5005	1/1	0.88	0.07	-2.54	32,32,32,32	0
2	CA	S	5037	1/1	0.84	0.09	-3.17	22,22,22,22	0
2	CA	T	5039	1/1	0.93	0.07	-	45,45,45,45	0
2	CA	L	5024	1/1	0.91	0.16	-	52,52,52,52	0
2	CA	G	5013	1/1	0.83	0.11	-	48,48,48,48	0
2	CA	O	5030	1/1	0.95	0.27	-	54,54,54,54	0
2	CA	O	5029	1/1	0.81	0.09	-	40,40,40,40	0
2	CA	R	5035	1/1	0.95	0.07	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	D	5007	1/1	0.92	0.16	-	25,25,25,25	0
2	CA	B	5004	1/1	0.80	0.15	-	55,55,55,55	0
2	CA	E	5009	1/1	0.96	0.07	-	23,23,23,23	0
2	CA	K	5021	1/1	0.80	0.11	-	32,32,32,32	0
2	CA	I	5017	1/1	0.92	0.10	-	35,35,35,35	0
2	CA	Q	5034	1/1	0.86	0.10	-	32,32,32,32	0
2	CA	N	5028	1/1	0.85	0.26	-	48,48,48,48	0
2	CA	C	5003	1/1	0.96	0.05	-	28,28,28,28	0
2	CA	E	5010	1/1	0.79	0.13	-	80,80,80,80	0
2	CA	B	5006	1/1	0.94	0.06	-	34,34,34,34	0
2	CA	L	5023	1/1	0.90	0.09	-	37,37,37,37	0
2	CA	J	5020	1/1	0.86	0.15	-	43,43,43,43	0
2	CA	P	5031	1/1	0.90	0.07	-	35,35,35,35	0
2	CA	H	5015	1/1	0.87	0.13	-	44,44,44,44	0
2	CA	J	5019	1/1	0.89	0.12	-	41,41,41,41	0
2	CA	M	5025	1/1	0.84	0.09	-	36,36,36,36	0
2	CA	N	5027	1/1	0.92	0.10	-	30,30,30,30	0
2	CA	H	5016	1/1	0.53	0.24	-	57,57,57,57	0
2	CA	R	5036	1/1	0.81	0.14	-	53,53,53,53	0
2	CA	F	5011	1/1	0.97	0.08	-	27,27,27,27	0
2	CA	A	5001	1/1	0.96	0.05	-	20,20,20,20	0
2	CA	Q	5033	1/1	0.95	0.11	-	36,36,36,36	0
2	CA	P	5032	1/1	0.72	0.14	-	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.