



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 AM GMT

PDB ID : 2J2P  
Title : L-ficolin complexed to N-acetyl-cystein (150mM)  
Authors : Garlatti, V.; Gaboriaud, C.  
Deposited on : 2006-08-17  
Resolution : 2.80 Å(reported)

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

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

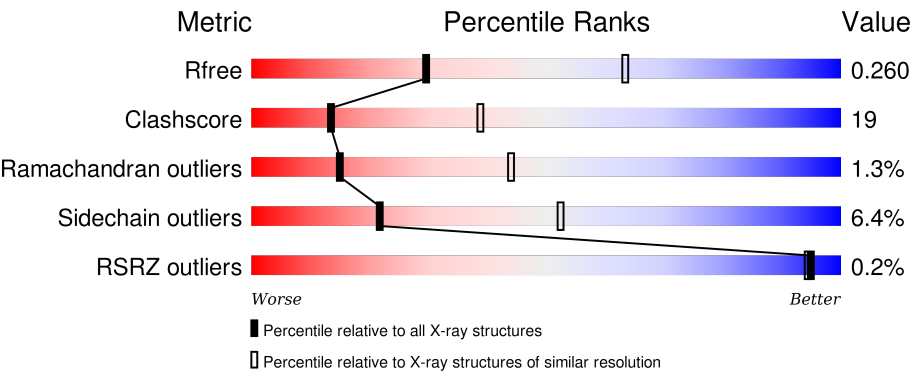
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div><div>%</div><div><div></div><div>61%</div><div>33%</div><div></div></div><div>...</div></div>
1	B	218	<div><div></div><div>76%</div><div>22%</div><div></div></div> <div>.</div>
1	C	218	<div><div></div><div>69%</div><div>25%</div><div></div></div> <div>..</div>
1	D	218	<div><div></div><div>61%</div><div>35%</div><div></div></div> <div>..</div>
1	E	218	<div><div></div><div>72%</div><div>25%</div><div></div></div> <div>.</div>

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Mol	Chain	Length	Quality of chain
1	F	218	 71% 23%

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	B	1291	-	-	-	X
3	SC2	B	1289	-	-	-	X
3	SC2	B	1290	-	-	-	X
3	SC2	B	1294	-	-	-	X
3	SC2	C	1289	-	-	-	X
3	SC2	C	1290	-	-	X	X
3	SC2	D	1290	-	-	X	X
3	SC2	E	1289	-	-	-	X
3	SC2	E	1290[A]	-	-	-	X
3	SC2	E	1290[B]	-	-	-	X
3	SC2	E	1291	-	-	X	-
3	SC2	F	1289	-	-	-	X
3	SC2	F	1290	-	-	X	X
3	SC2	F	1291	-	-	-	X
5	BMA	C	1291	X	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10628 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 FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	21	0	0
			1715	1078	302	327	8			
1	B	218	Total	C	N	O	S	0	0	0
			1744	1096	307	332	9			
1	C	212	Total	C	N	O	S	0	0	0
			1704	1072	300	324	8			
1	D	214	Total	C	N	O	S	4	0	0
			1715	1078	302	327	8			
1	E	218	Total	C	N	O	S	7	0	0
			1744	1096	307	332	9			
1	F	212	Total	C	N	O	S	0	1	0
			1715	1078	304	325	8			

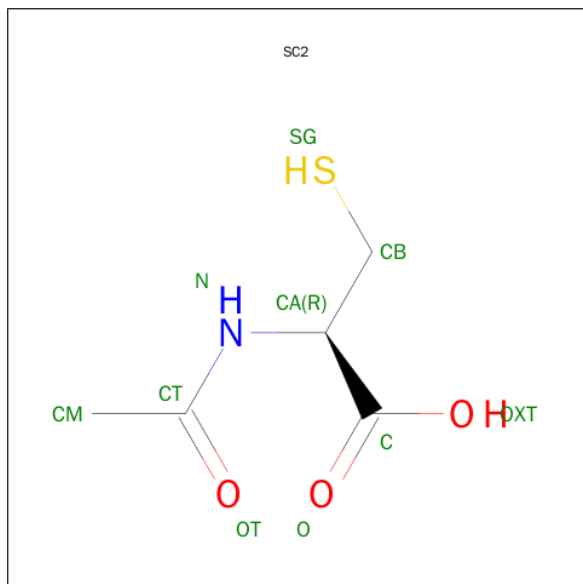
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	CONFLICT	UNP Q15485
A	247	THR	VAL	CONFLICT	UNP Q15485
B	168	THR	VAL	CONFLICT	UNP Q15485
B	247	THR	VAL	CONFLICT	UNP Q15485
C	168	THR	VAL	CONFLICT	UNP Q15485
C	247	THR	VAL	CONFLICT	UNP Q15485
D	168	THR	VAL	CONFLICT	UNP Q15485
D	247	THR	VAL	CONFLICT	UNP Q15485
E	168	THR	VAL	CONFLICT	UNP Q15485
E	247	THR	VAL	CONFLICT	UNP Q15485
F	168	THR	VAL	CONFLICT	UNP Q15485
F	247	THR	VAL	CONFLICT	UNP Q15485

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is N-ACETYL-L-CYSTEINE (three-letter code: SC2) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 10 5 1 3 1	0	0
3	B	1	Total C N O S 10 5 1 3 1	0	0
3	B	1	Total C N O S 10 5 1 3 1	0	0
3	B	1	Total C N O S 10 5 1 3 1	0	0
3	C	1	Total C N O S 10 5 1 3 1	0	0
3	C	1	Total C N O S 10 5 1 3 1	0	0

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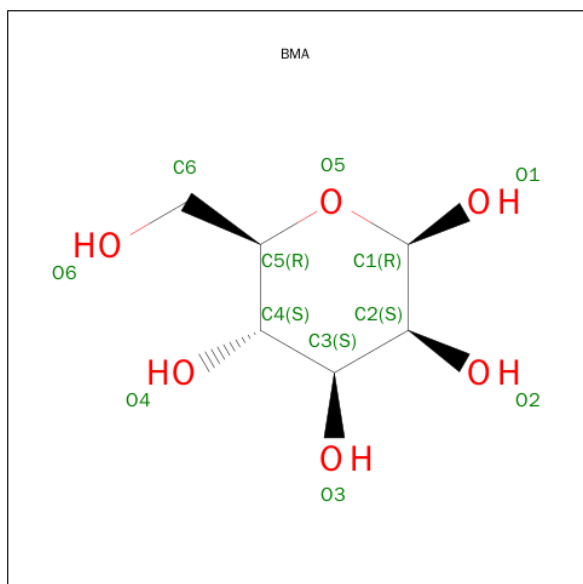
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
3	E	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
3	E	1	Total	C	N	O	S	0	1
			20	10	2	6	2		
3	E	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			10	5	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			10	5	1	3	1		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



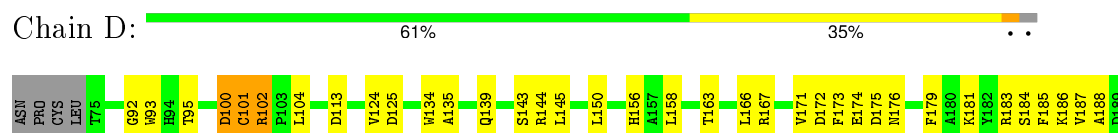
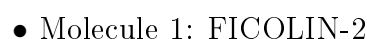
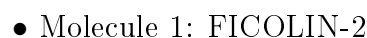
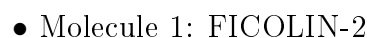
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is water.

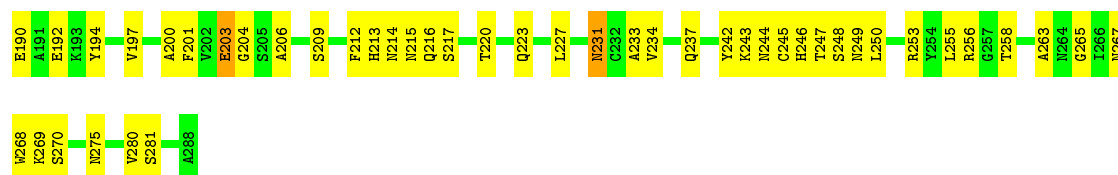
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	9	Total	O		0	0
			9	9			
6	B	14	Total	O		0	0
			14	14			
6	C	16	Total	O		0	0
			16	16			
6	D	9	Total	O		0	0
			9	9			
6	E	18	Total	O		0	0
			18	18			
6	F	12	Total	O		0	0
			12	12			



- Molecule 1: FICOLIN-2

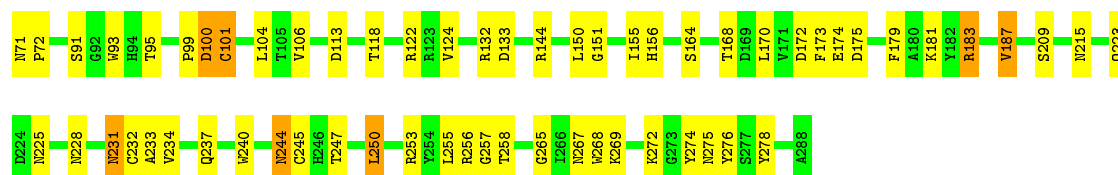






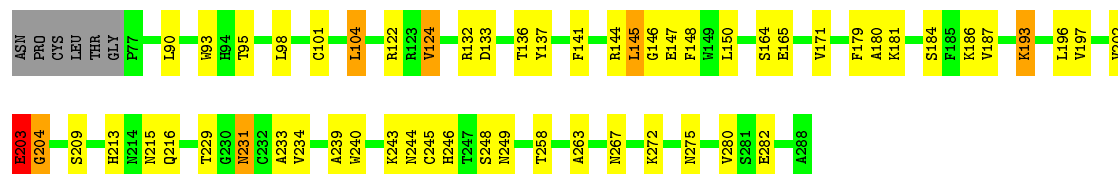
• Molecule 1: FICOLIN-2

Chain E: 72% 25% .



• Molecule 1: FICOLIN-2

Chain F: 71% 23% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.40 Å 96.40 Å 140.29 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.80 19.86 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.80) 92.4 (19.86-2.77)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.79 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.270 0.191 , 0.260	Depositor DCC
$R_{free}$ test set	1680 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 19.8	EDS
Estimated twinning fraction	0.029 for -h,-k,l 0.427 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 34164 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, BMA, NAG, SC2

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	0.65	2/1762 (0.1%)	0.68	2/2383 (0.1%)
1	B	0.43	0/1792	0.55	0/2425
1	C	0.42	0/1751	0.57	0/2367
1	D	0.50	1/1762 (0.1%)	0.54	0/2383
1	E	0.45	1/1792 (0.1%)	0.56	0/2425
1	F	0.43	0/1762	0.57	1/2381 (0.0%)
All	All	0.49	4/10621 (0.0%)	0.58	3/14364 (0.0%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	ARG	CA-CB	17.42	1.92	1.53
1	A	81	LYS	CA-CB	-9.69	1.32	1.53
1	D	158	LEU	CA-CB	-6.34	1.39	1.53
1	E	183	ARG	CA-CB	-6.12	1.40	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	CB-CA-C	-13.31	83.77	110.40
1	A	102	ARG	CA-CB-CG	-12.28	86.38	113.40
1	F	203	GLU	N-CA-C	5.26	125.21	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Peptide

## 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	1715	0	1585	83	5
1	B	1744	0	1611	42	0
1	C	1704	0	1576	60	0
1	D	1715	0	1585	78	0
1	E	1744	0	1612	48	3
1	F	1715	0	1588	54	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	10	0	8	2	0
3	B	30	0	24	3	0
3	C	20	0	16	5	0
3	D	10	0	8	19	0
3	E	40	0	32	9	0
3	F	30	0	24	12	0
4	B	28	0	25	1	0
4	E	28	0	25	2	0
5	C	11	0	10	5	0
6	A	9	0	0	2	0
6	B	14	0	0	1	0
6	C	16	0	0	0	0
6	D	9	0	0	0	0
6	E	18	0	0	1	0
6	F	12	0	0	1	0
All	All	10628	0	9729	376	5

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 19.

All (376) 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:215:ASN:HD21	4:E:1293:NAG:C1	1.11	1.56
1:B:183:ARG:CD	1:B:200:ALA:HB3	1.57	1.35
3:D:1290:SC2:HMC2	1:F:144:ARG:CD	1.58	1.33
3:D:1290:SC2:CM	1:F:144:ARG:HD2	1.59	1.31
1:D:183:ARG:HD2	1:D:200:ALA:HB3	1.24	1.09
1:B:183:ARG:HD2	1:B:200:ALA:HB3	1.10	1.06
1:E:228:ASN:HD22	1:E:244:ASN:ND2	1.54	1.04
1:D:183:ARG:CD	1:D:200:ALA:HB3	1.91	1.00
1:C:78:ARG:HG3	1:C:78:ARG:HH11	1.24	0.98
1:A:98:LEU:HD21	1:A:104:LEU:HD13	1.43	0.98
1:D:92:GLY:HA3	3:D:1290:SC2:CM	1.94	0.97
1:A:99:PRO:CB	1:A:161:GLN:HE22	1.78	0.97
1:B:183:ARG:HD3	1:B:200:ALA:HB3	1.46	0.96
1:B:71:ASN:N	1:B:72:PRO:HD3	1.85	0.91
1:C:78:ARG:CG	1:C:78:ARG:HH11	1.82	0.91
1:D:183:ARG:HG3	1:D:200:ALA:O	1.71	0.89
3:D:1290:SC2:CT	3:D:1290:SC2:SG	2.59	0.89
1:D:92:GLY:HA3	3:D:1290:SC2:HMC3	1.56	0.87
1:A:183:ARG:HD2	6:A:2006:HOH:O	1.74	0.87
1:D:188:ALA:HB1	1:D:192:GLU:HB2	1.55	0.87
1:B:183:ARG:CD	1:B:200:ALA:CB	2.50	0.85
1:A:99:PRO:HB3	1:A:161:GLN:HE22	1.37	0.85
1:C:216:GLN:HG3	1:C:243:LYS:HG3	1.59	0.84
1:A:99:PRO:HB3	1:A:161:GLN:NE2	1.93	0.84
1:A:99:PRO:CB	1:A:161:GLN:NE2	2.40	0.84
3:F:1291:SC2:SG	3:F:1291:SC2:OT	2.35	0.84
1:F:216:GLN:HG3	1:F:243:LYS:HG2	1.59	0.84
3:D:1290:SC2:HMC2	1:F:144:ARG:HD2	0.84	0.83
1:A:183:ARG:NE	1:A:200:ALA:HB3	1.93	0.83
1:D:156:HIS:HD2	1:D:187:VAL:O	1.60	0.83
1:A:98:LEU:O	1:A:101:CYS:HA	1.80	0.82
1:B:183:ARG:HD2	1:B:200:ALA:CB	2.04	0.81
1:F:146:GLY:HA3	3:F:1289:SC2:SG	2.21	0.80
1:A:188:ALA:HB1	1:A:192:GLU:HB2	1.63	0.80
1:B:163:THR:HG22	1:B:288:ALA:HB3	1.62	0.79
1:E:132:ARG:HD2	3:E:1289:SC2:HA	1.63	0.79
1:D:92:GLY:HA3	3:D:1290:SC2:HMC1	1.62	0.79
1:C:78:ARG:NH2	1:C:101:CYS:SG	2.58	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:CYS:H	5:C:1291:BMA:H62	1.48	0.77
1:A:244:ASN:N	1:A:245:CYS:HA	1.98	0.77
1:D:100:ASP:O	1:D:101:CYS:HB2	1.83	0.77
1:E:228:ASN:HD22	1:E:244:ASN:HD21	1.31	0.76
1:C:231:ASN:O	1:C:235:MET:HG3	1.85	0.76
1:C:132:ARG:HB3	3:C:1290:SC2:HMC1	1.68	0.76
1:A:98:LEU:O	1:A:101:CYS:CA	2.34	0.76
1:C:78:ARG:HG3	1:C:78:ARG:NH1	1.97	0.76
1:B:71:ASN:N	1:B:72:PRO:CD	2.48	0.76
3:D:1290:SC2:OT	3:D:1290:SC2:SG	2.44	0.75
1:F:216:GLN:HG3	1:F:243:LYS:CG	2.16	0.75
1:A:98:LEU:O	1:A:101:CYS:N	2.20	0.75
1:A:188:ALA:HB1	1:A:192:GLU:OE1	1.87	0.74
1:D:209:SER:HB2	1:D:268:TRP:CE2	2.23	0.74
1:A:133:ASP:N	1:A:221:LYS:HE2	2.02	0.74
1:A:99:PRO:HG3	1:A:161:GLN:OE1	1.86	0.74
1:F:136:THR:OG1	3:F:1290:SC2:HMC2	1.87	0.73
1:B:183:ARG:HG3	1:B:200:ALA:O	1.89	0.73
1:D:244:ASN:N	1:D:245:CYS:HA	2.02	0.73
1:B:183:ARG:HD3	1:B:200:ALA:CB	2.15	0.72
1:D:216:GLN:HE21	1:D:243:LYS:HG2	1.55	0.72
1:C:209:SER:HB2	1:C:268:TRP:CE2	2.24	0.72
1:D:188:ALA:O	1:D:194:TYR:HA	1.90	0.71
1:D:188:ALA:CB	1:D:192:GLU:HB2	2.20	0.71
1:D:188:ALA:HB1	1:D:192:GLU:CB	2.20	0.71
1:B:228:ASN:HD22	1:B:244:ASN:ND2	1.88	0.70
1:D:156:HIS:CD2	1:D:187:VAL:O	2.42	0.70
1:B:231:ASN:HD22	1:B:231:ASN:C	1.92	0.70
1:A:99:PRO:HB2	1:A:161:GLN:HE22	1.55	0.70
1:A:99:PRO:HB3	1:A:161:GLN:OE1	1.91	0.70
1:D:247:THR:HG22	1:D:269:LYS:HD2	1.72	0.70
1:C:98:LEU:HD21	1:C:104:LEU:HD12	1.74	0.69
1:A:188:ALA:HB1	1:A:192:GLU:CB	2.23	0.69
3:F:1290:SC2:CT	3:F:1290:SC2:OXT	2.40	0.69
1:D:237:GLN:HE22	1:D:253:ARG:NH1	1.91	0.69
1:C:216:GLN:HG2	1:C:243:LYS:HE3	1.74	0.69
1:C:245:CYS:H	5:C:1291:BMA:C6	2.06	0.69
1:D:100:ASP:O	1:D:101:CYS:CB	2.41	0.68
1:F:231:ASN:HD22	1:F:231:ASN:C	1.97	0.68
1:D:166:LEU:HD22	1:D:185:PHE:CD1	2.28	0.68
1:A:156:HIS:HD2	1:A:187:VAL:O	1.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLN:HG3	1:C:243:LYS:CG	2.24	0.67
1:E:71:ASN:N	1:E:72:PRO:HD2	2.09	0.67
1:A:135:ALA:O	1:A:139:GLN:HG2	1.94	0.67
1:E:228:ASN:ND2	1:E:244:ASN:ND2	2.37	0.67
1:C:231:ASN:C	1:C:231:ASN:HD22	1.97	0.67
1:E:231:ASN:HD22	1:E:231:ASN:C	1.96	0.67
1:C:216:GLN:CG	1:C:243:LYS:HE3	2.26	0.66
1:A:183:ARG:CZ	1:A:200:ALA:HB3	2.24	0.66
1:A:231:ASN:C	1:A:231:ASN:HD22	1.98	0.66
3:D:1290:SC2:CM	1:F:144:ARG:HB2	2.25	0.66
1:A:99:PRO:HB3	1:A:161:GLN:CD	2.16	0.66
1:B:93:TRP:CZ2	1:B:144:ARG:HA	2.32	0.65
1:F:132:ARG:HB3	3:F:1290:SC2:HMC1	1.77	0.65
1:C:244:ASN:N	1:C:245:CYS:HA	2.12	0.64
1:E:231:ASN:OD1	1:E:234:VAL:HG23	1.97	0.64
1:D:216:GLN:HG2	1:D:242:TYR:O	1.98	0.64
3:D:1290:SC2:HMC3	1:F:144:ARG:HD2	1.75	0.64
1:D:183:ARG:HD3	1:D:200:ALA:H	1.62	0.64
1:A:99:PRO:CG	1:A:161:GLN:OE1	2.46	0.64
1:C:171:VAL:HB	1:C:280:VAL:HB	1.79	0.64
3:D:1290:SC2:HMC2	1:F:144:ARG:CB	2.29	0.63
1:A:132:ARG:NH2	1:B:111:ASP:OD1	2.32	0.62
1:E:100:ASP:O	1:E:101:CYS:HB2	1.98	0.62
1:A:183:ARG:HG3	1:A:200:ALA:O	1.98	0.62
1:F:209:SER:O	1:F:248:SER:HB3	1.99	0.62
3:D:1290:SC2:HMC2	1:F:144:ARG:HB2	1.79	0.62
1:F:244:ASN:N	1:F:245:CYS:HA	2.14	0.61
1:E:269:LYS:HD2	1:E:274:TYR:CZ	2.35	0.61
1:A:174:GLU:O	1:A:175:ASP:HB2	2.00	0.61
1:B:156:HIS:HD2	1:B:187:VAL:O	1.82	0.61
1:A:188:ALA:CB	1:A:192:GLU:OE1	2.47	0.61
1:A:99:PRO:C	1:A:101:CYS:H	2.04	0.61
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.00	0.61
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.36	0.61
1:C:216:GLN:HG2	1:C:243:LYS:CE	2.31	0.61
1:F:216:GLN:CG	1:F:243:LYS:HG2	2.31	0.60
1:C:156:HIS:CE1	1:C:189:ASP:HB3	2.37	0.60
1:E:228:ASN:ND2	1:E:244:ASN:HD21	1.97	0.60
1:D:237:GLN:NE2	1:D:253:ARG:NH1	2.49	0.60
1:A:133:ASP:HB3	1:A:221:LYS:CE	2.32	0.60
1:C:132:ARG:HH11	3:C:1290:SC2:HMC2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1290:SC2:HMC2	1:F:144:ARG:CG	2.30	0.59
1:D:231:ASN:HD21	1:D:233:ALA:HB3	1.66	0.59
3:D:1290:SC2:H2	1:F:144:ARG:HH11	1.48	0.59
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.37	0.59
1:C:231:ASN:ND2	1:C:234:VAL:H	2.01	0.59
1:A:171:VAL:HB	1:A:280:VAL:HB	1.83	0.59
1:B:228:ASN:HD22	1:B:244:ASN:HD22	1.48	0.59
1:B:100:ASP:O	1:B:101:CYS:HB2	2.02	0.59
1:E:228:ASN:HD22	1:E:244:ASN:HD22	1.47	0.59
1:D:172:ASP:OD2	1:D:176:ASN:HB2	2.03	0.58
1:F:202:VAL:HG23	1:F:203:GLU:HG2	1.85	0.58
1:D:135:ALA:O	1:D:139:GLN:HG2	2.03	0.58
1:A:216:GLN:OE1	1:A:227:LEU:HG	2.03	0.58
1:C:245:CYS:HB2	5:C:1291:BMA:H61	1.86	0.58
4:E:1293:NAG:O3	4:E:1294:NAG:O5	2.22	0.57
1:C:216:GLN:HE21	1:C:243:LYS:HE2	1.67	0.57
1:D:216:GLN:NE2	1:D:243:LYS:HG2	2.18	0.57
1:A:133:ASP:CA	1:A:221:LYS:HE2	2.34	0.57
1:A:188:ALA:O	1:A:194:TYR:HA	2.04	0.57
1:D:213:HIS:CE1	1:D:246:HIS:HA	2.38	0.57
1:A:133:ASP:HB3	1:A:221:LYS:HE3	1.87	0.57
1:A:231:ASN:HD21	1:A:233:ALA:HB3	1.69	0.57
1:E:151:GLY:O	1:E:155:ILE:HG13	2.04	0.57
1:A:99:PRO:CB	1:A:161:GLN:OE1	2.52	0.57
1:B:134:TRP:HA	1:B:220:THR:HG21	1.87	0.57
4:B:1292:NAG:O3	4:B:1293:NAG:O5	2.17	0.56
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.40	0.56
1:A:247:THR:O	1:A:269:LYS:HB2	2.06	0.56
1:D:171:VAL:HB	1:D:280:VAL:HB	1.88	0.56
1:C:216:GLN:CG	1:C:243:LYS:CE	2.83	0.56
1:B:113:ASP:OD2	1:B:181:LYS:NZ	2.30	0.56
1:C:98:LEU:O	1:C:101:CYS:N	2.29	0.56
1:A:104:LEU:HD11	1:A:154:ASN:CG	2.25	0.56
3:F:1290:SC2:OT	3:F:1290:SC2:OXT	2.24	0.56
1:D:237:GLN:HE22	1:D:253:ARG:HH11	1.51	0.56
1:E:71:ASN:N	1:E:72:PRO:CD	2.69	0.56
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.40	0.56
1:E:93:TRP:CZ2	1:E:144:ARG:HA	2.41	0.56
1:D:201:PHE:CE2	1:D:203:GLU:HA	2.40	0.56
1:D:213:HIS:HE1	1:D:246:HIS:HA	1.70	0.55
1:A:198:LEU:HD23	1:A:211:THR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLN:CD	1:D:253:ARG:HD2	2.27	0.55
1:A:166:LEU:HD22	1:A:185:PHE:CD1	2.41	0.55
1:D:93:TRP:HB2	3:D:1290:SC2:HA	1.88	0.54
1:D:209:SER:O	1:D:248:SER:HB3	2.07	0.54
1:F:93:TRP:CZ2	1:F:144:ARG:HA	2.43	0.54
1:D:188:ALA:HB1	1:D:192:GLU:CD	2.28	0.54
1:E:99:PRO:C	1:E:101:CYS:H	2.12	0.53
1:C:146:GLY:HA3	3:C:1289:SC2:SG	2.49	0.53
1:C:172:ASP:OD2	1:C:176:ASN:HB2	2.09	0.53
1:C:117:TRP:HB3	1:C:284:LYS:HB2	1.90	0.53
1:E:231:ASN:C	1:E:231:ASN:ND2	2.61	0.53
1:D:231:ASN:HD22	1:D:231:ASN:C	2.12	0.53
1:D:206:ALA:O	1:D:270:SER:OG	2.25	0.53
1:D:212:PHE:O	1:D:243:LYS:HD2	2.09	0.52
1:E:113:ASP:OD2	1:E:181:LYS:NZ	2.33	0.52
1:D:179:PHE:CZ	1:D:204:GLY:HA2	2.45	0.52
1:A:99:PRO:CB	1:A:161:GLN:CD	2.76	0.52
1:E:231:ASN:HD21	1:E:233:ALA:HB3	1.74	0.52
1:A:156:HIS:CD2	1:A:187:VAL:O	2.59	0.52
1:B:231:ASN:ND2	1:B:231:ASN:C	2.62	0.52
3:F:1291:SC2:CB	3:F:1291:SC2:OT	2.58	0.51
1:D:263:ALA:HA	1:D:267:ASN:HD22	1.74	0.51
1:A:163:THR:O	1:A:163:THR:CG2	2.58	0.51
1:F:180:ALA:HA	1:F:204:GLY:HA3	1.91	0.51
1:A:209:SER:O	1:A:248:SER:HB3	2.11	0.51
1:C:202:VAL:O	1:C:203:GLU:HB3	2.11	0.51
1:A:93:TRP:CZ2	1:A:144:ARG:HA	2.44	0.51
1:B:100:ASP:OD2	1:B:102:ARG:NH2	2.40	0.51
1:A:216:GLN:NE2	1:A:243:LYS:HE3	2.25	0.51
1:D:92:GLY:CA	3:D:1290:SC2:HMC3	2.35	0.51
1:E:133:ASP:H	3:E:1289:SC2:HMC1	1.74	0.51
1:B:183:ARG:HD3	1:B:200:ALA:H	1.76	0.51
1:D:113:ASP:OD2	1:D:181:LYS:HE2	2.11	0.51
1:E:269:LYS:HD2	1:E:274:TYR:CE2	2.46	0.51
1:C:213:HIS:CE1	1:C:246:HIS:HA	2.46	0.51
1:A:99:PRO:C	1:A:101:CYS:N	2.65	0.50
1:C:78:ARG:CG	1:C:78:ARG:NH1	2.55	0.50
1:C:262:PHE:HZ	5:C:1291:BMA:C1	2.24	0.50
1:A:179:PHE:CE1	1:A:204:GLY:HA2	2.47	0.50
1:F:133:ASP:CG	3:F:1290:SC2:HMC3	2.32	0.50
3:A:1290:SC2:OXT	1:B:122:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:HIS:CE1	1:C:249:ASN:HB2	2.47	0.50
1:C:255:LEU:O	1:C:256:ARG:HB2	2.12	0.50
1:F:122:ARG:HD2	1:F:282:GLU:OE2	2.10	0.50
1:A:171:VAL:HG22	1:A:177:TYR:CD2	2.47	0.49
1:A:99:PRO:CG	1:A:161:GLN:CD	2.81	0.49
1:C:231:ASN:HD21	1:C:233:ALA:HB3	1.78	0.49
1:D:237:GLN:NE2	1:D:253:ARG:HH11	2.10	0.49
1:E:237:GLN:NE2	1:E:253:ARG:NH1	2.59	0.49
1:D:166:LEU:HD12	1:D:167:ARG:N	2.27	0.49
1:F:124:VAL:HG12	1:F:147:GLU:HG2	1.95	0.49
1:D:173:PHE:CE1	1:D:256:ARG:HA	2.47	0.49
3:B:1289:SC2:OT	3:B:1289:SC2:SG	2.69	0.49
1:F:213:HIS:CE1	1:F:246:HIS:HA	2.48	0.49
1:F:240:TRP:HE1	1:F:248:SER:HG	1.61	0.49
1:B:136:THR:HG22	1:B:141:PHE:CD1	2.48	0.49
1:D:214:ASN:ND2	1:D:215:ASN:HB2	2.27	0.49
1:A:188:ALA:HB3	1:A:195:ASN:H	1.78	0.48
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.47	0.48
3:B:1289:SC2:SG	3:B:1289:SC2:CT	3.01	0.48
1:A:103:PRO:O	1:A:104:LEU:CB	2.61	0.48
1:A:183:ARG:CD	1:A:200:ALA:HB3	2.44	0.48
1:D:216:GLN:HB2	1:D:243:LYS:NZ	2.28	0.48
1:D:231:ASN:HB3	1:D:234:VAL:HB	1.95	0.48
1:A:228:ASN:OD1	1:A:230:GLY:N	2.39	0.48
1:E:240:TRP:CH2	1:E:250:LEU:HB2	2.49	0.48
1:A:193:LYS:HB2	1:A:217:SER:OG	2.13	0.48
1:E:231:ASN:HD22	1:E:232:CYS:N	2.12	0.48
1:D:263:ALA:HA	1:D:267:ASN:ND2	2.28	0.48
1:B:263:ALA:HA	1:B:267:ASN:ND2	2.28	0.48
1:E:223:GLN:HE21	1:E:225:ASN:HD21	1.60	0.48
1:C:263:ALA:HA	1:C:267:ASN:ND2	2.28	0.48
1:A:136:THR:HG22	1:A:141:PHE:CD1	2.48	0.48
1:A:247:THR:HB	1:A:269:LYS:HD2	1.96	0.48
1:C:217:SER:O	1:C:241:TRP:HA	2.14	0.47
1:D:102:ARG:HH11	1:D:102:ARG:HG2	1.80	0.47
1:B:231:ASN:HD21	1:B:233:ALA:HB3	1.79	0.47
1:F:136:THR:HG22	1:F:141:PHE:CD1	2.49	0.47
1:D:171:VAL:HG12	1:D:172:ASP:O	2.14	0.47
1:D:237:GLN:NE2	1:D:253:ARG:HD2	2.29	0.47
1:F:231:ASN:HD21	1:F:233:ALA:HB3	1.80	0.47
1:C:78:ARG:HE	1:C:97:TYR:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.50	0.47
1:D:186:LYS:HG3	1:D:197:VAL:HB	1.97	0.47
1:D:216:GLN:HE21	1:D:243:LYS:CG	2.25	0.47
1:C:136:THR:HG22	1:C:141:PHE:CD1	2.50	0.46
1:E:237:GLN:CD	1:E:253:ARG:HH11	2.18	0.46
1:E:156:HIS:HD2	1:E:187:VAL:O	1.98	0.46
1:C:78:ARG:HD2	1:C:97:TYR:O	2.15	0.46
1:A:244:ASN:N	1:A:245:CYS:CA	2.75	0.46
1:B:112:THR:O	1:B:113:ASP:C	2.54	0.46
1:D:125:ASP:OD2	3:E:1291:SC2:HMC2	2.15	0.46
1:D:183:ARG:CD	1:D:200:ALA:CB	2.80	0.46
1:C:78:ARG:HA	1:C:78:ARG:HD2	1.56	0.46
1:D:92:GLY:CA	3:D:1290:SC2:CM	2.81	0.46
3:E:1289:SC2:SG	3:E:1289:SC2:O	2.71	0.46
1:F:215:ASN:ND2	6:F:2004:HOH:O	2.49	0.46
1:B:216:GLN:HE22	1:B:227:LEU:HD11	1.81	0.46
1:F:263:ALA:HA	1:F:267:ASN:ND2	2.30	0.46
1:F:231:ASN:CG	1:F:234:VAL:HG23	2.35	0.46
1:D:172:ASP:CG	1:D:176:ASN:HB2	2.36	0.46
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.51	0.46
1:E:244:ASN:C	1:E:244:ASN:ND2	2.68	0.46
1:D:227:LEU:O	1:D:244:ASN:HB3	2.16	0.46
3:E:1291:SC2:OT	3:E:1291:SC2:SG	2.73	0.46
1:E:255:LEU:O	1:E:256:ARG:HB2	2.16	0.46
1:A:173:PHE:CZ	1:A:256:ARG:HA	2.51	0.46
1:D:216:GLN:HE22	1:D:227:LEU:HD11	1.81	0.46
1:B:265:GLY:H	1:B:267:ASN:HD21	1.63	0.46
1:E:173:PHE:CE1	1:E:256:ARG:HA	2.51	0.46
1:D:143:SER:HA	1:E:91:SER:HB2	1.97	0.45
1:E:265:GLY:H	1:E:267:ASN:HD21	1.65	0.45
1:D:183:ARG:HD3	1:D:200:ALA:HB3	1.88	0.45
1:C:124:VAL:HG23	1:C:280:VAL:HG22	1.98	0.45
1:E:122:ARG:NH2	3:E:1291:SC2:SG	2.89	0.45
1:A:133:ASP:HB3	1:A:221:LYS:HE2	1.97	0.45
1:E:168:THR:O	1:E:179:PHE:HA	2.15	0.45
1:D:93:TRP:CZ2	1:D:144:ARG:HA	2.52	0.45
1:B:163:THR:O	1:B:288:ALA:N	2.38	0.45
1:A:143:SER:HA	1:B:91:SER:HB2	1.99	0.45
1:F:171:VAL:HB	1:F:280:VAL:HB	1.98	0.45
1:F:136:THR:OG1	3:F:1290:SC2:CM	2.62	0.45
1:C:132:ARG:HD2	3:C:1290:SC2:CM	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:PHE:O	1:F:204:GLY:HA3	2.17	0.45
1:F:263:ALA:HA	1:F:267:ASN:HD22	1.80	0.45
1:C:272:LYS:HB2	1:C:276:TYR:HB3	1.98	0.45
1:A:113:ASP:OD2	1:A:181:LYS:HE3	2.17	0.45
1:C:78:ARG:HE	1:C:97:TYR:CB	2.30	0.44
1:C:216:GLN:HG3	1:C:243:LYS:HE3	1.97	0.44
1:D:231:ASN:ND2	1:D:233:ALA:HB3	2.32	0.44
1:B:255:LEU:HA	1:B:255:LEU:HD23	1.83	0.44
3:D:1290:SC2:HMC1	1:F:144:ARG:HB2	1.96	0.44
1:E:244:ASN:C	1:E:244:ASN:HD22	2.21	0.44
1:D:209:SER:HB2	1:D:268:TRP:CD2	2.51	0.44
1:C:171:VAL:HG22	1:C:177:TYR:CD2	2.52	0.44
1:A:159:THR:O	1:A:186:LYS:HG2	2.18	0.44
1:F:202:VAL:O	1:F:203:GLU:HB3	2.17	0.44
1:C:236:PHE:CZ	5:C:1291:BMA:H5	2.53	0.44
1:E:93:TRP:HA	1:E:106:VAL:O	2.18	0.44
1:A:231:ASN:C	1:A:231:ASN:ND2	2.70	0.44
1:C:240:TRP:CH2	1:C:250:LEU:HB2	2.52	0.44
1:F:216:GLN:HG3	1:F:243:LYS:HG3	1.96	0.43
1:A:132:ARG:C	1:A:221:LYS:HE2	2.39	0.43
1:F:179:PHE:CZ	1:F:204:GLY:HA2	2.53	0.43
3:E:1291:SC2:CB	3:E:1291:SC2:OT	2.66	0.43
1:F:216:GLN:HG2	1:F:243:LYS:HE2	1.98	0.43
1:A:101:CYS:HB2	1:A:102:ARG:H	1.73	0.43
1:A:93:TRP:HA	1:A:106:VAL:O	2.18	0.43
1:C:216:GLN:HE22	1:C:227:LEU:HD11	1.83	0.43
1:F:258:THR:HA	1:F:275:ASN:O	2.17	0.43
1:A:263:ALA:HA	1:A:267:ASN:ND2	2.33	0.43
1:A:104:LEU:CD2	1:A:106:VAL:CG1	2.96	0.43
1:A:183:ARG:CD	6:A:2006:HOH:O	2.50	0.43
1:B:126:GLY:HA2	6:B:2006:HOH:O	2.18	0.43
1:A:118:THR:HG21	1:A:158:LEU:HD21	2.01	0.43
1:A:98:LEU:HB2	1:A:101:CYS:O	2.18	0.43
1:F:164:SER:O	1:F:184:SER:HA	2.19	0.43
1:D:102:ARG:NH1	1:D:102:ARG:HG2	2.34	0.43
1:D:216:GLN:HB2	1:D:243:LYS:HZ2	1.84	0.43
1:F:246:HIS:CE1	1:F:249:ASN:HB2	2.54	0.43
1:E:170:LEU:HD13	1:E:278:TYR:CZ	2.53	0.43
1:A:163:THR:O	1:A:163:THR:HG22	2.19	0.43
1:C:196:LEU:HB2	1:C:241:TRP:CD1	2.54	0.43
1:A:192:GLU:O	1:A:193:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:ASN:C	1:F:231:ASN:ND2	2.70	0.42
1:F:98:LEU:HD21	1:F:104:LEU:HD12	1.99	0.42
1:A:103:PRO:O	1:A:104:LEU:HB3	2.19	0.42
1:E:99:PRO:C	1:E:101:CYS:N	2.72	0.42
1:E:122:ARG:HH12	3:E:1290[B]:SC2:HA	1.83	0.42
1:B:143:SER:OG	1:B:145:LEU:HB2	2.20	0.42
1:C:231:ASN:HD22	1:C:232:CYS:N	2.17	0.42
1:D:220:THR:OG1	1:D:223:GLN:HB2	2.19	0.42
1:D:247:THR:O	1:D:269:LYS:HB2	2.20	0.42
1:C:272:LYS:HG2	1:C:278:TYR:OH	2.20	0.42
1:A:165:GLU:OE2	1:A:181:LYS:HE2	2.20	0.42
1:D:255:LEU:HD12	1:D:265:GLY:CA	2.50	0.42
1:C:136:THR:OG1	3:C:1290:SC2:HMC3	2.20	0.42
1:E:99:PRO:O	1:E:101:CYS:N	2.53	0.42
1:E:122:ARG:NH1	3:E:1290[B]:SC2:HA	2.34	0.42
1:D:186:LYS:CG	1:D:197:VAL:HB	2.50	0.42
1:B:117:TRP:HB3	1:B:284:LYS:HB2	2.02	0.42
1:A:98:LEU:HD11	1:A:104:LEU:HD12	2.02	0.41
1:E:71:ASN:N	6:E:2001:HOH:O	2.52	0.41
1:D:258:THR:HA	1:D:275:ASN:O	2.19	0.41
1:F:145:LEU:O	3:F:1289:SC2:HA	2.21	0.41
1:D:246:HIS:CD2	1:D:249:ASN:HB2	2.56	0.41
1:D:93:TRP:H	3:D:1290:SC2:CT	2.34	0.41
1:D:93:TRP:CD2	1:D:144:ARG:HD3	2.54	0.41
1:E:244:ASN:HA	1:E:245:CYS:HA	1.90	0.41
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.63	0.41
3:A:1290:SC2:OT	3:A:1290:SC2:HBC2	2.20	0.41
1:F:98:LEU:O	1:F:101:CYS:N	2.44	0.41
1:F:193:LYS:HA	1:F:193:LYS:NZ	2.36	0.41
1:A:75:THR:OG1	1:A:76:GLY:N	2.52	0.41
1:F:132:ARG:HD2	3:F:1290:SC2:HMC1	2.03	0.41
1:E:106:VAL:HG21	1:E:118:THR:HG23	2.03	0.41
1:C:187:VAL:HA	1:C:195:ASN:O	2.21	0.41
1:F:148:PHE:C	1:F:148:PHE:CD2	2.94	0.41
1:B:104:LEU:HD13	1:B:106:VAL:HG12	2.03	0.41
1:C:244:ASN:N	1:C:245:CYS:CA	2.83	0.41
1:E:257:GLY:HA2	1:E:276:TYR:CZ	2.55	0.41
1:F:165:GLU:OE2	1:F:181:LYS:HE3	2.21	0.41
1:C:112:THR:O	1:C:113:ASP:C	2.58	0.41
1:D:174:GLU:O	1:D:175:ASP:HB2	2.21	0.41
1:A:103:PRO:HB2	1:A:104:LEU:H	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASN:HD22	1:B:232:CYS:N	2.19	0.41
1:B:156:HIS:CD2	1:B:187:VAL:O	2.69	0.41
1:E:172:ASP:C	1:E:172:ASP:OD1	2.58	0.41
1:B:143:SER:HB2	3:B:1294:SC2:HA	2.02	0.40
1:C:272:LYS:CB	1:C:276:TYR:HB3	2.52	0.40
1:F:137:TYR:CZ	1:F:239:ALA:HB3	2.56	0.40
1:F:186:LYS:HB3	1:F:197:VAL:HB	2.03	0.40
1:F:133:ASP:H	3:F:1290:SC2:HMC3	1.85	0.40
1:D:134:TRP:HZ2	1:D:190:GLU:HG3	1.86	0.40
1:E:258:THR:HA	1:E:275:ASN:O	2.21	0.40

All (5) 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:A:288:ALA:OXT	1:E:183:ARG:NH1[3_665]	0.89	1.31
1:A:288:ALA:OXT	1:E:183:ARG:CZ[3_665]	1.84	0.36
1:A:183:ARG:NH2	1:F:272:LYS:CD[1_665]	1.95	0.25
1:A:288:ALA:C	1:E:183:ARG:NH1[3_665]	2.10	0.10
1:A:183:ARG:NH2	1:F:272:LYS:CE[1_665]	2.14	0.06

## 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	212/218 (97%)	184 (87%)	22 (10%)	6 (3%)	6	21
1	B	216/218 (99%)	196 (91%)	19 (9%)	1 (0%)	34	69
1	C	210/218 (96%)	193 (92%)	15 (7%)	2 (1%)	19	52
1	D	212/218 (97%)	185 (87%)	24 (11%)	3 (1%)	14	42
1	E	216/218 (99%)	200 (93%)	14 (6%)	2 (1%)	21	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	211/218 (97%)	191 (90%)	17 (8%)	3 (1%)	14	42
All	All	1277/1308 (98%)	1149 (90%)	111 (9%)	17 (1%)	15	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
1	D	101	CYS
1	D	102	ARG
1	A	100	ASP
1	A	101	CYS
1	F	203	GLU
1	A	104	LEU
1	E	100	ASP
1	B	124	VAL
1	A	102	ARG
1	C	256	ARG
1	C	124	VAL
1	D	124	VAL
1	E	124	VAL
1	F	124	VAL
1	F	204	GLY
1	A	202	VAL

### 5.3.2 Protein sidechains ⓘ

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	179/183 (98%)	167 (93%)	12 (7%)	20	50
1	B	183/183 (100%)	171 (93%)	12 (7%)	21	51
1	C	178/183 (97%)	168 (94%)	10 (6%)	26	59
1	D	179/183 (98%)	167 (93%)	12 (7%)	20	50
1	E	183/183 (100%)	170 (93%)	13 (7%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	179/183 (98%)	169 (94%)	10 (6%)	26	59
All	All	1081/1098 (98%)	1012 (94%)	69 (6%)	22	52

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	95	THR
1	A	101	CYS
1	A	145	LEU
1	A	150	LEU
1	A	163	THR
1	A	165	GLU
1	A	214	ASN
1	A	223	GLN
1	A	231	ASN
1	A	250	LEU
1	A	281	SER
1	B	95	THR
1	B	104	LEU
1	B	124	VAL
1	B	150	LEU
1	B	164	SER
1	B	166	LEU
1	B	175	ASP
1	B	187	VAL
1	B	231	ASN
1	B	247	THR
1	B	250	LEU
1	B	281	SER
1	C	78	ARG
1	C	90	LEU
1	C	95	THR
1	C	104	LEU
1	C	150	LEU
1	C	196	LEU
1	C	202	VAL
1	C	231	ASN
1	C	247	THR
1	C	250	LEU
1	D	95	THR
1	D	100	ASP

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Mol	Chain	Res	Type
1	D	104	LEU
1	D	145	LEU
1	D	150	LEU
1	D	163	THR
1	D	184	SER
1	D	203	GLU
1	D	217	SER
1	D	231	ASN
1	D	250	LEU
1	D	281	SER
1	E	95	THR
1	E	101	CYS
1	E	104	LEU
1	E	150	LEU
1	E	164	SER
1	E	174	GLU
1	E	175	ASP
1	E	187	VAL
1	E	231	ASN
1	E	244	ASN
1	E	247	THR
1	E	250	LEU
1	E	272	LYS
1	F	90	LEU
1	F	95	THR
1	F	104	LEU
1	F	145	LEU
1	F	150	LEU
1	F	187	VAL
1	F	193	LYS
1	F	196	LEU
1	F	229	THR
1	F	231	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	178	GLN
1	A	223	GLN
1	A	231	ASN
1	A	246	HIS

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Mol	Chain	Res	Type
1	A	267	ASN
1	B	71	ASN
1	B	121	GLN
1	B	156	HIS
1	B	195	ASN
1	B	223	GLN
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	C	156	HIS
1	C	216	GLN
1	C	231	ASN
1	C	267	ASN
1	D	156	HIS
1	D	195	ASN
1	D	216	GLN
1	D	231	ASN
1	D	246	HIS
1	D	267	ASN
1	E	139	GLN
1	E	156	HIS
1	E	195	ASN
1	E	215	ASN
1	E	225	ASN
1	E	231	ASN
1	E	244	ASN
1	E	246	HIS
1	F	139	GLN
1	F	156	HIS
1	F	215	ASN
1	F	231	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

4 carbohydrates 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	$\# Z  > 2$
4	NAG	B	1292	1,4	14,14,15	0.52	0	15,19,21	0.87	0
4	NAG	B	1293	4	14,14,15	0.44	0	15,19,21	1.46	3 (20%)
4	NAG	E	1293	1,4	14,14,15	0.67	0	15,19,21	0.95	0
4	NAG	E	1294	4	14,14,15	0.55	0	15,19,21	1.05	1 (6%)

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
4	NAG	B	1292	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1293	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1293	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1294	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1293	NAG	C4-C3-C2	-3.55	105.72	111.23
4	B	1293	NAG	C2-N2-C7	-2.08	120.36	123.04
4	E	1294	NAG	C4-C3-C2	-2.03	108.07	111.23
4	B	1293	NAG	C1-O5-C5	3.03	116.10	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1292	NAG	1	0
4	B	1293	NAG	1	0
4	E	1293	NAG	2	0
4	E	1294	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SC2	A	1290	-	6,9,9	0.39	0	5,11,11	0.27	0
3	SC2	B	1289	-	6,9,9	0.16	0	5,11,11	1.06	1 (20%)
3	SC2	B	1290	-	6,9,9	0.30	0	5,11,11	0.60	0
3	SC2	B	1294	-	6,9,9	0.24	0	5,11,11	0.53	0
3	SC2	C	1289	-	6,9,9	0.47	0	5,11,11	1.12	0
3	SC2	C	1290	-	6,9,9	0.50	0	5,11,11	0.53	0
5	BMA	C	1291	-	11,11,12	0.58	0	14,15,17	0.71	0
3	SC2	D	1290	-	6,9,9	0.33	0	5,11,11	1.72	1 (20%)
3	SC2	E	1289	-	6,9,9	0.26	0	5,11,11	1.79	1 (20%)
3	SC2	E	1290[A]	-	6,9,9	0.34	0	5,11,11	0.58	0
3	SC2	E	1290[B]	-	6,9,9	0.29	0	5,11,11	0.49	0
3	SC2	E	1291	-	6,9,9	0.19	0	5,11,11	1.51	1 (20%)
3	SC2	F	1289	-	6,9,9	0.50	0	5,11,11	1.24	1 (20%)
3	SC2	F	1290	-	6,9,9	0.71	0	5,11,11	1.26	1 (20%)
3	SC2	F	1291	-	6,9,9	0.29	0	5,11,11	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SC2	A	1290	-	-	0/6/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SC2	B	1289	-	-	0/6/10/10	0/0/0/0
3	SC2	B	1290	-	-	1/6/10/10	0/0/0/0
3	SC2	B	1294	-	-	0/6/10/10	0/0/0/0
3	SC2	C	1289	-	-	0/6/10/10	0/0/0/0
3	SC2	C	1290	-	-	0/6/10/10	0/0/0/0
5	BMA	C	1291	-	1/1/4/5	0/2/19/22	0/1/1/1
3	SC2	D	1290	-	-	0/6/10/10	0/0/0/0
3	SC2	E	1289	-	-	0/6/10/10	0/0/0/0
3	SC2	E	1290[A]	-	-	0/6/10/10	0/0/0/0
3	SC2	E	1290[B]	-	-	0/6/10/10	0/0/0/0
3	SC2	E	1291	-	-	0/6/10/10	0/0/0/0
3	SC2	F	1289	-	-	0/6/10/10	0/0/0/0
3	SC2	F	1290	-	-	0/6/10/10	0/0/0/0
3	SC2	F	1291	-	-	0/6/10/10	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1289	SC2	CA-CB-SG	-3.96	109.30	114.16
3	D	1290	SC2	CA-CB-SG	-3.09	110.36	114.16
3	E	1291	SC2	CA-CB-SG	-2.90	110.60	114.16
3	F	1290	SC2	CA-CB-SG	-2.67	110.87	114.16
3	B	1289	SC2	CA-CB-SG	-2.31	111.31	114.16
3	F	1289	SC2	CB-CA-N	-2.26	108.22	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	1291	BMA	C5

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1290	SC2	OT-CT-N-CA

There are no ring outliers.

13 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1290	SC2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1289	SC2	2	0
3	B	1294	SC2	1	0
3	C	1289	SC2	1	0
3	C	1290	SC2	4	0
5	C	1291	BMA	5	0
3	D	1290	SC2	19	0
3	E	1289	SC2	3	0
3	E	1290[B]	SC2	2	0
3	E	1291	SC2	4	0
3	F	1289	SC2	2	0
3	F	1290	SC2	8	0
3	F	1291	SC2	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	214/218 (98%)	-0.11	2 (0%) 85 79	18, 32, 47, 52	4 (1%)
1	B	218/218 (100%)	-0.49	0 100 100	15, 25, 40, 48	0
1	C	212/218 (97%)	-0.51	0 100 100	16, 25, 37, 51	0
1	D	214/218 (98%)	-0.45	0 100 100	19, 35, 50, 54	1 (0%)
1	E	218/218 (100%)	-0.59	0 100 100	16, 26, 39, 49	1 (0%)
1	F	212/218 (97%)	-0.52	0 100 100	16, 26, 38, 50	0
All	All	1288/1308 (98%)	-0.45	2 (0%) 95 94	15, 28, 45, 54	6 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ALA	2.7
1	A	271	GLY	2.2

### 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](#)

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1293	14/15	0.94	0.13	-	39,42,43,44	0
4	NAG	E	1293	14/15	0.96	0.13	-	32,33,34,34	0
4	NAG	B	1292	14/15	0.90	0.21	-	35,39,41,42	0
4	NAG	E	1294	14/15	0.95	0.12	-	31,33,35,35	0

## 6.4 Ligands

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	SC2	B	1289	10/10	0.87	0.33	11.65	29,30,30,31	10
3	SC2	D	1290	10/10	0.89	0.33	10.27	54,56,56,57	10
3	SC2	E	1290[B]	10/10	0.92	0.30	8.13	23,23,23,23	10
3	SC2	E	1290[A]	10/10	0.92	0.30	7.85	31,31,31,31	10
3	SC2	B	1290	10/10	0.87	0.36	7.10	44,44,44,44	10
3	SC2	C	1290	10/10	0.84	0.25	5.55	34,38,39,41	10
3	SC2	B	1294	10/10	0.87	0.28	5.30	30,31,32,33	10
3	SC2	F	1289	10/10	0.90	0.24	4.81	36,37,38,39	10
3	SC2	E	1289	10/10	0.90	0.22	4.20	46,48,49,50	10
3	SC2	F	1291	10/10	0.95	0.24	3.70	20,20,21,21	10
3	SC2	C	1289	10/10	0.79	0.23	3.05	64,66,66,66	0
2	CA	B	1291	1/1	0.96	0.16	2.54	12,12,12,12	1
5	BMA	C	1291	11/12	0.87	0.19	2.41	56,56,57,57	0
3	SC2	F	1290	10/10	0.93	0.20	2.21	41,42,42,43	10
3	SC2	A	1290	10/10	0.88	0.20	1.26	64,64,65,67	0
3	SC2	E	1291	10/10	0.91	0.18	1.22	54,55,56,56	0
2	CA	E	1292	1/1	0.98	0.12	-1.07	18,18,18,18	0
2	CA	C	1292	1/1	0.97	0.09	-1.63	32,32,32,32	0
2	CA	F	1292	1/1	0.98	0.06	-2.83	35,35,35,35	0
2	CA	D	1289	1/1	0.92	0.11	-	59,59,59,59	0
2	CA	A	1289	1/1	0.84	0.08	-	51,51,51,51	1

## 6.5 Other polymers

There are no such residues in this entry.