



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:51 AM GMT

PDB ID : 2J0H
Title : L-FICOLIN COMPLEXED TO ACETYL-CHOLINE
Authors : Garlatti, V.; Gaboriaud, C.
Deposited on : 2006-08-03
Resolution : 2.85 Å(reported)

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

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

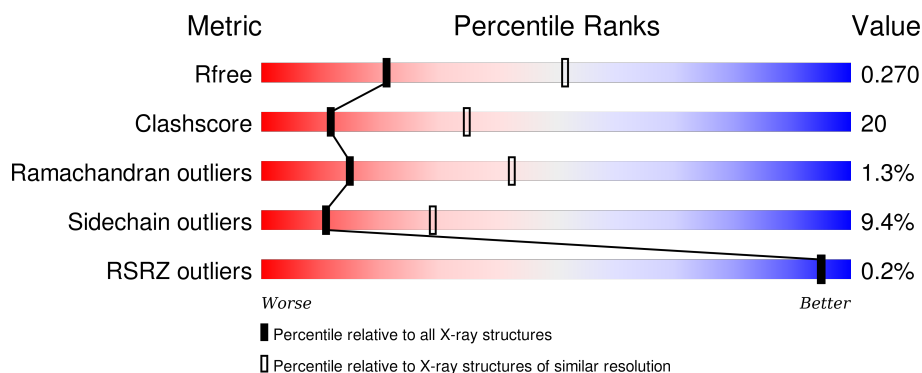
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 $\leq 5\%$. 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>59%</div> <div>35%</div> <div>• •</div> </div>
1	B	218	<div> <div>68%</div> <div>28%</div> <div>•</div> </div>
1	C	218	<div> <div>64%</div> <div>32%</div> <div>• •</div> </div>
1	D	218	<div> <div>55%</div> <div>38%</div> <div>5% •</div> </div>
1	E	218	<div> <div>66%</div> <div>30%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	218	

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	1290	-	-	-	X
2	CA	C	1290	-	-	-	X
2	CA	E	1290	-	-	-	X
3	ACH	B	1289	-	-	X	-
3	ACH	C	1289	-	-	X	X
3	ACH	F	1289	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10586 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	12	1	0
			1727	1087	303	329	8			
1	B	217	Total	C	N	O	S	0	0	0
			1736	1092	305	330	9			
1	C	216	Total	C	N	O	S	5	0	0
			1729	1087	304	329	9			
1	D	214	Total	C	N	O	S	26	2	0
			1733	1090	304	331	8			
1	E	218	Total	C	N	O	S	10	0	0
			1744	1096	307	332	9			
1	F	212	Total	C	N	O	S	5	0	0
			1704	1072	300	324	8			

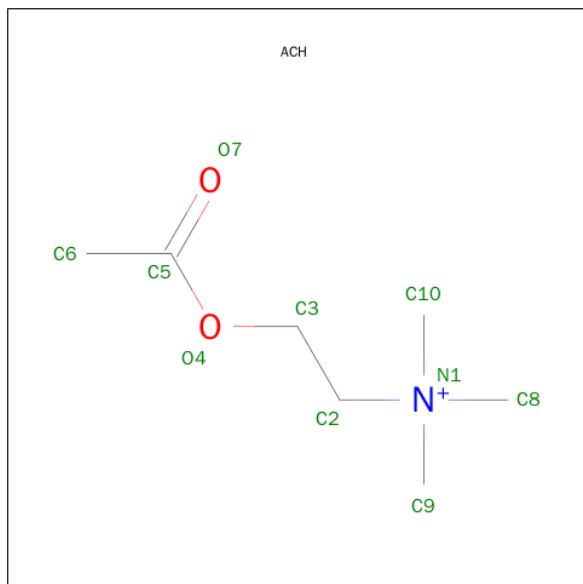
There are 13 discrepancies between the modelled and reference sequences:

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	71	ASN	GLN	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 ACETYLCHOLINE (three-letter code: ACH) (formula: $C_7H_{16}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 7 1 2	0	0
3	B	1	Total C N O 10 7 1 2	0	0
3	C	1	Total C N O 10 7 1 2	0	0
3	E	1	Total C N O 10 7 1 2	0	0
3	F	1	Total C N O 10 7 1 2	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

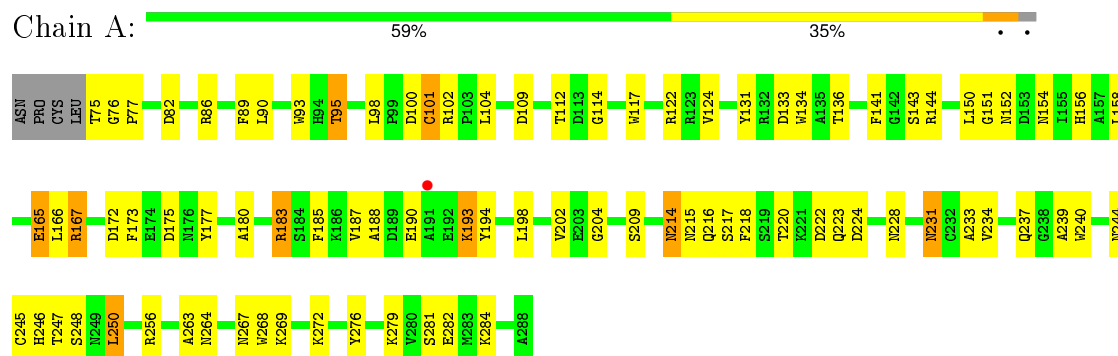
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	15	Total	O	0	0
			15	15		
6	C	17	Total	O	0	0
			17	17		
6	D	13	Total	O	0	0
			13	13		
6	E	13	Total	O	0	0
			13	13		
6	F	16	Total	O	0	0
			16	16		

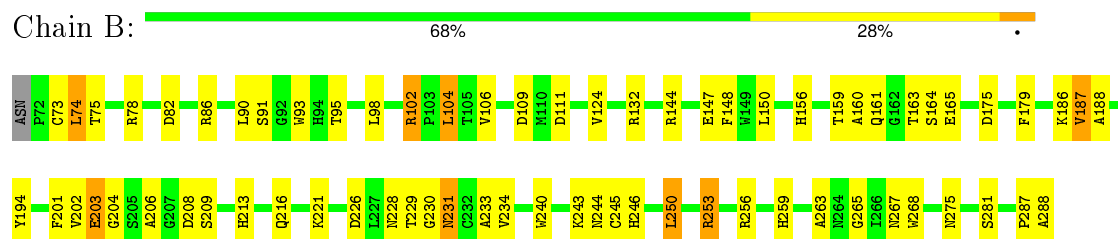
3 Residue-property plots [i](#)

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.

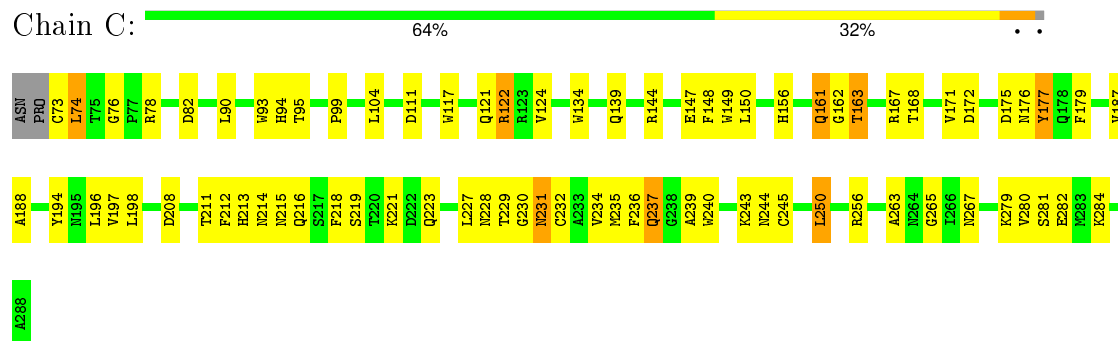
• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2

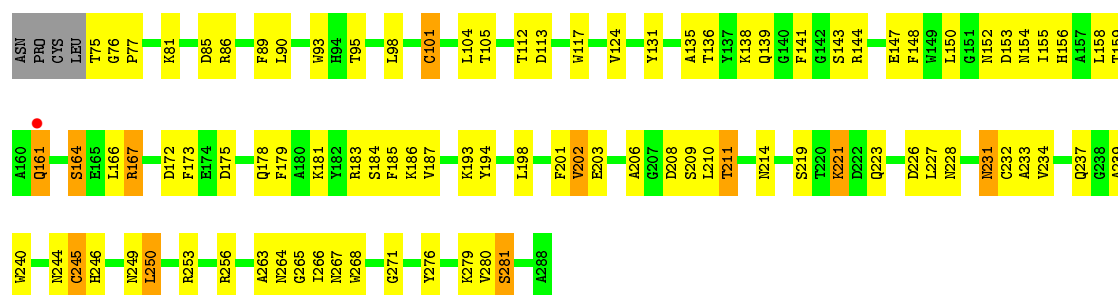


• Molecule 1: FICOLIN-2

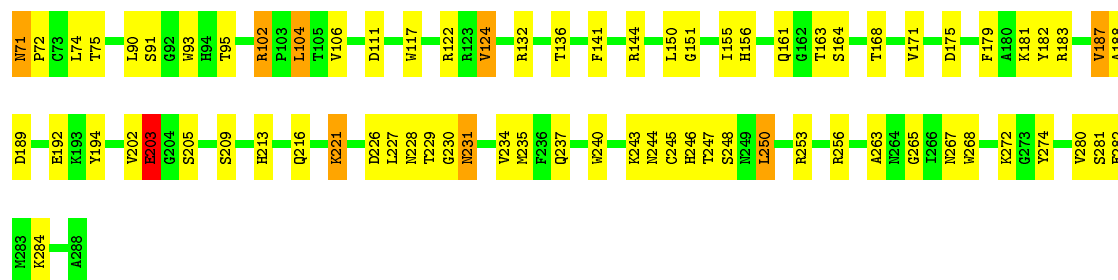


• Molecule 1: FICOLIN-2

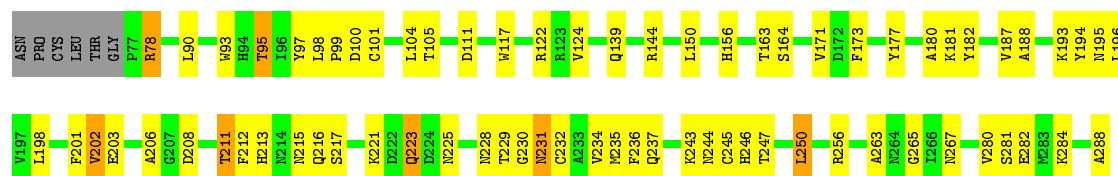




• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	97.06 Å 97.06 Å 140.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.85 19.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.85) 96.8 (19.94-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.83 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.275 0.205 , 0.270	Depositor DCC
R_{free} test set	1655 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 4.6	EDS
Estimated twinning fraction	0.027 for -h,-k,l 0.467 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33234 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10586	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACH, CA, BMA, NAG

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	0.60	0/1775	0.67	0/2401
1	B	0.57	0/1784	0.72	2/2413 (0.1%)
1	C	0.57	0/1776	0.69	0/2402
1	D	0.63	1/1781 (0.1%)	0.70	2/2409 (0.1%)
1	E	0.61	0/1792	0.77	2/2425 (0.1%)
1	F	0.60	0/1751	0.68	0/2367
All	All	0.60	1/10659 (0.0%)	0.70	6/14417 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	CYS	CA-CB	-5.55	1.41	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	161	GLN	CB-CA-C	-10.00	90.41	110.40
1	E	226	ASP	CB-CG-OD1	6.70	124.33	118.30
1	D	232	CYS	N-CA-CB	5.90	121.22	110.60
1	D	161	GLN	N-CA-CB	-5.77	100.21	110.60
1	B	104	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	226	ASP	CB-CG-OD1	5.17	122.95	118.30

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	1727	0	1593	83	0
1	B	1736	0	1606	69	0
1	C	1729	0	1599	58	0
1	D	1733	0	1599	75	0
1	E	1744	0	1611	62	0
1	F	1704	0	1576	63	0
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	16	5	0
3	B	10	0	16	6	0
3	C	10	0	16	6	0
3	E	10	0	16	4	0
3	F	10	0	16	8	0
4	B	39	0	34	0	0
5	E	28	0	25	0	0
6	A	16	0	0	4	0
6	B	15	0	0	1	0
6	C	17	0	0	4	0
6	D	13	0	0	3	0
6	E	13	0	0	1	0
6	F	16	0	0	2	0
All	All	10586	0	9723	405	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 20.

All (405) 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:112:THR:HG22	1:D:167:ARG:HH21	1.14	1.11
1:A:112:THR:CG2	1:A:167:ARG:HH21	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG22	1:A:167:ARG:HH21	1.13	1.09
1:D:155:ILE:HB	6:D:2008:HOH:O	1.61	0.99
1:A:133:ASP:HB2	1:A:222:ASP:OD1	1.65	0.96
1:D:152:ASN:HA	6:D:2008:HOH:O	1.65	0.95
1:A:112:THR:HG22	1:A:167:ARG:NH2	1.84	0.93
1:D:231:ASN:ND2	1:D:234:VAL:H	1.68	0.92
1:A:231:ASN:HD22	1:A:234:VAL:H	1.15	0.91
1:B:163:THR:HG22	1:B:288:ALA:HB3	1.52	0.90
1:D:112:THR:CG2	1:D:167:ARG:HH21	1.84	0.90
3:F:1289:ACH:H81	6:F:2016:HOH:O	1.72	0.89
1:F:78:ARG:HH11	1:F:78:ARG:CG	1.87	0.88
1:A:231:ASN:ND2	1:A:234:VAL:H	1.72	0.86
1:F:78:ARG:NH2	1:F:101:CYS:SG	2.49	0.84
1:B:202:VAL:HG12	1:B:203:GLU:HG2	1.59	0.83
1:D:112:THR:HG22	1:D:167:ARG:NH2	1.92	0.83
1:C:231:ASN:C	1:C:231:ASN:HD22	1.82	0.82
1:E:231:ASN:HD22	1:E:231:ASN:C	1.82	0.82
1:F:78:ARG:HD2	1:F:97:TYR:O	1.80	0.81
1:D:246:HIS:CE1	1:D:263:ALA:HB1	2.14	0.81
1:F:216:GLN:HG3	1:F:243:LYS:HG3	1.62	0.81
1:A:112:THR:CG2	1:A:167:ARG:NH2	2.40	0.81
1:C:73:CYS:SG	1:C:74:LEU:N	2.54	0.80
1:D:156:HIS:HD2	1:D:187:VAL:O	1.64	0.80
1:C:216:GLN:HE21	1:C:243:LYS:HZ2	1.29	0.80
1:F:244:ASN:N	1:F:245:CYS:HA	1.97	0.80
1:E:71:ASN:N	1:E:72:PRO:HD2	1.96	0.80
1:F:231:ASN:HD22	1:F:231:ASN:C	1.86	0.79
1:E:102:ARG:HH11	1:E:102:ARG:HG2	1.46	0.78
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.18	0.78
1:B:231:ASN:HD22	1:B:231:ASN:C	1.84	0.77
1:B:221:LYS:NZ	3:B:1289:ACH:H63	1.99	0.77
1:B:228:ASN:HD22	1:B:244:ASN:HD22	1.31	0.77
1:E:156:HIS:HD2	1:E:187:VAL:O	1.68	0.76
1:E:228:ASN:HD22	1:E:244:ASN:ND2	1.83	0.76
1:A:134:TRP:HB2	1:A:223:GLN:HG3	1.67	0.75
1:D:240:TRP:CH2	1:D:250:LEU:HB2	2.21	0.75
1:A:95:THR:HG22	6:A:2002:HOH:O	1.85	0.75
1:B:228:ASN:HD22	1:B:244:ASN:ND2	1.83	0.75
1:A:156:HIS:HD2	1:A:187:VAL:O	1.70	0.75
1:A:134:TRP:HE3	1:A:220:THR:HG23	1.52	0.74
1:D:231:ASN:HD22	1:D:234:VAL:H	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:HIS:HD2	1:B:187:VAL:O	1.71	0.74
1:A:134:TRP:HA	1:A:220:THR:HG21	1.69	0.72
1:E:228:ASN:HD22	1:E:244:ASN:HD22	1.37	0.72
1:F:216:GLN:HG2	1:F:243:LYS:HE3	1.72	0.71
1:F:163:THR:HG22	1:F:288:ALA:HB2	1.72	0.71
1:F:78:ARG:HG3	1:F:78:ARG:HH11	1.55	0.70
1:A:222:ASP:OD2	1:A:223:GLN:HG2	1.92	0.70
1:E:228:ASN:O	1:E:230:GLY:N	2.24	0.70
1:B:104:LEU:CD1	1:B:106:VAL:HG12	2.21	0.69
1:A:154:ASN:O	1:A:158:LEU:HB2	1.92	0.69
1:A:114:GLY:CA	3:A:1290:ACH:H103	2.22	0.69
1:A:263:ALA:HA	1:A:267:ASN:ND2	2.08	0.68
1:A:246:HIS:HE1	1:A:263:ALA:O	1.77	0.68
1:B:216:GLN:NE2	1:B:243:LYS:HG3	2.08	0.68
1:E:71:ASN:HA	6:E:2001:HOH:O	1.94	0.67
1:B:104:LEU:CD1	1:B:106:VAL:CG1	2.73	0.66
1:F:228:ASN:O	1:F:230:GLY:N	2.28	0.66
1:A:100:ASP:OD1	1:A:102:ARG:N	2.24	0.66
1:A:144:ARG:HG3	1:B:91:SER:O	1.94	0.66
1:E:171:VAL:HB	1:E:280:VAL:HB	1.78	0.66
1:F:221:LYS:NZ	3:F:1289:ACH:H63	2.11	0.65
1:C:244:ASN:N	1:C:245:CYS:HA	2.11	0.65
1:E:104:LEU:HD13	1:E:106:VAL:HG12	1.78	0.65
1:C:156:HIS:HD2	1:C:187:VAL:O	1.78	0.65
1:C:228:ASN:O	1:C:230:GLY:N	2.30	0.64
1:A:112:THR:HG21	1:A:167:ARG:HH21	1.57	0.64
1:E:124:VAL:HG23	1:E:280:VAL:HG22	1.79	0.64
1:F:231:ASN:ND2	1:F:234:VAL:H	1.96	0.64
1:A:231:ASN:ND2	1:A:234:VAL:N	2.44	0.64
1:D:143:SER:HA	1:E:91:SER:HB2	1.80	0.64
1:B:221:LYS:HZ3	3:B:1289:ACH:H63	1.62	0.64
1:B:228:ASN:O	1:B:230:GLY:N	2.32	0.63
1:B:102:ARG:HG2	1:B:102:ARG:HH11	1.63	0.63
1:D:246:HIS:HE1	1:D:263:ALA:HB1	1.59	0.63
1:A:172:ASP:HB2	1:A:276:TYR:CE1	2.34	0.63
1:A:134:TRP:CE3	1:A:220:THR:HG23	2.33	0.63
1:F:221:LYS:NZ	3:F:1289:ACH:C6	2.62	0.63
1:E:102:ARG:CG	1:E:102:ARG:HH11	2.12	0.62
1:B:221:LYS:NZ	3:B:1289:ACH:C6	2.62	0.62
1:A:246:HIS:CE1	1:A:263:ALA:HB1	2.35	0.62
1:F:156:HIS:HD2	1:F:187:VAL:O	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:CYS:SG	1:B:78:ARG:NH1	2.73	0.62
1:D:164[A]:SER:O	1:D:184:SER:HA	2.00	0.61
1:C:167:ARG:NH2	1:C:177:TYR:OH	2.33	0.61
1:B:102:ARG:CG	1:B:102:ARG:HH11	2.14	0.61
1:B:74:LEU:HD12	1:B:74:LEU:H	1.65	0.61
1:B:132:ARG:NH2	1:C:111:ASP:OD2	2.34	0.61
1:A:263:ALA:HA	1:A:267:ASN:HD22	1.66	0.61
1:D:144:ARG:HG3	1:E:91:SER:O	2.01	0.60
1:D:240:TRP:HH2	1:D:250:LEU:HB2	1.65	0.60
1:D:178:GLN:HE21	1:D:206:ALA:HA	1.66	0.60
1:E:104:LEU:HD13	1:E:106:VAL:CG1	2.31	0.60
1:D:156:HIS:CD2	1:D:187:VAL:O	2.51	0.60
1:A:143:SER:HA	1:B:91:SER:HB2	1.83	0.60
1:B:263:ALA:HA	1:B:267:ASN:ND2	2.16	0.60
1:B:104:LEU:HD13	1:B:106:VAL:CG1	2.32	0.60
1:E:132:ARG:NH2	1:F:111:ASP:OD2	2.35	0.60
1:C:172:ASP:OD2	1:C:176:ASN:HB2	2.02	0.59
1:B:156:HIS:CD2	1:B:187:VAL:O	2.54	0.59
1:E:228:ASN:O	1:E:230:GLY:O	2.19	0.59
1:A:165:GLU:O	1:A:165:GLU:HG2	2.01	0.59
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.38	0.59
1:F:228:ASN:O	1:F:230:GLY:O	2.20	0.59
1:B:244:ASN:HB3	6:B:2014:HOH:O	2.00	0.59
1:A:228:ASN:HB2	1:A:244:ASN:OD1	2.03	0.59
1:F:78:ARG:HG2	1:F:78:ARG:HH11	1.65	0.58
1:F:78:ARG:CG	1:F:78:ARG:NH1	2.59	0.58
3:C:1289:ACH:H101	6:C:2017:HOH:O	2.02	0.58
1:A:272:LYS:HG3	6:A:2010:HOH:O	2.02	0.58
1:C:236:PHE:O	1:C:237:GLN:C	2.42	0.58
1:D:164[B]:SER:O	1:D:184:SER:HA	2.02	0.58
1:D:166:LEU:HD12	1:D:167:ARG:H	1.69	0.58
1:C:161:GLN:O	1:C:163:THR:N	2.36	0.57
1:E:231:ASN:C	1:E:231:ASN:ND2	2.56	0.57
1:A:218:PHE:CE2	1:A:239:ALA:HB1	2.39	0.57
1:D:198:LEU:HD23	1:D:211:THR:HA	1.85	0.57
1:D:239:ALA:O	1:D:240:TRP:HE3	1.86	0.57
1:C:228:ASN:O	1:C:230:GLY:O	2.22	0.57
1:B:231:ASN:ND2	1:B:231:ASN:C	2.57	0.57
1:E:202:VAL:O	1:E:203:GLU:HB3	2.04	0.57
1:D:198:LEU:H	1:D:214:ASN:ND2	2.03	0.57
1:B:231:ASN:ND2	1:B:233:ALA:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ASN:OD1	1:E:71:ASN:N	2.38	0.56
1:A:166:LEU:HD22	1:A:185:PHE:CD1	2.40	0.56
1:B:221:LYS:HZ1	3:B:1289:ACH:H63	1.68	0.56
1:A:156:HIS:CD2	1:A:187:VAL:O	2.56	0.56
1:E:263:ALA:HA	1:E:267:ASN:ND2	2.20	0.56
1:F:215:ASN:ND2	6:F:2010:HOH:O	2.39	0.56
1:A:175:ASP:OD1	1:A:279:LYS:NZ	2.39	0.56
1:F:231:ASN:C	1:F:231:ASN:ND2	2.59	0.56
1:D:237:GLN:NE2	1:D:264:ASN:HD22	2.02	0.56
1:C:78:ARG:HB2	1:C:82:ASP:OD2	2.04	0.56
1:C:221:LYS:NZ	3:C:1289:ACH:C6	2.68	0.56
1:D:198:LEU:H	1:D:214:ASN:HD22	1.53	0.56
1:F:193:LYS:HB2	1:F:217:SER:OG	2.05	0.56
1:E:156:HIS:CD2	1:E:187:VAL:O	2.54	0.56
1:B:228:ASN:O	1:B:230:GLY:O	2.24	0.56
1:D:178:GLN:NE2	1:D:206:ALA:HA	2.21	0.55
1:A:173:PHE:CZ	1:A:256:ARG:HA	2.41	0.55
1:F:180:ALA:HB2	1:F:206:ALA:HB3	1.88	0.55
1:F:182:TYR:HE2	1:F:208:ASP:OD1	1.89	0.55
1:D:98:LEU:O	1:D:101:CYS:N	2.32	0.55
1:D:181:LYS:HB3	1:D:202:VAL:HB	1.89	0.55
1:A:131:TYR:CE1	1:A:237:GLN:HA	2.42	0.55
1:D:263:ALA:HA	1:D:267:ASN:ND2	2.22	0.55
1:D:179:PHE:HZ	1:D:203:GLU:OE2	1.90	0.55
1:F:201:PHE:HB2	1:F:208:ASP:OD1	2.07	0.55
1:C:198:LEU:H	1:C:214:ASN:ND2	2.04	0.55
1:C:231:ASN:ND2	1:C:234:VAL:H	2.05	0.54
1:A:240:TRP:HH2	1:A:250:LEU:HB2	1.70	0.54
1:C:156:HIS:CD2	1:C:187:VAL:O	2.60	0.54
1:D:244:ASN:N	1:D:245:CYS:HA	2.22	0.54
1:C:221:LYS:NZ	3:C:1289:ACH:H61	2.22	0.54
1:D:93:TRP:CD2	1:D:144:ARG:HD3	2.43	0.54
1:D:198:LEU:HD22	1:D:210:LEU:HD23	1.90	0.54
1:D:221:LYS:HA	1:D:233:ALA:HB3	1.90	0.54
1:A:75:THR:HG23	1:A:76:GLY:H	1.72	0.54
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.42	0.54
1:F:163:THR:CG2	1:F:288:ALA:HB2	2.36	0.54
1:E:221:LYS:HE2	3:E:1289:ACH:C6	2.38	0.54
1:A:133:ASP:CB	1:A:222:ASP:OD1	2.48	0.54
1:E:216:GLN:OE1	1:E:216:GLN:HA	2.05	0.53
1:A:166:LEU:HB2	1:A:185:PHE:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:HIS:HD2	1:E:248:SER:N	2.06	0.53
1:E:256:ARG:HG3	1:E:256:ARG:HH11	1.73	0.53
1:C:93:TRP:CD2	1:C:144:ARG:HD3	2.44	0.53
1:E:71:ASN:N	1:E:72:PRO:CD	2.70	0.53
1:E:221:LYS:CE	3:E:1289:ACH:C6	2.86	0.53
1:D:166:LEU:HD22	1:D:185:PHE:CD1	2.44	0.53
1:F:216:GLN:CG	1:F:243:LYS:HE3	2.39	0.53
1:E:213:HIS:CD2	1:E:247:THR:HG22	2.44	0.53
1:D:93:TRP:CZ2	1:D:144:ARG:HA	2.44	0.53
1:A:114:GLY:HA3	3:A:1290:ACH:H103	1.91	0.52
1:E:265:GLY:H	1:E:267:ASN:HD21	1.57	0.52
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.44	0.52
1:D:131:TYR:CE1	1:D:237:GLN:HA	2.45	0.52
1:B:179:PHE:CZ	1:B:204:GLY:HA2	2.45	0.52
1:A:244:ASN:N	1:A:245:CYS:HA	2.23	0.52
1:F:246:HIS:CE1	1:F:263:ALA:HB1	2.44	0.52
1:E:228:ASN:ND2	1:E:244:ASN:ND2	2.57	0.52
1:D:175:ASP:OD1	1:D:279:LYS:NZ	2.43	0.51
1:A:89:PHE:CE2	1:C:139:GLN:HB2	2.45	0.51
1:B:104:LEU:HD13	1:B:106:VAL:HG12	1.91	0.51
1:C:231:ASN:C	1:C:231:ASN:ND2	2.56	0.51
1:F:156:HIS:CD2	1:F:187:VAL:O	2.64	0.51
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.45	0.51
1:D:246:HIS:CE1	1:D:263:ALA:O	2.64	0.51
1:D:233:ALA:O	1:D:237:GLN:N	2.42	0.51
1:D:154:ASN:O	1:D:158:LEU:HB2	2.11	0.51
1:A:247:THR:HG22	1:A:269:LYS:HD2	1.92	0.51
1:E:93:TRP:CZ2	1:E:144:ARG:HA	2.46	0.51
1:F:221:LYS:HZ3	3:F:1289:ACH:H63	1.75	0.51
1:D:135:ALA:O	1:D:139:GLN:HG2	2.11	0.50
1:F:211:THR:O	1:F:213:HIS:N	2.43	0.50
3:A:1290:ACH:H31	3:C:1289:ACH:H91	1.93	0.50
1:F:263:ALA:HA	1:F:267:ASN:ND2	2.26	0.50
1:D:201:PHE:CD1	1:D:208:ASP:HB2	2.47	0.50
3:A:1290:ACH:H31	3:C:1289:ACH:C9	2.40	0.50
1:D:173:PHE:CZ	1:D:256:ARG:HA	2.47	0.50
1:F:122:ARG:HD2	1:F:282:GLU:OE2	2.12	0.50
1:A:231:ASN:ND2	1:A:234:VAL:HB	2.26	0.50
1:E:183:ARG:HG2	1:E:183:ARG:O	2.11	0.50
1:F:93:TRP:CD2	1:F:144:ARG:HD3	2.46	0.50
1:F:221:LYS:CE	3:F:1289:ACH:H61	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:O	1:A:177[A]:TYR:CE2	2.66	0.49
1:D:246:HIS:CD2	1:D:249:ASN:HB2	2.48	0.49
1:E:231:ASN:ND2	1:E:234:VAL:H	2.11	0.49
1:E:216:GLN:HE22	1:E:227:LEU:HD11	1.78	0.49
1:D:246:HIS:HE1	1:D:263:ALA:O	1.96	0.49
1:D:231:ASN:HD21	1:D:234:VAL:H	1.57	0.49
1:B:231:ASN:ND2	1:B:234:VAL:H	2.11	0.49
1:C:263:ALA:HA	1:C:267:ASN:ND2	2.28	0.49
1:A:166:LEU:HG	1:A:167:ARG:N	2.28	0.48
1:E:228:ASN:C	1:E:230:GLY:N	2.64	0.48
1:E:168:THR:O	1:E:179:PHE:HA	2.13	0.48
1:E:122:ARG:HG3	1:E:282:GLU:HG2	1.94	0.48
1:F:211:THR:C	1:F:213:HIS:N	2.66	0.48
1:A:122:ARG:NH1	1:A:282:GLU:OE2	2.46	0.48
1:E:240:TRP:CH2	1:E:250:LEU:HB2	2.48	0.48
1:C:73:CYS:SG	1:C:78:ARG:NH2	2.67	0.48
1:C:239:ALA:O	1:C:240:TRP:HE3	1.97	0.48
1:C:168:THR:O	1:C:179:PHE:HA	2.14	0.48
1:A:246:HIS:CE1	1:A:263:ALA:O	2.62	0.48
1:D:75:THR:HG21	1:D:101:CYS:SG	2.53	0.48
1:C:231:ASN:CG	1:C:234:VAL:HG23	2.34	0.48
1:B:231:ASN:HD22	1:B:233:ALA:H	1.62	0.48
1:F:221:LYS:HZ1	3:F:1289:ACH:C6	2.26	0.47
1:C:163:THR:HA	6:C:2009:HOH:O	2.14	0.47
1:F:182:TYR:CE2	1:F:208:ASP:OD1	2.67	0.47
1:A:237:GLN:NE2	1:A:264:ASN:HD22	2.12	0.47
1:F:93:TRP:CZ2	1:F:144:ARG:HA	2.49	0.47
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.15	0.47
1:F:228:ASN:C	1:F:230:GLY:N	2.67	0.47
1:F:202:VAL:HG22	1:F:203:GLU:HG2	1.96	0.47
1:F:236:PHE:O	1:F:237:GLN:C	2.52	0.47
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.49	0.47
3:A:1290:ACH:H83	3:A:1290:ACH:H32	1.53	0.47
1:C:265:GLY:H	1:C:267:ASN:HD21	1.63	0.47
1:B:228:ASN:C	1:B:230:GLY:N	2.67	0.47
1:F:211:THR:C	1:F:213:HIS:H	2.18	0.47
1:D:152:ASN:HB3	1:D:194:TYR:CD1	2.50	0.47
1:B:244:ASN:N	1:B:245:CYS:HA	2.29	0.47
1:E:228:ASN:C	1:E:230:GLY:H	2.18	0.47
1:B:216:GLN:HA	1:B:216:GLN:OE1	2.15	0.47
1:A:93:TRP:CZ2	1:A:144:ARG:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ALA:HB2	1:E:274:TYR:CD1	2.50	0.47
1:D:75:THR:HG23	1:D:76:GLY:H	1.80	0.47
1:A:82:ASP:O	1:A:86:ARG:HG3	2.14	0.47
1:C:171:VAL:HB	1:C:280:VAL:HB	1.97	0.47
1:D:173:PHE:HB2	1:D:276:TYR:OH	2.15	0.47
1:D:178:GLN:HE22	1:D:271:GLY:HA2	1.81	0.46
1:F:265:GLY:H	1:F:267:ASN:HD21	1.64	0.46
1:F:181:LYS:O	1:F:202:VAL:HG13	2.15	0.46
1:F:188:ALA:O	1:F:194:TYR:HA	2.14	0.46
1:C:228:ASN:C	1:C:230:GLY:N	2.68	0.46
1:C:161:GLN:CA	1:C:161:GLN:OE1	2.63	0.46
1:D:117:TRP:CZ3	1:D:167:ARG:HB3	2.50	0.46
1:B:102:ARG:HB3	1:B:102:ARG:NH1	2.31	0.46
1:D:231:ASN:ND2	1:D:234:VAL:HB	2.29	0.46
1:B:213:HIS:CE1	1:B:246:HIS:HA	2.51	0.46
1:D:228:ASN:ND2	1:D:244:ASN:OD1	2.48	0.46
1:A:216:GLN:HA	1:A:216:GLN:OE1	2.15	0.46
1:E:102:ARG:CG	1:E:102:ARG:NH1	2.77	0.46
1:A:198:LEU:H	1:A:214:ASN:ND2	2.12	0.46
1:F:117:TRP:HB3	1:F:284:LYS:HB2	1.98	0.46
1:D:265:GLY:H	1:D:267:ASN:HD21	1.64	0.46
1:C:93:TRP:CE2	1:C:144:ARG:HB3	2.50	0.46
1:C:215:ASN:ND2	6:C:2010:HOH:O	2.37	0.46
1:B:78:ARG:NH2	1:B:98:LEU:O	2.49	0.46
1:E:179:PHE:HD1	1:E:205:SER:HG	1.62	0.46
1:D:209:SER:HB2	1:D:268:TRP:CE2	2.52	0.45
1:A:98:LEU:O	1:A:101:CYS:N	2.37	0.45
1:B:253:ARG:CZ	1:B:253:ARG:HB3	2.46	0.45
1:C:221:LYS:HZ3	3:C:1289:ACH:H61	1.81	0.45
1:F:195:ASN:HD21	1:F:215:ASN:C	2.20	0.45
1:A:231:ASN:HD22	1:A:234:VAL:N	1.96	0.45
1:D:279:LYS:HE3	6:D:2013:HOH:O	2.16	0.45
1:A:233:ALA:O	1:A:237:GLN:N	2.50	0.45
1:C:93:TRP:NE1	1:C:144:ARG:HB3	2.32	0.45
1:A:193:LYS:HB3	1:A:217:SER:HB3	1.98	0.45
1:F:232:CYS:HA	1:F:235:MET:HE2	1.99	0.45
1:B:165:GLU:HG2	1:B:288:ALA:HA	1.97	0.45
1:F:231:ASN:CG	1:F:234:VAL:HG23	2.37	0.45
1:B:221:LYS:HZ1	3:B:1289:ACH:C6	2.26	0.45
1:F:228:ASN:C	1:F:230:GLY:H	2.21	0.45
1:D:105:THR:HG22	1:D:105:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:PHE:CZ	1:F:256:ARG:HA	2.52	0.45
1:B:159:THR:O	1:B:186:LYS:HG3	2.17	0.45
1:A:224:ASP:C	1:A:224:ASP:OD1	2.55	0.45
1:F:171:VAL:HG22	1:F:177:TYR:CD2	2.52	0.45
1:B:104:LEU:HD13	1:B:106:VAL:HG13	1.98	0.45
1:D:226:ASP:OD1	1:D:227:LEU:N	2.50	0.45
1:D:166:LEU:HB2	1:D:185:PHE:HB2	1.99	0.44
1:C:163:THR:CA	6:C:2009:HOH:O	2.66	0.44
1:F:263:ALA:HA	1:F:267:ASN:HD22	1.82	0.44
1:B:179:PHE:O	1:B:206:ALA:HB3	2.17	0.44
1:A:193:LYS:HB3	1:A:217:SER:CB	2.46	0.44
1:F:223:GLN:OE1	1:F:225:ASN:ND2	2.42	0.44
1:E:216:GLN:HE22	1:E:227:LEU:CD1	2.30	0.44
1:A:209:SER:O	1:A:248:SER:HB3	2.18	0.44
1:B:228:ASN:C	1:B:230:GLY:H	2.21	0.44
1:A:198:LEU:H	1:A:214:ASN:HD21	1.66	0.44
1:B:93:TRP:CD2	1:B:144:ARG:HD3	2.52	0.44
1:A:180:ALA:HA	1:A:204:GLY:HA3	2.00	0.44
1:D:159:THR:O	1:D:186:LYS:HG3	2.17	0.44
1:E:246:HIS:CE1	1:E:263:ALA:HB1	2.52	0.44
1:D:136:THR:HG22	1:D:141:PHE:CD1	2.53	0.44
1:B:201:PHE:HB2	1:B:208:ASP:OD2	2.18	0.44
1:B:93:TRP:CZ2	1:B:144:ARG:HA	2.52	0.44
1:E:117:TRP:HB3	1:E:284:LYS:HB2	1.99	0.44
1:F:78:ARG:HD2	1:F:78:ARG:HA	1.80	0.43
1:A:117:TRP:HB3	1:A:284:LYS:HB2	2.01	0.43
1:C:147:GLU:O	1:C:148:PHE:HB3	2.19	0.43
1:E:136:THR:HG22	1:E:141:PHE:CD1	2.53	0.43
1:C:117:TRP:HB3	1:C:284:LYS:HB2	2.00	0.43
1:E:189:ASP:OD1	1:E:192:GLU:HG2	2.18	0.43
1:D:113:ASP:HB2	1:D:167:ARG:NH2	2.32	0.43
1:B:144:ARG:NH2	1:C:94:HIS:NE2	2.66	0.43
1:F:98:LEU:C	1:F:100:ASP:H	2.21	0.43
1:E:151:GLY:O	1:E:155:ILE:HG13	2.18	0.43
1:E:202:VAL:HG12	1:E:203:GLU:HG2	1.99	0.43
1:C:240:TRP:CH2	1:C:250:LEU:HB2	2.54	0.43
1:A:214:ASN:HD22	1:A:215:ASN:H	1.65	0.43
1:B:111:ASP:C	1:B:111:ASP:OD1	2.56	0.43
1:E:244:ASN:N	1:E:245:CYS:HA	2.32	0.43
1:A:93:TRP:CD2	1:A:144:ARG:HD3	2.52	0.43
1:E:256:ARG:HG3	1:E:256:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.60	0.43
1:C:244:ASN:N	1:C:245:CYS:CA	2.81	0.43
1:C:228:ASN:C	1:C:230:GLY:H	2.22	0.43
1:C:198:LEU:HD23	1:C:211:THR:HA	2.00	0.43
1:B:144:ARG:HH22	1:C:94:HIS:CD2	2.37	0.43
1:E:221:LYS:HE2	3:E:1289:ACH:H63	2.01	0.43
1:A:216:GLN:OE1	1:A:217:SER:N	2.50	0.43
1:C:232:CYS:HA	1:C:235:MET:HE2	2.00	0.43
1:D:166:LEU:HB2	1:D:185:PHE:CB	2.49	0.42
1:B:263:ALA:HA	1:B:267:ASN:HD22	1.81	0.42
1:A:190:GLU:HG3	1:A:194:TYR:CE2	2.54	0.42
1:B:82:ASP:O	1:B:86:ARG:HG3	2.19	0.42
1:B:246:HIS:CE1	1:B:263:ALA:HB1	2.54	0.42
1:A:231:ASN:HD22	1:A:234:VAL:HB	1.83	0.42
1:B:102:ARG:CG	1:B:102:ARG:NH1	2.79	0.42
1:E:209:SER:HB2	1:E:268:TRP:CD2	2.54	0.42
1:A:151:GLY:HA3	6:A:2007:HOH:O	2.20	0.42
1:F:221:LYS:CE	3:F:1289:ACH:C6	2.97	0.42
1:A:172:ASP:HB2	1:A:276:TYR:HE1	1.83	0.42
1:C:211:THR:C	1:C:213:HIS:N	2.72	0.42
1:F:171:VAL:HB	1:F:280:VAL:HB	2.01	0.42
1:D:186:LYS:HB3	1:D:186:LYS:HE2	1.90	0.42
1:F:221:LYS:HZ1	3:F:1289:ACH:H63	1.82	0.42
1:D:147:GLU:O	1:D:148:PHE:HB3	2.19	0.42
1:C:188:ALA:O	1:C:194:TYR:HA	2.20	0.42
1:E:188:ALA:O	1:E:194:TYR:HA	2.19	0.42
1:B:147:GLU:O	1:B:148:PHE:HB3	2.20	0.42
1:D:81:LYS:NZ	1:D:85:ASP:OD1	2.46	0.42
1:B:244:ASN:O	1:B:244:ASN:ND2	2.53	0.42
1:D:172:ASP:HB2	1:D:276:TYR:CE1	2.54	0.42
1:C:265:GLY:H	1:C:267:ASN:ND2	2.17	0.42
1:A:183:ARG:HB3	6:A:2011:HOH:O	2.19	0.42
1:A:166:LEU:HB2	1:A:185:PHE:HB2	2.00	0.42
1:A:272:LYS:HB3	1:A:272:LYS:NZ	2.35	0.42
1:F:182:TYR:CD2	1:F:198:LEU:HD21	2.55	0.42
1:B:109:ASP:C	1:B:109:ASP:OD1	2.59	0.42
1:D:89:PHE:CE2	1:F:139:GLN:HB2	2.55	0.42
1:C:99:PRO:CB	1:C:161:GLN:HE21	2.33	0.41
1:D:76:GLY:HA3	1:D:77:PRO:HD3	1.83	0.41
1:D:265:GLY:H	1:D:267:ASN:ND2	2.18	0.41
1:B:188:ALA:O	1:B:194:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:OD1	1:C:208:ASP:C	2.58	0.41
1:E:111:ASP:OD1	1:E:111:ASP:C	2.58	0.41
1:C:134:TRP:HZ3	1:C:218:PHE:O	2.03	0.41
1:A:188:ALA:O	1:A:194:TYR:HA	2.20	0.41
1:A:100:ASP:OD1	1:A:100:ASP:C	2.58	0.41
1:E:93:TRP:CD2	1:E:144:ARG:HD3	2.56	0.41
1:A:152:ASN:HB3	1:A:194:TYR:CD1	2.55	0.41
1:C:256:ARG:HH11	1:C:256:ARG:HG3	1.86	0.41
1:E:231:ASN:N	1:E:235:MET:HE2	2.36	0.41
1:B:265:GLY:H	1:B:267:ASN:HD21	1.67	0.41
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.86	0.41
1:C:263:ALA:HA	1:C:267:ASN:HD22	1.86	0.41
1:D:138:LYS:HG2	1:D:153:ASP:OD2	2.21	0.41
1:B:221:LYS:HG2	1:B:221:LYS:H	1.61	0.41
1:D:280:VAL:HG12	1:D:281:SER:N	2.35	0.41
1:B:231:ASN:HD22	1:B:233:ALA:N	2.19	0.41
1:B:259:HIS:CE1	1:B:275:ASN:HA	2.56	0.41
1:C:175:ASP:OD2	1:C:279:LYS:NZ	2.53	0.41
1:A:136:THR:HG22	1:A:141:PHE:CD1	2.56	0.41
1:C:121:GLN:HG3	1:C:149:TRP:CE3	2.56	0.41
1:F:250:LEU:HD12	1:F:250:LEU:HA	1.91	0.41
1:E:74:LEU:HD23	1:E:74:LEU:HA	1.75	0.41
1:A:134:TRP:CB	1:A:223:GLN:HG3	2.44	0.40
1:C:227:LEU:HD12	1:C:243:LYS:HG2	2.03	0.40
1:D:250:LEU:HD12	1:D:266:ILE:HG22	2.03	0.40
1:E:181:LYS:HG2	1:E:182:TYR:N	2.36	0.40
1:D:77:PRO:HG3	1:D:86:ARG:NH1	2.36	0.40
1:E:221:LYS:HE2	3:E:1289:ACH:H61	2.02	0.40
1:A:109:ASP:C	1:A:109:ASP:OD1	2.59	0.40
1:F:95:THR:HA	1:F:105:THR:HA	2.02	0.40
1:B:221:LYS:HZ3	3:B:1289:ACH:C6	2.31	0.40
1:A:222:ASP:OD2	1:A:222:ASP:C	2.59	0.40
1:B:231:ASN:HD21	1:B:233:ALA:HB3	1.86	0.40
1:A:100:ASP:O	1:A:101:CYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	213/218 (98%)	187 (88%)	24 (11%)	2 (1%)	21	52
1	B	215/218 (99%)	195 (91%)	16 (7%)	4 (2%)	10	32
1	C	214/218 (98%)	189 (88%)	21 (10%)	4 (2%)	10	32
1	D	214/218 (98%)	189 (88%)	24 (11%)	1 (0%)	34	67
1	E	216/218 (99%)	191 (88%)	22 (10%)	3 (1%)	14	40
1	F	210/218 (96%)	192 (91%)	15 (7%)	3 (1%)	14	40
All	All	1282/1308 (98%)	1143 (89%)	122 (10%)	17 (1%)	15	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ALA
1	C	162	GLY
1	F	212	PHE
1	A	77	PRO
1	C	76	GLY
1	E	229	THR
1	A	202	VAL
1	B	203	GLU
1	B	229	THR
1	C	229	THR
1	E	164	SER
1	E	203	GLU
1	F	229	THR
1	F	99	PRO
1	B	287	PRO
1	C	212	PHE
1	D	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	180/183 (98%)	166 (92%)	14 (8%)	16	39
1	B	182/183 (100%)	167 (92%)	15 (8%)	14	36
1	C	181/183 (99%)	163 (90%)	18 (10%)	10	27
1	D	181/183 (99%)	160 (88%)	21 (12%)	7	18
1	E	183/183 (100%)	163 (89%)	20 (11%)	8	21
1	F	178/183 (97%)	163 (92%)	15 (8%)	14	35
All	All	1085/1098 (99%)	982 (90%)	103 (10%)	11	28

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	95	THR
1	A	101	CYS
1	A	104	LEU
1	A	124	VAL
1	A	150	LEU
1	A	165	GLU
1	A	167	ARG
1	A	183	ARG
1	A	193	LYS
1	A	214	ASN
1	A	231	ASN
1	A	250	LEU
1	A	281	SER
1	B	74	LEU
1	B	75	THR
1	B	90	LEU
1	B	95	THR
1	B	102	ARG
1	B	124	VAL
1	B	150	LEU
1	B	161	GLN

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Mol	Chain	Res	Type
1	B	164	SER
1	B	175	ASP
1	B	187	VAL
1	B	231	ASN
1	B	250	LEU
1	B	253	ARG
1	B	281	SER
1	C	74	LEU
1	C	90	LEU
1	C	95	THR
1	C	104	LEU
1	C	122	ARG
1	C	124	VAL
1	C	150	LEU
1	C	161	GLN
1	C	163	THR
1	C	177	TYR
1	C	196	LEU
1	C	197	VAL
1	C	219	SER
1	C	223	GLN
1	C	231	ASN
1	C	237	GLN
1	C	250	LEU
1	C	281	SER
1	D	90	LEU
1	D	95	THR
1	D	101	CYS
1	D	104	LEU
1	D	124	VAL
1	D	150	LEU
1	D	161	GLN
1	D	164[A]	SER
1	D	164[B]	SER
1	D	167	ARG
1	D	183	ARG
1	D	193	LYS
1	D	211	THR
1	D	219	SER
1	D	221	LYS
1	D	223	GLN
1	D	231	ASN

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Mol	Chain	Res	Type
1	D	245	CYS
1	D	250	LEU
1	D	253	ARG
1	D	281	SER
1	E	71	ASN
1	E	75	THR
1	E	90	LEU
1	E	95	THR
1	E	102	ARG
1	E	104	LEU
1	E	124	VAL
1	E	150	LEU
1	E	163	THR
1	E	175	ASP
1	E	187	VAL
1	E	203	GLU
1	E	221	LYS
1	E	231	ASN
1	E	237	GLN
1	E	243	LYS
1	E	250	LEU
1	E	253	ARG
1	E	272	LYS
1	E	281	SER
1	F	78	ARG
1	F	90	LEU
1	F	95	THR
1	F	104	LEU
1	F	124	VAL
1	F	150	LEU
1	F	164	SER
1	F	196	LEU
1	F	202	VAL
1	F	211	THR
1	F	223	GLN
1	F	231	ASN
1	F	247	THR
1	F	250	LEU
1	F	281	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	161	GLN
1	A	176	ASN
1	A	195	ASN
1	A	214	ASN
1	A	231	ASN
1	A	237	GLN
1	A	246	HIS
1	A	267	ASN
1	B	139	GLN
1	B	156	HIS
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	C	139	GLN
1	C	156	HIS
1	C	214	ASN
1	C	216	GLN
1	C	231	ASN
1	C	267	ASN
1	D	156	HIS
1	D	178	GLN
1	D	195	ASN
1	D	214	ASN
1	D	216	GLN
1	D	231	ASN
1	D	237	GLN
1	D	246	HIS
1	D	267	ASN
1	E	139	GLN
1	E	156	HIS
1	E	216	GLN
1	E	231	ASN
1	E	244	ASN
1	E	246	HIS
1	E	267	ASN
1	F	156	HIS
1	F	195	ASN
1	F	215	ASN
1	F	216	GLN
1	F	231	ASN
1	F	267	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 ⓘ

5 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	1291	1,4	14,14,15	0.74	0	15,19,21	1.94	3 (20%)
4	NAG	B	1292	4	14,14,15	0.55	0	15,19,21	1.10	2 (13%)
4	BMA	B	1293	4	11,11,12	0.53	0	14,15,17	2.42	4 (28%)
5	NAG	E	1291	1,5	14,14,15	0.78	0	15,19,21	1.50	3 (20%)
5	NAG	E	1292	5	14,14,15	0.68	0	15,19,21	1.47	3 (20%)

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	1291	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1292	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1293	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1291	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1292	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1291	NAG	C2-N2-C7	-4.98	116.64	123.04
4	B	1291	NAG	O4-C4-C3	-3.24	103.04	110.34
4	B	1293	BMA	C2-C3-C4	-3.01	105.94	111.04
4	B	1291	NAG	C3-C4-C5	-2.84	105.24	110.20
4	B	1292	NAG	C3-C4-C5	-2.38	106.06	110.20
5	E	1291	NAG	O4-C4-C3	-2.33	105.09	110.34
5	E	1291	NAG	O6-C6-C5	-2.02	104.65	111.33
4	B	1292	NAG	O4-C4-C5	2.05	114.67	109.24
5	E	1292	NAG	O4-C4-C5	2.11	114.83	109.24
5	E	1292	NAG	C2-N2-C7	2.16	125.82	123.04
5	E	1292	NAG	C1-O5-C5	2.70	115.68	112.25
5	E	1291	NAG	C1-O5-C5	3.00	116.06	112.25
4	B	1293	BMA	C1-C2-C3	3.02	113.11	109.54
4	B	1293	BMA	O5-C1-C2	3.48	116.50	110.86
4	B	1293	BMA	C1-O5-C5	6.35	120.31	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	ACH	A	1290	-	9,9,9	1.08	1 (11%)	12,12,12	0.66	0
3	ACH	B	1289	-	9,9,9	1.08	1 (11%)	12,12,12	0.78	0
3	ACH	C	1289	-	9,9,9	0.85	1 (11%)	12,12,12	0.79	0
3	ACH	E	1289	-	9,9,9	1.02	1 (11%)	12,12,12	0.59	0
3	ACH	F	1289	-	9,9,9	0.73	0	12,12,12	0.86	1 (8%)

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	ACH	A	1290	-	-	0/7/7/7	0/0/0/0
3	ACH	B	1289	-	-	0/7/7/7	0/0/0/0
3	ACH	C	1289	-	-	0/7/7/7	0/0/0/0
3	ACH	E	1289	-	-	0/7/7/7	0/0/0/0
3	ACH	F	1289	-	-	0/7/7/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1289	ACH	O4-C5	2.12	1.44	1.33
3	A	1290	ACH	O4-C5	2.47	1.46	1.33
3	E	1289	ACH	O4-C5	2.54	1.46	1.33
3	B	1289	ACH	O4-C5	2.65	1.47	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1289	ACH	C3-C2-N1	-2.06	109.41	116.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1290	ACH	5	0
3	B	1289	ACH	6	0
3	C	1289	ACH	6	0
3	E	1289	ACH	4	0
3	F	1289	ACH	8	0

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/218 (98%)	-0.26	1 (0%) 91 90	25, 39, 62, 66	2 (0%)
1	B	217/218 (99%)	-0.44	0 100 100	16, 32, 45, 51	0
1	C	216/218 (99%)	-0.50	0 100 100	22, 33, 54, 64	1 (0%)
1	D	214/218 (98%)	-0.23	1 (0%) 91 90	25, 39, 63, 66	5 (2%)
1	E	218/218 (100%)	-0.46	0 100 100	16, 32, 43, 48	2 (0%)
1	F	212/218 (97%)	-0.47	0 100 100	20, 33, 44, 56	1 (0%)
All	All	1291/1308 (98%)	-0.39	2 (0%) 95 95	16, 34, 58, 66	11 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	GLN	2.9
1	A	191	ALA	2.5

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	E	1291	14/15	0.94	0.15	-	25,29,33,34	0
5	NAG	E	1292	14/15	0.95	0.17	-	36,38,40,41	0
4	NAG	B	1292	14/15	0.91	0.25	-	44,46,49,52	0
4	NAG	B	1291	14/15	0.90	0.20	-	32,36,39,42	0
4	BMA	B	1293	11/12	0.91	0.16	-	55,57,58,59	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	1290	1/1	0.86	0.18	5.85	33,33,33,33	0
2	CA	E	1290	1/1	0.84	0.20	3.77	32,32,32,32	0
3	ACH	C	1289	10/10	0.94	0.18	2.44	23,36,39,40	0
3	ACH	F	1289	10/10	0.94	0.21	2.39	14,29,35,37	0
2	CA	C	1290	1/1	0.91	0.18	2.01	35,35,35,35	0
2	CA	F	1290	1/1	0.89	0.13	0.02	35,35,35,35	0
2	CA	D	1289	1/1	0.94	0.10	-1.84	64,64,64,64	0
2	CA	A	1289	1/1	0.73	0.07	-4.52	69,69,69,69	0
3	ACH	E	1289	10/10	0.89	0.24	-	31,41,42,43	6
3	ACH	B	1289	10/10	0.91	0.25	-	27,39,40,41	6
3	ACH	A	1290	10/10	0.91	0.35	-	76,76,77,77	6

6.5 Other polymers

There are no such residues in this entry.