Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:59 AM EDT

PDB ID	:	6FGA
Title	:	Crystal structure of TRIM21 E3 ligase, RING domain in complex with its cognate E2 conjugating enzyme UBE2E1
Authors	:	Anandapadamanaban, M.; Moche, M.; Sunnerhagen, M.
Deposited on	:	2018-01-10
Resolution	:	2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

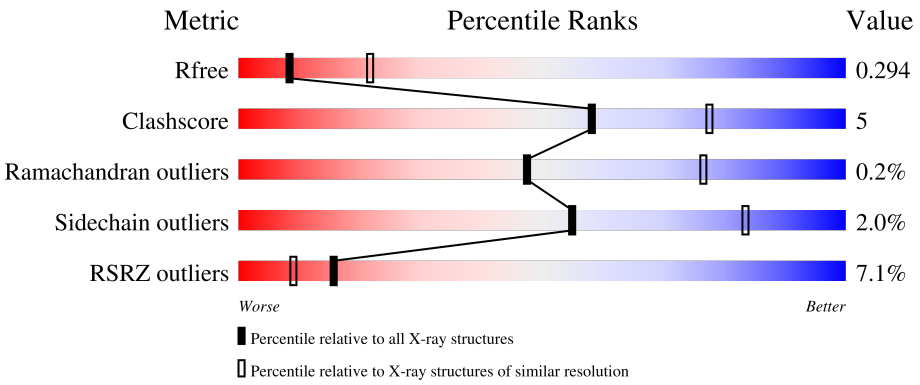
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.82 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	101	8%, 68%, 7%, 25%
1	B	101	10%, 69%, 5%, 25%
1	C	101	7%, 62%, 13%, 22%
1	D	101	9%, 60%, 10%, 30%
1	E	101	3%, 65%, 10%, 22%

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Mol	Chain	Length	Quality of chain
1	F	101	9% 65% 10% 24%
1	G	101	3% 70% 5% 24%
1	H	101	5% 73% 24%
2	I	158	83% 12% 5%
2	J	158	3% 96%
2	K	158	33% 91%
2	L	158	3% 89% 5% 6%
2	M	158	87% 8% 5%
2	N	158	2% 90% 6%
2	O	158	87% 7% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13206 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 E3 ubiquitin-protein ligase TRIM21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	76	591	368	104	109	10	0	0	0
1	B	76	593	369	107	107	10	0	0	0
1	C	79	612	380	110	112	10	0	0	0
1	D	71	552	345	98	99	10	0	0	0
1	E	79	612	380	110	112	10	0	0	0
1	F	77	602	374	108	110	10	0	0	0
1	G	77	602	374	108	110	10	0	0	0
1	H	77	602	374	108	110	10	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P19474
A	-1	SER	-	expression tag	UNP P19474
A	0	HIS	-	expression tag	UNP P19474
B	-2	GLY	-	expression tag	UNP P19474
B	-1	SER	-	expression tag	UNP P19474
B	0	HIS	-	expression tag	UNP P19474
C	-2	GLY	-	expression tag	UNP P19474
C	-1	SER	-	expression tag	UNP P19474
C	0	HIS	-	expression tag	UNP P19474
D	-2	GLY	-	expression tag	UNP P19474
D	-1	SER	-	expression tag	UNP P19474
D	0	HIS	-	expression tag	UNP P19474
E	-2	GLY	-	expression tag	UNP P19474

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP P19474
E	0	HIS	-	expression tag	UNP P19474
F	-2	GLY	-	expression tag	UNP P19474
F	-1	SER	-	expression tag	UNP P19474
F	0	HIS	-	expression tag	UNP P19474
G	-2	GLY	-	expression tag	UNP P19474
G	-1	SER	-	expression tag	UNP P19474
G	0	HIS	-	expression tag	UNP P19474
H	-2	GLY	-	expression tag	UNP P19474
H	-1	SER	-	expression tag	UNP P19474
H	0	HIS	-	expression tag	UNP P19474

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	150	1179	753	200	219	7	0	0	0
			Total	C	N	O	S			
2	J	156	1225	780	209	228	8	0	0	0
			Total	C	N	O	S			
2	K	151	1188	759	202	220	7	0	0	0
			Total	C	N	O	S			
2	L	148	1163	741	198	217	7	0	0	0
			Total	C	N	O	S			
2	M	150	1179	753	200	219	7	0	0	0
			Total	C	N	O	S			
2	N	152	1194	762	203	222	7	0	0	0
			Total	C	N	O	S			
2	O	148	1163	741	198	217	7	0	0	0

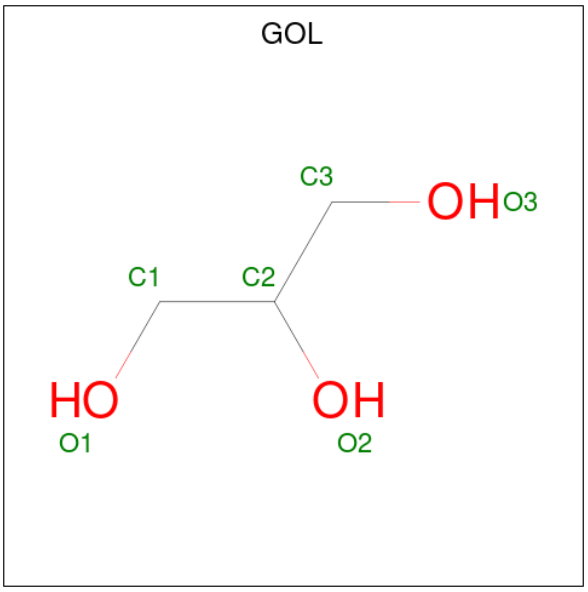
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	36	GLY	-	expression tag	UNP P51965
J	36	GLY	-	expression tag	UNP P51965
K	36	GLY	-	expression tag	UNP P51965
L	36	GLY	-	expression tag	UNP P51965
M	36	GLY	-	expression tag	UNP P51965
N	36	GLY	-	expression tag	UNP P51965
O	36	GLY	-	expression tag	UNP P51965

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

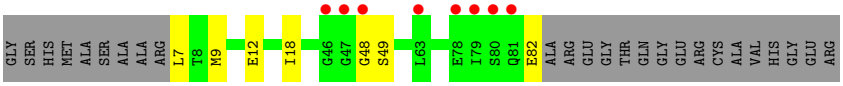
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	D	1	1	1	0	0
			Total	O		
5	E	1	1	1	0	0
			Total	O		
5	F	1	1	1	0	0
			Total	O		
5	H	1	1	1	0	0
			Total	O		
5	I	32	32	32	0	0
			Total	O		
5	J	16	16	16	0	0
			Total	O		
5	L	10	10	10	0	0
			Total	O		
5	M	5	5	5	0	0
			Total	O		
5	N	21	21	21	0	0
			Total	O		
5	O	21	21	21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

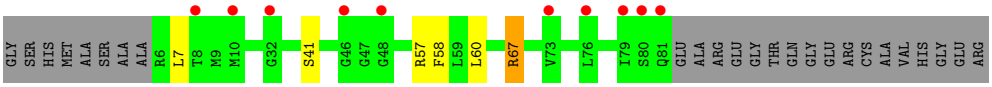
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain A:



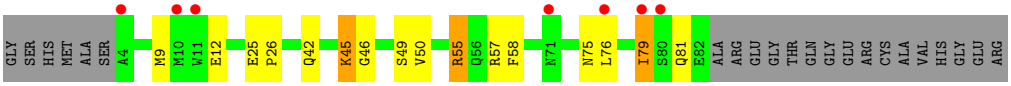
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain B:



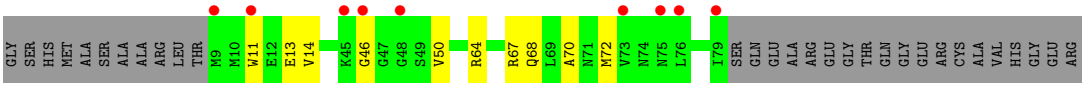
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain C:



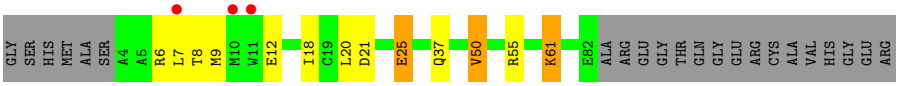
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain D:



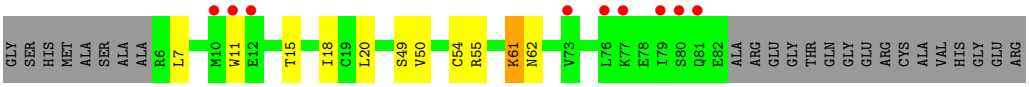
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain E:



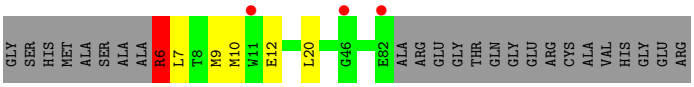
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain F:



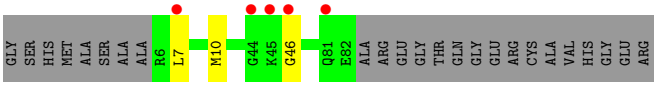
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain G:



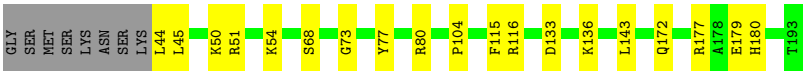
• Molecule 1: E3 ubiquitin-protein ligase TRIM21

Chain H:



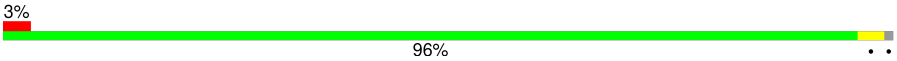
• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain I:



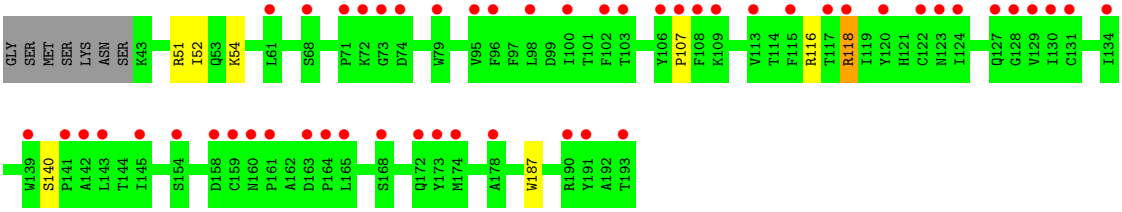
• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain J:



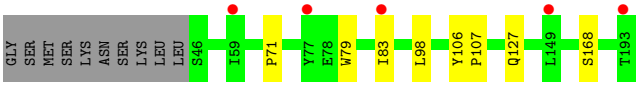
• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain K:



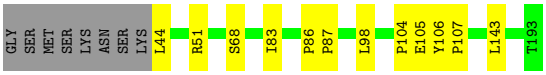
• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain L:



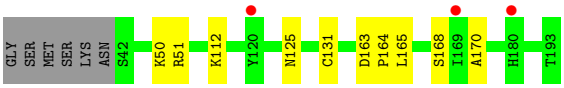
• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain M:



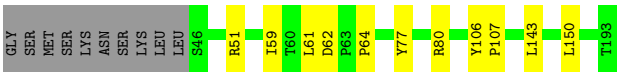
• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain N:



• Molecule 2: Ubiquitin-conjugating enzyme E2 E1

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.83Å 95.87Å 235.10Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	47.90 – 2.82 47.94 – 2.82	Depositor EDS
% Data completeness (in resolution range)	91.2 (47.90-2.82) 91.2 (47.94-2.82)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.253 , 0.294 0.255 , 0.294	Depositor DCC
R_{free} test set	2549 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13206	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL

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	0.67	0/601	0.69	0/811
1	B	0.67	0/603	0.69	0/813
1	C	0.67	0/622	0.70	0/839
1	D	0.71	0/562	0.78	0/758
1	E	0.71	0/622	0.84	0/839
1	F	0.75	0/612	0.82	0/825
1	G	0.64	0/612	0.75	1/825 (0.1%)
1	H	0.67	0/612	0.73	0/825
2	I	0.70	0/1210	0.84	0/1651
2	J	0.65	0/1256	0.73	0/1710
2	K	0.67	0/1219	0.76	1/1662 (0.1%)
2	L	0.65	0/1194	0.72	0/1629
2	M	0.63	0/1210	0.73	0/1651
2	N	0.70	0/1225	0.79	0/1670
2	O	0.65	0/1194	0.73	0/1629
All	All	0.67	0/13354	0.75	2/18137 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	118	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	G	6	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	591	0	584	4	0
1	B	593	0	590	4	0
1	C	612	0	606	16	0
1	D	552	0	546	9	0
1	E	612	0	606	20	0
1	F	602	0	596	12	0
1	G	602	0	596	15	1
1	H	602	0	596	0	0
2	I	1179	0	1179	15	0
2	J	1225	0	1230	3	0
2	K	1188	0	1192	6	1
2	L	1163	0	1157	5	0
2	M	1179	0	1179	8	0
2	N	1194	0	1197	13	0
2	O	1163	0	1157	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	I	12	0	16	1	0
4	J	6	0	8	1	0
4	N	6	0	8	1	0
5	D	1	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	I	32	0	0	1	0
5	J	16	0	0	1	0
5	L	10	0	0	2	0
5	M	5	0	0	0	0
5	N	21	0	0	0	0
5	O	21	0	0	0	0
All	All	13206	0	13043	125	1

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 5.

All (125) 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:G:6:ARG:HD3	1:G:7:LEU:N	1.46	1.28
1:G:6:ARG:CD	1:G:7:LEU:H	1.61	1.14
1:G:6:ARG:CD	1:G:7:LEU:HD23	1.87	1.03
1:G:6:ARG:HD3	1:G:7:LEU:H	0.85	1.01
1:D:68:GLN:OE1	1:D:68:GLN:N	2.05	0.90
1:G:6:ARG:HD2	1:G:7:LEU:HD23	1.54	0.88
2:M:44:LEU:HD13	2:M:104:PRO:HB2	1.57	0.85
2:K:51:ARG:NH1	2:K:107:PRO:HG3	1.93	0.84
1:C:45:LYS:CG	1:C:46:GLY:N	2.49	0.74
2:J:47:THR:O	5:J:301:HOH:O	2.04	0.73
1:E:25:GLU:CG	1:E:37:GLN:HB3	2.18	0.72
1:B:57:ARG:HG3	1:B:58:PHE:N	2.05	0.71
1:G:6:ARG:NH1	1:G:6:ARG:HA	2.06	0.70
1:C:45:LYS:HG2	1:C:46:GLY:N	2.06	0.70
2:K:51:ARG:O	2:K:54:LYS:N	2.25	0.69
1:G:6:ARG:HA	1:G:6:ARG:HH11	1.56	0.68
1:A:18:ILE:O	2:K:51:ARG:NH1	2.27	0.68
1:C:81:GLN:OE1	1:C:81:GLN:HA	1.92	0.67
2:I:172:GLN:HG2	2:I:180:HIS:HB2	1.75	0.67
1:C:45:LYS:HG2	1:C:46:GLY:H	1.60	0.67
1:E:9:MET:HA	1:E:12:GLU:HG3	1.78	0.65
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.61	0.65
2:M:44:LEU:CD1	2:M:104:PRO:HB2	2.28	0.64
2:M:104:PRO:HG2	2:M:105:GLU:OE2	1.99	0.63
1:C:75:ASN:O	1:C:79:ILE:HG13	1.99	0.62
1:D:13:GLU:HA	1:D:13:GLU:OE1	1.99	0.61
1:G:6:ARG:HH11	1:G:6:ARG:CA	2.13	0.61
1:A:82:GLU:OE2	1:E:6:ARG:NH1	2.34	0.61
1:E:25:GLU:HG3	1:E:37:GLN:HB3	1.82	0.61
1:G:6:ARG:CD	1:G:7:LEU:N	2.36	0.60
2:I:44:LEU:HD12	2:I:44:LEU:O	2.02	0.60
1:G:6:ARG:NE	1:G:7:LEU:HD23	2.16	0.59
1:F:50:VAL:CG1	1:F:55:ARG:C	2.71	0.59
1:D:68:GLN:NE2	5:D:201:HOH:O	2.36	0.58
1:C:57:ARG:HG3	1:C:58:PHE:N	2.18	0.58
1:E:61:LYS:HE3	2:I:133:ASP:OD1	2.04	0.58
1:E:25:GLU:O	1:E:25:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:HD3	1:G:7:LEU:HD23	1.83	0.57
1:B:67:ARG:HG2	1:B:67:ARG:NH1	2.19	0.57
1:F:50:VAL:HG12	1:F:55:ARG:C	2.24	0.57
2:N:125:ASN:HB3	2:N:165:LEU:CD2	2.36	0.56
1:G:7:LEU:O	1:G:10:MET:HB2	2.05	0.56
2:K:118:ARG:NH1	2:K:187:TRP:CH2	2.74	0.56
1:F:54:CYS:O	1:F:55:ARG:HB2	2.05	0.55
2:L:168:SER:HB3	5:L:203:HOH:O	2.05	0.55
1:G:6:ARG:HH11	1:G:6:ARG:CB	2.19	0.55
1:A:9:MET:O	1:A:12:GLU:HB3	2.06	0.55
1:E:21:ASP:OD2	2:N:50:LYS:HE2	2.07	0.54
1:C:75:ASN:O	1:C:79:ILE:CG1	2.55	0.54
2:K:51:ARG:HH11	2:K:107:PRO:HG3	1.71	0.54
1:C:50:VAL:HG13	1:C:55:ARG:HA	1.91	0.53
1:D:64:ARG:NH2	1:F:62:ASN:O	2.22	0.53
2:O:64:PRO:HB3	2:O:150:LEU:HD21	1.90	0.53
1:E:9:MET:HA	1:E:12:GLU:CG	2.39	0.53
1:F:50:VAL:CG1	1:F:55:ARG:O	2.57	0.53
1:G:7:LEU:H	1:G:7:LEU:HD23	1.75	0.52
1:E:8:THR:O	1:E:12:GLU:HG3	2.09	0.51
2:N:131:CYS:SG	2:N:163:ASP:OD2	2.67	0.51
2:I:115:PHE:O	4:I:202:GOL:H31	2.09	0.51
2:N:164:PRO:HB3	2:N:170:ALA:HB2	1.93	0.51
1:E:50:VAL:CG1	1:E:55:ARG:O	2.58	0.51
1:E:20:LEU:HD12	2:N:51:ARG:HD2	1.92	0.50
1:C:42:GLN:OE1	1:C:45:LYS:HD3	2.11	0.50
1:C:25:GLU:N	1:C:26:PRO:CD	2.75	0.50
1:E:9:MET:HA	1:E:12:GLU:CD	2.32	0.50
1:F:18:ILE:O	2:I:51:ARG:NH1	2.44	0.50
2:I:44:LEU:HD12	2:I:44:LEU:C	2.32	0.49
1:C:50:VAL:CG1	1:C:55:ARG:HA	2.43	0.49
2:I:45:LEU:HD22	2:I:77:TYR:OH	2.12	0.49
2:I:177:ARG:O	2:I:177:ARG:HG3	2.13	0.49
2:M:83:ILE:HD12	2:M:98:LEU:CD1	2.43	0.49
1:G:9:MET:O	1:G:12:GLU:HB2	2.11	0.49
1:F:11:TRP:O	1:F:15:THR:HG23	2.13	0.48
1:D:11:TRP:HA	1:D:14:VAL:HG22	1.96	0.48
1:F:61:LYS:HE2	2:N:163:ASP:CG	2.34	0.48
1:E:50:VAL:HG12	1:E:55:ARG:O	2.13	0.48
1:F:50:VAL:HG11	1:F:55:ARG:O	2.14	0.47
1:E:9:MET:CA	1:E:12:GLU:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:125:ASN:ND2	2:N:165:LEU:HD21	2.30	0.46
2:I:44:LEU:HD11	2:I:104:PRO:O	2.16	0.46
1:D:67:ARG:O	1:D:70:ALA:HB3	2.17	0.45
1:C:9:MET:H	1:C:9:MET:HG2	1.54	0.45
1:D:67:ARG:O	1:D:70:ALA:N	2.49	0.45
2:N:125:ASN:HB3	2:N:165:LEU:HG	1.99	0.44
1:E:18:ILE:O	2:N:51:ARG:NH1	2.50	0.44
1:E:25:GLU:HG3	1:E:37:GLN:CB	2.48	0.44
2:L:71:PRO:HA	2:L:79:TRP:HA	1.99	0.44
1:F:20:LEU:HB2	2:I:54:LYS:HE2	1.98	0.44
2:N:125:ASN:CG	2:N:165:LEU:HD21	2.38	0.44
2:L:83:ILE:HD12	2:L:98:LEU:HD11	1.99	0.44
2:O:61:LEU:HD23	2:O:62:ASP:HB2	2.00	0.44
2:N:125:ASN:N	2:N:165:LEU:HD23	2.33	0.43
1:C:76:LEU:HA	1:C:79:ILE:HG13	1.99	0.43
2:J:130:ILE:H	4:J:201:GOL:H12	1.83	0.43
1:B:41:SER:HA	1:B:60:LEU:HD11	2.00	0.43
1:C:9:MET:O	1:C:12:GLU:N	2.51	0.43
1:D:72:MET:HB3	1:D:72:MET:HE2	1.83	0.43
2:I:50:LYS:O	2:I:54:LYS:HG3	2.19	0.43
2:I:51:ARG:NH2	2:I:143:LEU:O	2.51	0.43
1:D:67:ARG:HB2	1:D:68:GLN:OE1	2.19	0.43
2:J:51:ARG:NH1	2:J:141:PRO:O	2.50	0.43
1:C:55:ARG:HH11	1:C:55:ARG:HG3	1.84	0.43
1:E:9:MET:O	1:E:12:GLU:HB2	2.19	0.43
2:O:106:TYR:CD1	2:O:107:PRO:HA	2.54	0.43
2:K:51:ARG:O	2:K:52:ILE:C	2.57	0.42
2:I:73:GLY:N	5:I:302:HOH:O	2.53	0.42
2:I:179:GLU:OE1	2:I:179:GLU:HA	2.19	0.42
2:M:51:ARG:NH2	2:M:143:LEU:O	2.53	0.42
2:O:77:TYR:CD1	2:O:77:TYR:N	2.88	0.42
2:N:112:LYS:HA	4:N:201:GOL:H32	2.02	0.42
2:N:163:ASP:HA	2:N:164:PRO:HD3	1.85	0.41
1:A:9:MET:O	1:A:12:GLU:CB	2.69	0.41
2:L:106:TYR:CD1	2:L:107:PRO:HA	2.56	0.41
2:M:86:PRO:HA	2:M:87:PRO:HD3	1.98	0.41
1:C:45:LYS:HG3	1:C:46:GLY:N	2.31	0.41
1:F:50:VAL:HG12	1:F:55:ARG:HA	2.03	0.41
2:M:106:TYR:CD1	2:M:107:PRO:HA	2.56	0.41
2:O:51:ARG:NH2	2:O:143:LEU:O	2.53	0.41
2:I:45:LEU:CD2	2:I:77:TYR:OH	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:VAL:HG11	1:E:55:ARG:O	2.22	0.40
1:E:25:GLU:HG2	1:E:37:GLN:HB3	2.01	0.40
1:E:25:GLU:CG	1:E:37:GLN:CB	2.95	0.40
1:F:61:LYS:HE3	1:F:61:LYS:HB2	1.72	0.40
2:L:168:SER:CB	5:L:203:HOH:O	2.67	0.40
2:M:83:ILE:HD12	2:M:98:LEU:HD13	2.03	0.40

All (1) 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:G:20:LEU:CD1	2:K:118:ARG:NH2[1_565]	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	74/101 (73%)	71 (96%)	2 (3%)	1 (1%)	11	32
1	B	74/101 (73%)	70 (95%)	4 (5%)	0	100	100
1	C	77/101 (76%)	73 (95%)	3 (4%)	1 (1%)	12	34
1	D	69/101 (68%)	65 (94%)	3 (4%)	1 (1%)	11	32
1	E	77/101 (76%)	74 (96%)	3 (4%)	0	100	100
1	F	75/101 (74%)	72 (96%)	3 (4%)	0	100	100
1	G	75/101 (74%)	69 (92%)	6 (8%)	0	100	100
1	H	75/101 (74%)	72 (96%)	2 (3%)	1 (1%)	12	34
2	I	148/158 (94%)	145 (98%)	3 (2%)	0	100	100
2	J	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
2	K	149/158 (94%)	145 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	146/158 (92%)	143 (98%)	3 (2%)	0	100	100
2	M	148/158 (94%)	146 (99%)	2 (1%)	0	100	100
2	N	150/158 (95%)	144 (96%)	6 (4%)	0	100	100
2	O	146/158 (92%)	142 (97%)	4 (3%)	0	100	100
All	All	1637/1914 (86%)	1581 (97%)	52 (3%)	4 (0%)	47	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	46	GLY
1	C	49	SER
1	A	48	GLY
1	H	46	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	70/86 (81%)	68 (97%)	2 (3%)	42	74
1	B	70/86 (81%)	68 (97%)	2 (3%)	42	74
1	C	71/86 (83%)	68 (96%)	3 (4%)	30	62
1	D	65/86 (76%)	64 (98%)	1 (2%)	65	88
1	E	71/86 (83%)	67 (94%)	4 (6%)	21	49
1	F	71/86 (83%)	68 (96%)	3 (4%)	30	62
1	G	71/86 (83%)	70 (99%)	1 (1%)	67	89
1	H	71/86 (83%)	69 (97%)	2 (3%)	43	76
2	I	133/140 (95%)	129 (97%)	4 (3%)	41	73
2	J	139/140 (99%)	138 (99%)	1 (1%)	84	95
2	K	134/140 (96%)	132 (98%)	2 (2%)	65	88
2	L	131/140 (94%)	130 (99%)	1 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	133/140 (95%)	132 (99%)	1 (1%)	81	94
2	N	135/140 (96%)	134 (99%)	1 (1%)	84	95
2	O	131/140 (94%)	129 (98%)	2 (2%)	65	88
All	All	1496/1668 (90%)	1466 (98%)	30 (2%)	55	83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	49	SER
1	B	7	LEU
1	B	67	ARG
1	C	45	LYS
1	C	55	ARG
1	C	79	ILE
1	D	50	VAL
1	E	7	LEU
1	E	25	GLU
1	E	50	VAL
1	E	61	LYS
1	F	7	LEU
1	F	49	SER
1	F	61	LYS
1	G	6	ARG
1	H	7	LEU
1	H	10	MET
2	I	68	SER
2	I	80	ARG
2	I	116	ARG
2	I	136	LYS
2	J	146	SER
2	K	116	ARG
2	K	140	SER
2	L	127	GLN
2	M	68	SER
2	N	168	SER
2	O	59	ILE
2	O	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	68	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	GOL	N	201	-	5,5,5	0.10	0	5,5,5	0.31	0
4	GOL	J	201	-	5,5,5	0.10	0	5,5,5	0.40	0
4	GOL	I	202	-	5,5,5	0.21	0	5,5,5	0.48	0
4	GOL	I	201	-	5,5,5	0.13	0	5,5,5	0.45	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
4	GOL	N	201	-	-	2/4/4/4	-
4	GOL	J	201	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	I	202	-	-	0/4/4/4	-
4	GOL	I	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	201	GOL	O1-C1-C2-C3
4	N	201	GOL	O1-C1-C2-O2
4	I	201	GOL	O1-C1-C2-O2
4	I	201	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	201	GOL	1	0
4	J	201	GOL	1	0
4	I	202	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	76/101 (75%)	0.48	8 (10%) 6 3	68, 122, 180, 206	0
1	B	76/101 (75%)	0.69	10 (13%) 3 2	80, 112, 167, 178	0
1	C	79/101 (78%)	0.55	7 (8%) 9 5	78, 117, 198, 227	0
1	D	71/101 (70%)	0.70	9 (12%) 3 2	51, 95, 180, 222	0
1	E	79/101 (78%)	0.25	3 (3%) 40 30	45, 80, 133, 160	0
1	F	77/101 (76%)	0.56	9 (11%) 4 2	43, 73, 189, 209	0
1	G	77/101 (76%)	0.30	3 (3%) 39 29	73, 108, 150, 161	0
1	H	77/101 (76%)	0.21	5 (6%) 18 11	59, 85, 141, 154	0
2	I	150/158 (94%)	-0.08	0 100 100	14, 58, 87, 139	0
2	J	156/158 (98%)	0.17	4 (2%) 56 46	42, 81, 143, 159	0
2	K	151/158 (95%)	1.68	52 (34%) 0 0	117, 169, 200, 222	0
2	L	148/158 (93%)	0.18	5 (3%) 45 35	44, 88, 144, 161	0
2	M	150/158 (94%)	0.25	0 100 100	43, 86, 147, 184	0
2	N	152/158 (96%)	0.18	3 (1%) 65 56	14, 68, 109, 124	0
2	O	148/158 (93%)	0.09	0 100 100	38, 70, 99, 123	0
All	All	1667/1914 (87%)	0.39	118 (7%) 16 9	14, 90, 176, 227	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	74	ASP	8.6
2	K	163	ASP	6.7
1	D	48	GLY	6.3
2	K	165	LEU	6.0
2	K	113	VAL	5.7
2	K	130	ILE	5.4
1	D	46	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
2	K	115	PHE	4.9
2	K	127	GLN	4.8
2	K	96	PHE	4.7
2	K	98	LEU	4.7
2	K	160	ASN	4.7
1	F	80	SER	4.6
2	K	161	PRO	4.5
1	D	9	MET	4.5
2	K	61	LEU	4.5
2	K	164	PRO	4.4
1	C	10	MET	4.4
2	K	159	CYS	4.3
2	K	134	ILE	4.2
2	K	118	ARG	4.2
1	D	79	ILE	4.1
1	F	73	VAL	4.1
2	K	73	GLY	4.0
1	A	80	SER	4.0
1	B	48	GLY	4.0
1	D	76	LEU	4.0
2	K	174	MET	3.9
1	B	32	GLY	3.8
2	K	193	THR	3.8
2	K	107	PRO	3.8
2	K	131	CYS	3.7
1	B	76	LEU	3.7
2	K	191	TYR	3.7
1	B	80	SER	3.7
1	A	48	GLY	3.6
1	G	46	GLY	3.6
2	K	68	SER	3.6
1	C	80	SER	3.6
2	K	100	ILE	3.5
2	K	190	ARG	3.5
2	K	103	THR	3.5
2	K	128	GLY	3.4
2	K	168	SER	3.4
1	B	46	GLY	3.4
2	K	178	ALA	3.4
1	H	44	GLY	3.4
1	H	45	LYS	3.4
2	K	120	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
2	N	180	HIS	3.3
2	N	120	TYR	3.1
1	F	79	ILE	3.1
1	G	11	TRP	3.1
2	K	124	ILE	3.1
2	K	141	PRO	3.1
1	F	10	MET	3.1
1	D	11	TRP	3.0
1	F	11	TRP	3.0
1	C	76	LEU	3.0
2	K	172	GLN	2.9
2	K	72	LYS	2.9
2	L	59	ILE	2.9
2	K	143	LEU	2.9
2	K	102	PHE	2.9
2	L	193	THR	2.8
1	B	73	VAL	2.8
2	K	106	TYR	2.8
1	G	82	GLU	2.7
1	F	77	LYS	2.7
1	E	7	LEU	2.7
1	E	10	MET	2.6
2	L	77	TYR	2.6
2	K	109	LYS	2.6
2	J	173	TYR	2.6
1	F	76	LEU	2.6
1	B	81	GLN	2.6
2	K	173	TYR	2.6
2	K	129	VAL	2.6
1	B	8	THR	2.6
1	H	7	LEU	2.5
2	J	167	GLY	2.5
1	D	75	ASN	2.5
1	B	10	MET	2.5
1	F	12	GLU	2.5
1	D	45	LYS	2.4
2	K	123	ASN	2.4
1	D	73	VAL	2.4
1	A	79	ILE	2.4
1	B	79	ILE	2.4
2	N	169	ILE	2.4
1	A	46	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	122	CYS	2.3
2	J	120	TYR	2.3
2	K	139	TRP	2.3
1	A	81	GLN	2.3
1	F	81	GLN	2.3
2	K	71	PRO	2.3
1	E	11	TRP	2.3
1	H	81	GLN	2.3
2	K	154	SER	2.2
1	A	47	GLY	2.2
1	C	79	ILE	2.2
1	A	63	LEU	2.2
2	K	108	PHE	2.2
2	K	79	TRP	2.2
2	L	149	LEU	2.1
1	C	71	ASN	2.1
2	K	158	ASP	2.1
2	K	95	VAL	2.1
1	H	46	GLY	2.1
2	K	145	ILE	2.1
1	C	11	TRP	2.0
1	A	78	GLU	2.0
2	L	83	ILE	2.0
2	K	142	ALA	2.0
2	J	90	VAL	2.0
1	C	4	ALA	2.0
2	K	117	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	B-factors(Å^2)	Q<0.9
4	GOL	N	201	6/6	0.77	0.34	104,114,114,115	0
4	GOL	I	202	6/6	0.82	0.49	78,85,86,94	0
4	GOL	I	201	6/6	0.85	0.29	94,97,99,103	0
4	GOL	J	201	6/6	0.89	0.36	97,99,103,105	0
3	ZN	A	102	1/1	0.89	0.04	133,133,133,133	0
3	ZN	C	102	1/1	0.94	0.03	87,87,87,87	0
3	ZN	D	101	1/1	0.95	0.06	51,51,51,51	0
3	ZN	E	102	1/1	0.97	0.08	49,49,49,49	0
3	ZN	B	101	1/1	0.97	0.03	93,93,93,93	0
3	ZN	C	101	1/1	0.97	0.07	80,80,80,80	0
3	ZN	D	102	1/1	0.97	0.06	85,85,85,85	0
3	ZN	E	101	1/1	0.97	0.07	46,46,46,46	0
3	ZN	G	102	1/1	0.98	0.03	100,100,100,100	0
3	ZN	A	101	1/1	0.98	0.04	66,66,66,66	0
3	ZN	B	102	1/1	0.98	0.02	89,89,89,89	0
3	ZN	F	102	1/1	0.98	0.08	53,53,53,53	0
3	ZN	G	101	1/1	0.98	0.03	67,67,67,67	0
3	ZN	H	101	1/1	0.99	0.03	69,69,69,69	0
3	ZN	H	102	1/1	0.99	0.06	54,54,54,54	0
3	ZN	F	101	1/1	0.99	0.08	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.