Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 12:20 pm GMT

PDB ID	:	6ZBU
Title	:	Crystal structure of an NCoR1BBD2-BCL6BTB chimera in complex with the NcoR1 BBD1 corepressor peptide
Authors	:	Zacharchenko, T.; Wright, S.C.
Deposited on	:	2020-06-09
Resolution	:	2.46 Å(reported)

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

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

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

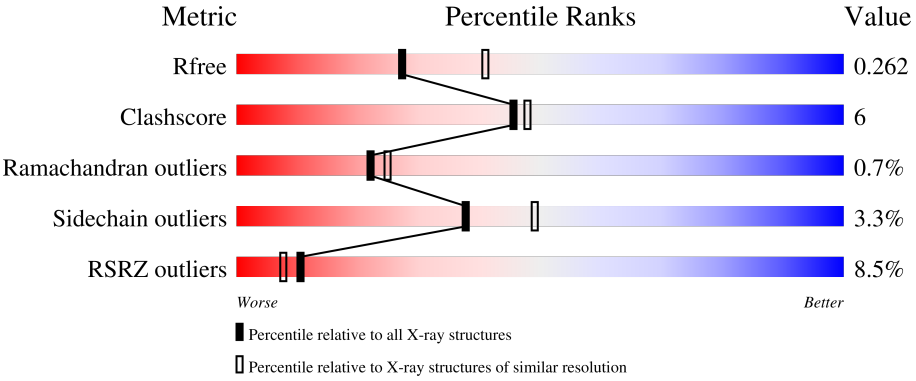
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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

Mol	Chain	Length	Quality of chain
1	A	137	2% 80% 15%
1	B	137	% 88% 7%
1	E	137	6% 78% 16% 5%
1	F	137	15% 78% 16%
1	I	137	7% 80% 13% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	137	16% 81% 13%
2	C	17	76% 12% 12%
2	D	17	65% 29% 6%
2	G	17	6% 76% 12% 12%
2	H	17	29% 71% 18% 6% 6%
2	K	17	71% 18% 12%
2	L	17	35% 71% 24% 6%

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
3	SO4	A	204	-	-	-	X
3	SO4	B	204	-	-	-	X
3	SO4	J	201	-	-	X	-
4	GOL	A	205	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7421 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 Nuclear receptor corepressor 1,B-cell lymphoma 6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	2	0
			1084	686	191	199	8			
1	B	134	Total	C	N	O	S	0	1	0
			1090	688	194	200	8			
1	E	130	Total	C	N	O	S	0	0	0
			1048	663	186	191	8			
1	F	131	Total	C	N	O	S	0	0	0
			1051	664	186	193	8			
1	I	130	Total	C	N	O	S	0	0	0
			1048	663	186	191	8			
1	J	132	Total	C	N	O	S	0	0	0
			1054	665	187	194	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O75376
A	-6	PRO	-	expression tag	UNP O75376
A	4	GLY	-	linker	UNP O75376
A	5	GLY	-	linker	UNP O75376
A	8	GLN	CYS	conflict	UNP P41182
A	67	ARG	CYS	conflict	UNP P41182
A	84	ASN	CYS	conflict	UNP P41182
B	-7	GLY	-	expression tag	UNP O75376
B	-6	PRO	-	expression tag	UNP O75376
B	4	GLY	-	linker	UNP O75376
B	5	GLY	-	linker	UNP O75376
B	8	GLN	CYS	conflict	UNP P41182
B	67	ARG	CYS	conflict	UNP P41182
B	84	ASN	CYS	conflict	UNP P41182
E	-7	GLY	-	expression tag	UNP O75376
E	-6	PRO	-	expression tag	UNP O75376
E	4	GLY	-	linker	UNP O75376

Continued on next page...

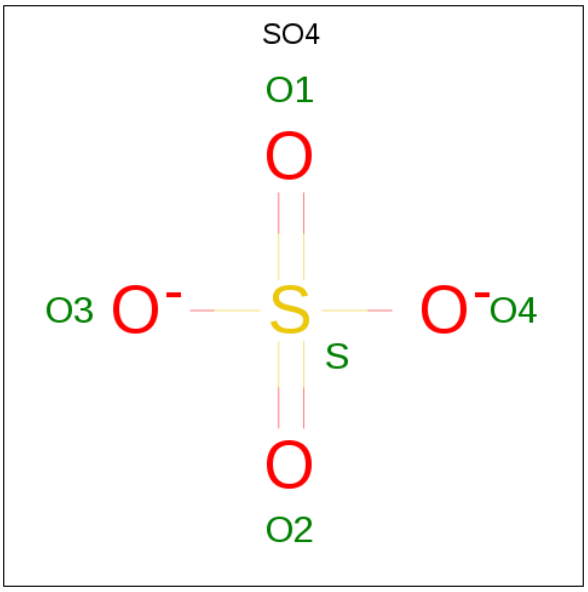
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	5	GLY	-	linker	UNP O75376
E	8	GLN	CYS	conflict	UNP P41182
E	67	ARG	CYS	conflict	UNP P41182
E	84	ASN	CYS	conflict	UNP P41182
F	-7	GLY	-	expression tag	UNP O75376
F	-6	PRO	-	expression tag	UNP O75376
F	4	GLY	-	linker	UNP O75376
F	5	GLY	-	linker	UNP O75376
F	8	GLN	CYS	conflict	UNP P41182
F	67	ARG	CYS	conflict	UNP P41182
F	84	ASN	CYS	conflict	UNP P41182
I	-7	GLY	-	expression tag	UNP O75376
I	-6	PRO	-	expression tag	UNP O75376
I	4	GLY	-	linker	UNP O75376
I	5	GLY	-	linker	UNP O75376
I	8	GLN	CYS	conflict	UNP P41182
I	67	ARG	CYS	conflict	UNP P41182
I	84	ASN	CYS	conflict	UNP P41182
J	-7	GLY	-	expression tag	UNP O75376
J	-6	PRO	-	expression tag	UNP O75376
J	4	GLY	-	linker	UNP O75376
J	5	GLY	-	linker	UNP O75376
J	8	GLN	CYS	conflict	UNP P41182
J	67	ARG	CYS	conflict	UNP P41182
J	84	ASN	CYS	conflict	UNP P41182

- Molecule 2 is a protein called Nuclear receptor corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	0	0	0
			123	75	24	23	1			
2	D	16	Total	C	N	O	S	0	0	0
			131	81	25	24	1			
2	G	15	Total	C	N	O	S	0	0	0
			123	75	24	23	1			
2	K	15	Total	C	N	O	S	0	0	0
			123	75	24	23	1			
2	L	16	Total	C	N	O	S	0	0	0
			131	81	25	24	1			
2	H	16	Total	C	N	O	S	0	0	0
			131	81	25	24	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



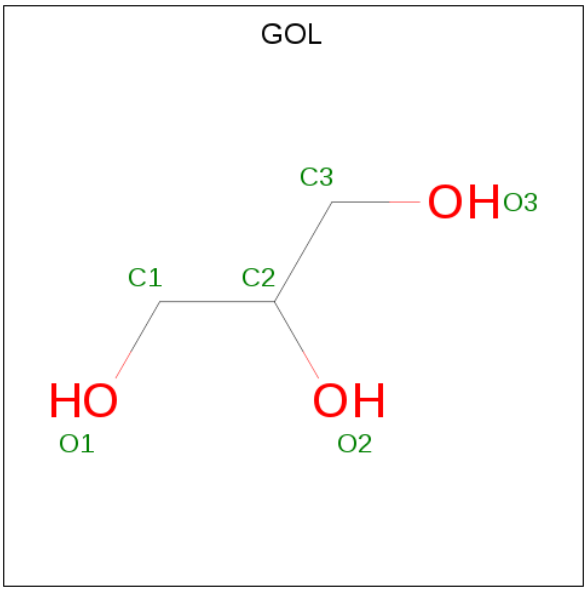
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	30	Total O 30 30	0	0
5	C	7	Total O 7 7	0	0
5	D	4	Total O 4 4	0	0
5	E	23	Total O 23 23	0	0
5	F	8	Total O 8 8	0	0
5	G	2	Total O 2 2	0	0
5	I	16	Total O 16 16	0	0

Continued on next page...

Continued from previous page...

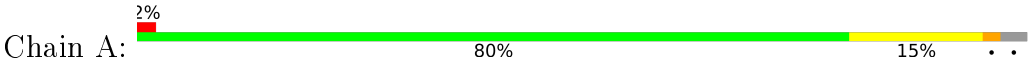
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	9	Total O 9 9	0	0
5	K	3	Total O 3 3	0	0

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.

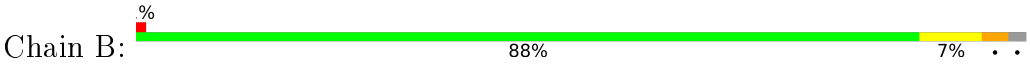
- Molecule 1: Nuclear receptor corepressor 1,B-cell lymphoma 6 protein

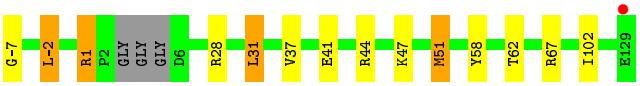
Chain A:



- Molecule 1: Nuclear receptor corepressor 1,B-cell lymphoma 6 protein

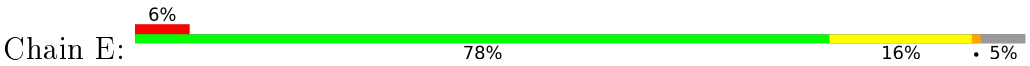
Chain B:





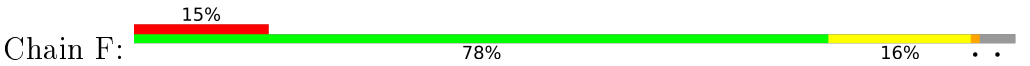
- Molecule 1: Nuclear receptor corepressor 1,B-cell lymphoma 6 protein

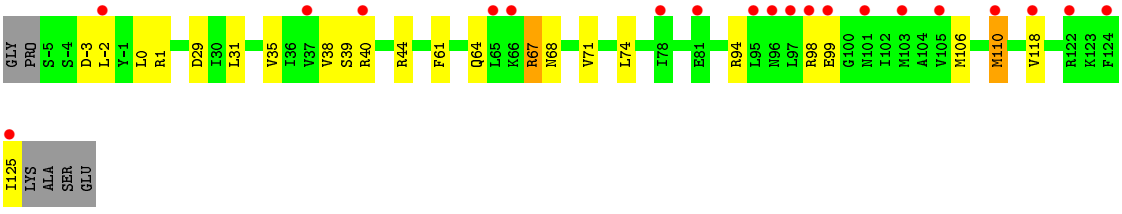
Chain E:



- Molecule 1: Nuclear receptor corepressor 1,B-cell lymphoma 6 protein

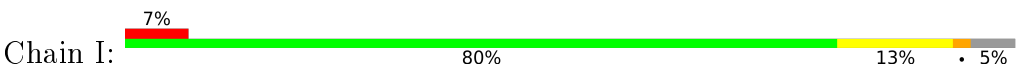
Chain F:

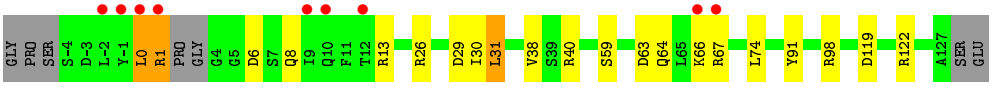




- Molecule 1: Nuclear receptor corepressor 1,B-cell lymphoma 6 protein

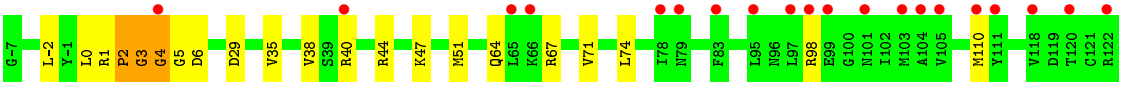
Chain I:

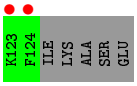




• Molecule 1: Nuclear receptor corepressor 1,B-cell lymphoma 6 protein

Chain J:



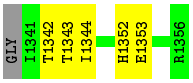


• Molecule 2: Nuclear receptor corepressor 1

Chain C:

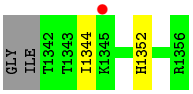
• Molecule 2: Nuclear receptor corepressor 1

Chain D:



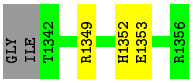
• Molecule 2: Nuclear receptor corepressor 1

Chain G:



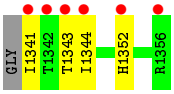
• Molecule 2: Nuclear receptor corepressor 1

Chain K:



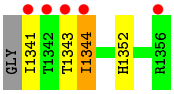
• Molecule 2: Nuclear receptor corepressor 1

Chain L:



• Molecule 2: Nuclear receptor corepressor 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	198.57Å 198.57Å 113.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.81 – 2.46 98.26 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.6 (88.81-2.46) 99.9 (98.26-2.46)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.224 , 0.259 0.228 , 0.262	Depositor DCC
R_{free} test set	4028 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7421	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9946e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.53	0/1100	0.78	1/1484 (0.1%)
1	B	0.53	0/1106	0.74	1/1491 (0.1%)
1	E	0.52	0/1062	0.67	0/1430
1	F	0.43	0/1067	0.63	0/1440
1	I	0.52	0/1062	0.68	1/1430 (0.1%)
1	J	0.44	0/1071	0.63	0/1446
2	C	0.46	0/124	0.64	0/163
2	D	0.45	0/132	0.55	0/174
2	G	0.47	0/124	0.68	0/163
2	H	0.31	0/132	0.57	0/174
2	K	0.37	0/124	0.59	0/163
2	L	0.32	0/132	0.60	0/174
All	All	0.49	0/7236	0.68	3/9732 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	0	LEU	CA-CB-CG	7.67	132.94	115.30
1	B	-2	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	A	0	LEU	CA-CB-CG	-5.10	103.58	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1084	0	1103	22	0
1	B	1090	0	1107	12	0
1	E	1048	0	1068	28	0
1	F	1051	0	1066	18	0
1	I	1048	0	1068	24	0
1	J	1054	0	1065	17	0
2	C	123	0	128	1	0
2	D	131	0	139	4	0
2	G	123	0	128	0	0
2	H	131	0	139	3	0
2	K	123	0	128	1	0
2	L	131	0	139	2	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	D	5	0	0	0	0
3	E	20	0	0	0	0
3	F	5	0	0	0	0
3	G	15	0	0	0	0
3	H	5	0	0	0	0
3	I	15	0	0	1	0
3	J	25	0	0	2	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	6	0	8	1	0
4	C	6	0	7	0	0
4	D	6	0	7	2	0
4	I	6	0	8	0	0
5	A	18	0	0	1	0
5	B	30	0	0	0	0
5	C	7	0	0	0	0
5	D	4	0	0	0	0
5	E	23	0	0	0	0
5	F	8	0	0	0	0
5	G	2	0	0	0	0
5	I	16	0	0	1	0
5	J	9	0	0	0	0
5	K	3	0	0	0	0
All	All	7421	0	7308	94	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 6.

All (94) 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)
2:D:1353:GLU:H	4:D:1402:GOL:H11	1.27	0.94
1:E:40:ARG:HH21	1:I:40:ARG:HD3	1.37	0.88
1:A:106:MET:HE2	1:A:121:CYS:HB3	1.59	0.84
1:B:-2:LEU:HD11	1:E:60:ILE:HD11	1.58	0.83
1:E:40:ARG:HH21	1:I:40:ARG:HH21	1.28	0.79
1:A:67:ARG:NH2	1:B:31:LEU:H	1.82	0.76
1:E:40:ARG:NH2	1:I:40:ARG:HD3	2.02	0.74
1:J:3:GLY:O	1:J:5:GLY:N	2.19	0.74
1:I:119:ASP:OD1	1:I:122:ARG:NH2	2.21	0.73
1:F:61:PHE:O	1:F:67:ARG:HD2	1.87	0.72
1:F:29:ASP:OD1	1:F:44:ARG:HD2	1.97	0.65
1:F:110:MET:HG3	1:F:118:VAL:HG21	1.79	0.64
1:E:40:ARG:HB3	1:I:40:ARG:HG2	1.79	0.64
2:D:1353:GLU:N	4:D:1402:GOL:H11	2.09	0.62
1:A:47:LYS:O	1:A:51:MET:HG3	2.00	0.62
1:J:29:ASP:OD1	1:J:44:ARG:HD2	2.01	0.61
1:F:0:LEU:O	1:F:1:ARG:NH1	2.32	0.60
1:E:1:ARG:HB2	1:F:99:GLU:HB2	1.82	0.60
1:A:99:GLU:OE2	5:A:301:HOH:O	2.17	0.60
1:I:30:ILE:HA	1:J:67:ARG:HH22	1.66	0.60
1:B:-2:LEU:HD13	1:E:56:LEU:HD21	1.84	0.58
1:J:0:LEU:O	1:J:1:ARG:NH1	2.37	0.58
1:I:6:ASP:OD1	1:J:98:ARG:HG3	2.05	0.57
1:I:63:ASP:OD2	1:I:66:LYS:HE3	2.05	0.56
1:A:106:MET:SD	1:E:110:MET:HG2	2.48	0.54
1:A:110:MET:SD	1:E:106:MET:HG2	2.47	0.54
1:J:47:LYS:O	1:J:51:MET:HG3	2.06	0.54
1:E:65:LEU:HD22	1:J:64:GLN:HG3	1.89	0.54
1:E:1:ARG:HB3	1:E:4:GLY:HA2	1.90	0.53
1:I:38:VAL:HG22	1:I:74:LEU:HD12	1.90	0.53
1:E:40:ARG:HG2	1:I:40:ARG:HB3	1.90	0.52
1:E:0:LEU:O	1:E:1:ARG:NH2	2.42	0.52
1:E:40:ARG:NH2	1:I:40:ARG:HH21	2.03	0.52
1:A:31[A]:LEU:HD12	1:B:67:ARG:HD3	1.93	0.52
1:J:35:VAL:CG1	1:J:71:VAL:HG22	2.41	0.51
1:E:8:GLN:HB3	2:H:1343:THR:HG22	1.93	0.50
1:E:-1:TYR:HB3	1:F:99:GLU:OE2	2.11	0.50
1:F:38:VAL:HG22	1:F:74:LEU:HD12	1.94	0.50
1:E:38:VAL:HG22	1:E:74:LEU:HD12	1.95	0.49
1:F:68:ASN:ND2	1:I:67:ARG:HD2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLN:OE1	1:F:94:ARG:HD2	2.13	0.49
1:J:3:GLY:C	1:J:5:GLY:H	2.11	0.48
1:A:26:ARG:HD3	1:A:91:TYR:CZ	2.48	0.48
1:I:13:ARG:NH2	3:I:202:SO4:O4	2.46	0.48
1:J:2:PRO:O	1:J:4:GLY:N	2.46	0.48
1:F:64:GLN:HE22	1:F:67:ARG:CZ	2.28	0.47
1:A:115:GLU:OE1	1:E:122:ARG:NH1	2.48	0.47
1:B:58:TYR:O	1:B:62:THR:HG23	2.14	0.47
1:J:67:ARG:NH2	3:J:201:SO4:O4	2.47	0.47
1:A:44:ARG:HB2	1:A:44:ARG:CZ	2.45	0.47
1:A:8:GLN:HB3	2:D:1343:THR:HG22	1.97	0.46
1:F:35:VAL:CG1	1:F:71:VAL:HG22	2.45	0.46
2:H:1341:ILE:HG22	2:H:1343:THR:HG23	1.97	0.46
1:B:37:VAL:HA	1:B:41:GLU:O	2.15	0.46
1:A:128:SER:HB2	1:B:1:ARG:H	1.80	0.45
1:A:60:ILE:HD11	1:F:-2:LEU:HD11	1.98	0.45
1:I:31:LEU:H	1:J:67:ARG:NH2	2.15	0.45
1:J:38:VAL:HG22	1:J:74:LEU:HD12	1.98	0.45
1:A:128:SER:HB2	1:B:1:ARG:N	2.31	0.45
1:I:8:GLN:O	2:L:1343:THR:HA	2.17	0.45
1:B:28:ARG:HH12	2:C:1355:PRO:HG2	1.82	0.45
1:E:40:ARG:HD3	1:I:40:ARG:HH21	1.82	0.45
1:A:66:LYS:HA	1:A:69:LEU:HD21	1.98	0.45
1:A:29:ASP:OD1	1:A:44:ARG:HD2	2.16	0.45
1:B:-7:GLY:HA3	1:I:29:ASP:OD2	2.17	0.44
1:E:6:ASP:CG	1:F:98:ARG:HG2	2.38	0.44
1:E:40:ARG:HD3	1:I:40:ARG:NH2	2.33	0.44
1:A:40:ARG:HG3	1:A:41:GLU:HG3	1.99	0.44
1:E:26:ARG:HD3	1:E:91:TYR:CZ	2.52	0.44
1:I:64:GLN:HG2	5:I:316:HOH:O	2.17	0.44
1:I:98:ARG:CZ	1:J:6:ASP:HB3	2.47	0.43
1:B:47:LYS:O	1:B:51:MET:HG2	2.18	0.43
1:E:6:ASP:OD1	1:F:98:ARG:HG2	2.18	0.43
2:K:1349:ARG:CZ	2:K:1353:GLU:HB2	2.49	0.43
1:A:2:PRO:HG2	1:B:102:ILE:HD11	2.01	0.43
1:A:61:PHE:O	1:A:67:ARG:HG3	2.19	0.42
1:I:1:ARG:HA	1:I:1:ARG:HD3	1.63	0.42
1:J:1:ARG:HA	1:J:1:ARG:HD3	1.84	0.42
1:J:-2:LEU:HD23	1:J:-2:LEU:HA	1.79	0.42
1:E:47:LYS:O	1:E:51:MET:HG3	2.20	0.42
1:A:44:ARG:HB2	1:A:44:ARG:NH2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:HB2	1:F:-3:ASP:HA	2.02	0.42
2:D:1342:THR:HG22	2:D:1344:ILE:HD11	2.02	0.42
4:A:205:GOL:H31	3:B:204:SO4:O2	2.21	0.41
1:I:6:ASP:O	2:L:1341:ILE:HA	2.20	0.41
1:A:106:MET:HE2	1:A:106:MET:HB2	1.80	0.41
1:F:1:ARG:HA	1:F:1:ARG:HD3	1.88	0.41
1:J:67:ARG:CZ	3:J:201:SO4:O4	2.68	0.41
1:F:31:LEU:HD23	1:F:31:LEU:HA	1.66	0.41
1:I:26:ARG:HD3	1:I:91:TYR:CZ	2.55	0.41
1:E:40:ARG:CG	1:I:40:ARG:HG2	2.51	0.41
1:E:8:GLN:O	2:H:1344:ILE:HD12	2.21	0.40
1:F:106:MET:HG3	1:F:110:MET:HE3	2.02	0.40
1:E:66:LYS:HB3	1:E:69:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	131/137 (96%)	124 (95%)	7 (5%)	0	100 100
1	B	131/137 (96%)	125 (95%)	6 (5%)	0	100 100
1	E	126/137 (92%)	121 (96%)	5 (4%)	0	100 100
1	F	129/137 (94%)	123 (95%)	4 (3%)	2 (2%)	9 8
1	I	126/137 (92%)	122 (97%)	4 (3%)	0	100 100
1	J	130/137 (95%)	124 (95%)	2 (2%)	4 (3%)	4 1
2	C	13/17 (76%)	13 (100%)	0	0	100 100
2	D	14/17 (82%)	13 (93%)	1 (7%)	0	100 100
2	G	13/17 (76%)	13 (100%)	0	0	100 100
2	H	14/17 (82%)	14 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	K	13/17 (76%)	13 (100%)	0	0	100 100
2	L	14/17 (82%)	14 (100%)	0	0	100 100
All	All	854/924 (92%)	819 (96%)	29 (3%)	6 (1%)	22 25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	40	ARG
1	J	40	ARG
1	J	3	GLY
1	J	4	GLY
1	F	39	SER
1	J	2	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	124/123 (101%)	121 (98%)	3 (2%)	49 61
1	B	124/123 (101%)	120 (97%)	4 (3%)	39 50
1	E	118/123 (96%)	115 (98%)	3 (2%)	47 60
1	F	119/123 (97%)	116 (98%)	3 (2%)	47 60
1	I	118/123 (96%)	114 (97%)	4 (3%)	37 48
1	J	119/123 (97%)	118 (99%)	1 (1%)	81 88
2	C	14/15 (93%)	13 (93%)	1 (7%)	14 17
2	D	15/15 (100%)	14 (93%)	1 (7%)	16 20
2	G	14/15 (93%)	12 (86%)	2 (14%)	3 2
2	H	15/15 (100%)	13 (87%)	2 (13%)	4 3
2	K	14/15 (93%)	13 (93%)	1 (7%)	14 17
2	L	15/15 (100%)	13 (87%)	2 (13%)	4 3
All	All	809/828 (98%)	782 (97%)	27 (3%)	38 49

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	67	ARG
1	A	69	LEU
1	B	1	ARG
1	B	31	LEU
1	B	44	ARG
1	B	51	MET
2	C	1352	HIS
2	D	1352	HIS
1	E	6	ASP
1	E	31	LEU
1	E	44	ARG
1	F	67	ARG
1	F	110	MET
1	F	125	ILE
2	G	1344	ILE
2	G	1352	HIS
1	I	0	LEU
1	I	1	ARG
1	I	31	LEU
1	I	59	SER
1	J	110	MET
2	K	1352	HIS
2	L	1344	ILE
2	L	1352	HIS
2	H	1344	ILE
2	H	1352	HIS

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

Mol	Chain	Res	Type
1	F	64	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	C	1401	-	5,5,5	1.78	1 (20%)	5,5,5	1.04	0
3	SO4	D	1401	-	4,4,4	0.21	0	6,6,6	0.28	0
3	SO4	B	203	-	4,4,4	0.09	0	6,6,6	0.16	0
3	SO4	G	1402	-	4,4,4	0.11	0	6,6,6	0.22	0
3	SO4	K	1401	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	B	204	-	4,4,4	0.12	0	6,6,6	0.20	0
3	SO4	G	1401	-	4,4,4	0.10	0	6,6,6	0.29	0
3	SO4	I	203	-	4,4,4	0.15	0	6,6,6	0.29	0
3	SO4	B	201	-	4,4,4	0.11	0	6,6,6	0.39	0
4	GOL	I	204	-	5,5,5	1.30	1 (20%)	5,5,5	0.83	0
3	SO4	J	205	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	E	203	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GOL	D	1402	-	5,5,5	1.58	1 (20%)	5,5,5	1.07	0
4	GOL	A	205	-	5,5,5	1.79	3 (60%)	5,5,5	1.66	2 (40%)
3	SO4	H	1401	-	4,4,4	0.12	0	6,6,6	0.30	0
3	SO4	J	204	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	E	201	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	F	201	-	4,4,4	0.17	0	6,6,6	0.31	0
3	SO4	I	201	-	4,4,4	0.11	0	6,6,6	0.21	0
3	SO4	J	201	-	4,4,4	0.45	0	6,6,6	0.66	0
3	SO4	A	203	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	A	204	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	J	202	-	4,4,4	0.15	0	6,6,6	0.27	0
3	SO4	E	202	-	4,4,4	0.16	0	6,6,6	0.24	0
3	SO4	A	202	-	4,4,4	0.13	0	6,6,6	0.19	0
3	SO4	A	201	-	4,4,4	0.20	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	E	204	-	4,4,4	0.12	0	6,6,6	0.24	0
3	SO4	B	202	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	J	203	-	4,4,4	0.14	0	6,6,6	0.20	0
3	SO4	L	1401	-	4,4,4	0.12	0	6,6,6	0.30	0
3	SO4	I	202	-	4,4,4	0.14	0	6,6,6	0.31	0
3	SO4	G	1403	-	4,4,4	0.16	0	6,6,6	0.20	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	C	1401	-	-	2/4/4/4	-
4	GOL	D	1402	-	-	3/4/4/4	-
4	GOL	A	205	-	-	0/4/4/4	-
4	GOL	I	204	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1401	GOL	O2-C2	-3.64	1.32	1.43
4	D	1402	GOL	O2-C2	-2.87	1.34	1.43
4	A	205	GOL	C3-C2	2.55	1.62	1.51
4	I	204	GOL	C1-C2	2.36	1.61	1.51
4	A	205	GOL	C1-C2	2.33	1.61	1.51
4	A	205	GOL	O2-C2	2.04	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	205	GOL	C3-C2-C1	-2.39	102.42	111.70
4	A	205	GOL	O2-C2-C3	2.17	118.70	109.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1402	GOL	C1-C2-C3-O3
4	D	1402	GOL	O2-C2-C3-O3
4	C	1401	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1401	GOL	C1-C2-C3-O3
4	D	1402	GOL	O1-C1-C2-O2
4	I	204	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	204	SO4	1	0
4	D	1402	GOL	2	0
4	A	205	GOL	1	0
3	J	201	SO4	2	0
3	I	202	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	133/137 (97%)	0.83	3 (2%) 60 56	32, 53, 105, 144	0
1	B	134/137 (97%)	0.79	1 (0%) 87 88	32, 51, 91, 115	0
1	E	130/137 (94%)	0.65	8 (6%) 20 17	38, 54, 120, 133	0
1	F	131/137 (95%)	1.03	20 (15%) 2 1	47, 75, 125, 147	0
1	I	130/137 (94%)	0.71	9 (6%) 16 13	37, 54, 128, 156	0
1	J	132/137 (96%)	1.18	22 (16%) 1 1	54, 82, 129, 156	0
2	C	15/17 (88%)	0.18	0 100 100	43, 60, 82, 95	0
2	D	16/17 (94%)	0.38	0 100 100	43, 60, 106, 125	0
2	G	15/17 (88%)	0.60	1 (6%) 17 14	54, 75, 97, 112	0
2	H	16/17 (94%)	1.74	5 (31%) 0 0	65, 84, 125, 126	0
2	K	15/17 (88%)	0.52	0 100 100	57, 75, 94, 113	0
2	L	16/17 (94%)	1.71	6 (37%) 0 0	73, 99, 126, 129	0
All	All	883/924 (95%)	0.87	75 (8%) 10 8	32, 63, 120, 156	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	97	LEU	6.6
1	I	0	LEU	5.4
1	I	67	ARG	5.0
1	I	-2	LEU	4.8
2	L	1341	ILE	4.7
2	H	1341	ILE	4.5
1	J	66	LYS	4.4
1	A	64	GLN	4.3
1	E	0	LEU	4.2
1	J	98	ARG	3.9
1	F	118	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	110	MET	3.8
1	F	66	LYS	3.7
1	F	122	ARG	3.7
1	J	4	GLY	3.5
1	J	122	ARG	3.4
1	J	99	GLU	3.4
1	B	129	GLU	3.4
2	L	1344	ILE	3.4
1	F	98	ARG	3.3
1	E	67	ARG	3.3
1	J	83	PHE	3.3
1	J	120	THR	3.3
1	F	105	VAL	3.2
1	J	95	LEU	3.2
2	H	1344	ILE	3.1
1	F	40	ARG	3.1
2	L	1356	ARG	3.1
1	J	65	LEU	3.1
1	J	40	ARG	3.0
1	J	78	ILE	3.0
1	J	105	VAL	3.0
2	L	1342	THR	3.0
1	F	65	LEU	2.9
1	I	-1	TYR	2.9
1	F	78	ILE	2.9
1	J	118	VAL	2.9
2	H	1356	ARG	2.9
1	F	-2	LEU	2.8
1	F	125	ILE	2.8
1	J	124	PHE	2.7
2	H	1342	THR	2.7
1	J	79	ASN	2.7
1	F	124	PHE	2.7
1	E	65	LEU	2.7
1	I	9	ILE	2.7
1	I	1	ARG	2.6
1	J	111	TYR	2.6
1	F	99	GLU	2.6
1	E	1	ARG	2.6
1	E	-2	LEU	2.5
1	F	103	MET	2.5
1	J	123	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	2.4
1	J	101	ASN	2.4
1	J	103	MET	2.4
1	F	81	GLU	2.4
1	F	97	LEU	2.3
2	L	1343	THR	2.3
1	F	101	ASN	2.3
1	J	110	MET	2.3
2	L	1352	HIS	2.3
1	F	96	ASN	2.3
1	E	-1	TYR	2.2
1	E	64	GLN	2.2
1	F	95	LEU	2.2
1	J	104	ALA	2.2
1	I	66	LYS	2.1
2	H	1343	THR	2.1
1	A	35	VAL	2.1
1	I	10	GLN	2.1
2	G	1345	LYS	2.1
1	E	5	GLY	2.1
1	I	12	THR	2.0
1	F	37	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	204	5/5	0.52	0.54	163,166,167,167	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	204	5/5	0.52	0.48	158,159,160,161	0
3	SO4	B	202	5/5	0.61	0.28	151,153,155,157	0
3	SO4	E	204	5/5	0.62	0.32	137,139,143,144	0
4	GOL	A	205	6/6	0.64	0.49	62,70,72,74	0
3	SO4	I	203	5/5	0.65	0.21	130,131,134,138	0
4	GOL	I	204	6/6	0.67	0.23	70,78,86,91	0
3	SO4	B	203	5/5	0.76	0.23	140,141,141,142	0
3	SO4	L	1401	5/5	0.79	0.15	121,122,124,128	0
3	SO4	E	202	5/5	0.80	0.17	109,116,117,118	0
3	SO4	G	1403	5/5	0.82	0.21	129,130,131,134	0
3	SO4	J	203	5/5	0.84	0.23	130,130,131,132	0
3	SO4	J	204	5/5	0.85	0.29	153,153,154,156	0
3	SO4	A	201	5/5	0.86	0.18	117,119,121,126	0
3	SO4	A	203	5/5	0.86	0.22	126,131,135,135	0
3	SO4	A	202	5/5	0.86	0.37	154,154,155,157	0
3	SO4	J	205	5/5	0.87	0.21	138,140,141,143	0
3	SO4	E	203	5/5	0.91	0.22	132,132,133,133	0
3	SO4	I	202	5/5	0.91	0.18	113,115,116,116	0
3	SO4	J	202	5/5	0.91	0.13	95,96,101,102	0
3	SO4	H	1401	5/5	0.92	0.15	113,116,117,118	0
4	GOL	C	1401	6/6	0.93	0.24	39,45,55,57	0
3	SO4	G	1402	5/5	0.93	0.14	99,101,104,109	0
3	SO4	G	1401	5/5	0.95	0.16	91,91,97,100	0
3	SO4	E	201	5/5	0.96	0.16	88,91,93,97	0
3	SO4	I	201	5/5	0.96	0.18	83,85,86,93	0
3	SO4	J	201	5/5	0.96	0.19	53,80,90,93	0
4	GOL	D	1402	6/6	0.96	0.24	45,47,51,53	0
3	SO4	K	1401	5/5	0.96	0.12	81,89,92,97	0
3	SO4	D	1401	5/5	0.97	0.20	80,81,88,90	0
3	SO4	B	201	5/5	0.97	0.14	80,84,88,92	0
3	SO4	F	201	5/5	0.98	0.17	56,74,81,82	0

6.5 Other polymers (i)

There are no such residues in this entry.