



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WO2
Title : Crystal structure of human interleukin-18
Authors : Tsutsumi, N.; Kimura, T.; Arita, K.; Ariyoshi, M.; Ohnishi, H.; Kondo, N.; Shirakawa, M.; Kato, Z.; Tochio, H.
Deposited on : 2013-12-19
Resolution : 2.33 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

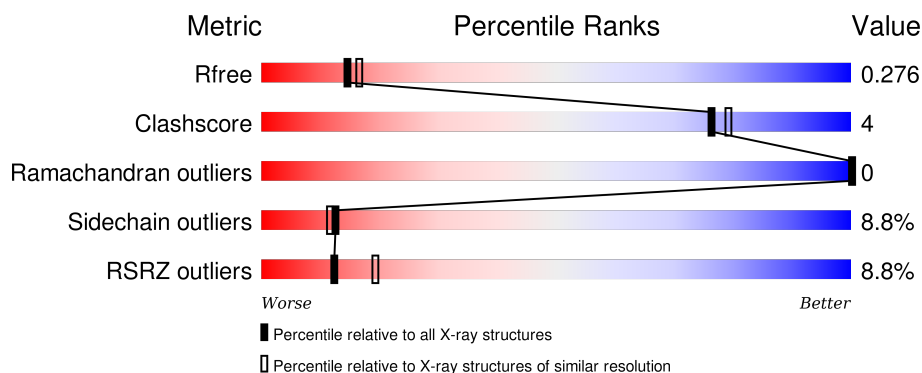
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	157	<div> <div>9%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	157	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	C	157	<div> <div>8%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	D	157	<div> <div>13%</div> <div>87%</div> <div>13%</div> </div>

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	CPS	A	203	-	-	-	X
2	CPS	B	203	-	-	-	X
2	CPS	C	201	-	-	-	X
2	CPS	C	202	-	-	-	X
2	CPS	D	203	-	-	-	X
3	SO4	A	204	-	-	-	X

2 Entry composition [i](#)

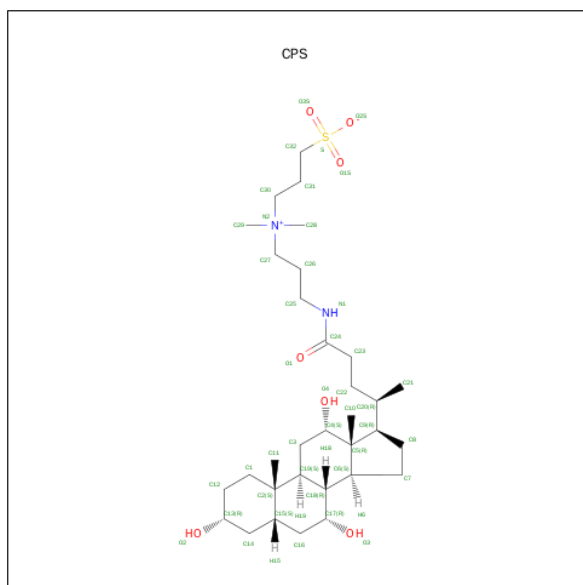
There are 4 unique types of molecules in this entry. The entry contains 5733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1257	793	208	246	10			
1	B	156	Total	C	N	O	S	0	0	0
			1233	779	204	240	10			
1	C	157	Total	C	N	O	S	0	0	0
			1266	796	211	250	9			
1	D	157	Total	C	N	O	S	0	1	0
			1266	801	211	244	10			

- Molecule 2 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



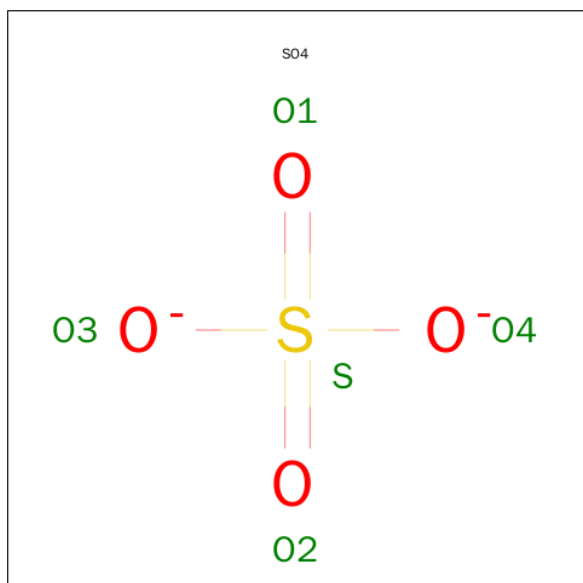
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			28	24	4			
2	A	1	Total	C	N	O	0	0
			30	25	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 28 24 4	0	0
2	B	1	Total C N O 29 24 1 4	0	0
2	B	1	Total C O 23 20 3	0	0
2	B	1	Total C N O S 42 32 2 7 1	0	0
2	C	1	Total C O 26 23 3	0	0
2	C	1	Total C N O S 42 32 2 7 1	0	0
2	C	1	Total C O 26 23 3	0	0
2	D	1	Total C N O S 42 32 2 7 1	0	0
2	D	1	Total C O 23 20 3	0	0
2	D	1	Total C N O S 42 32 2 7 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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

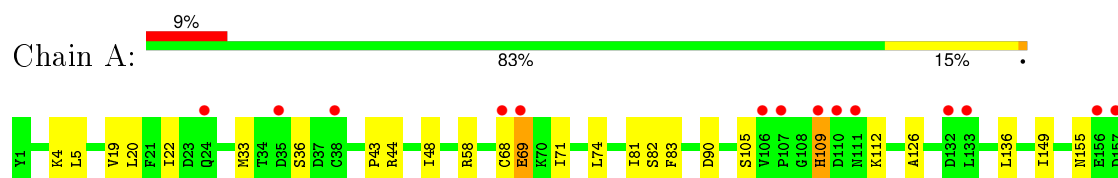
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	93	Total	O	0	0
			93	93		
4	C	82	Total	O	0	0
			82	82		
4	D	56	Total	O	0	0
			56	56		

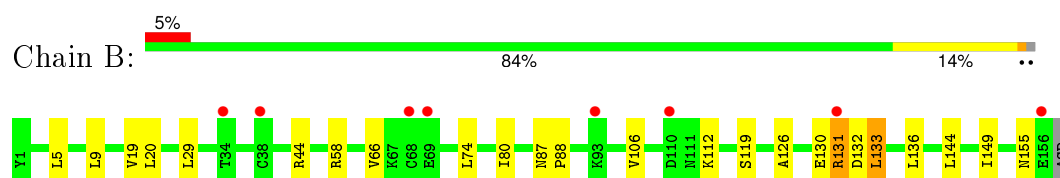
3 Residue-property plots [i](#)

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.

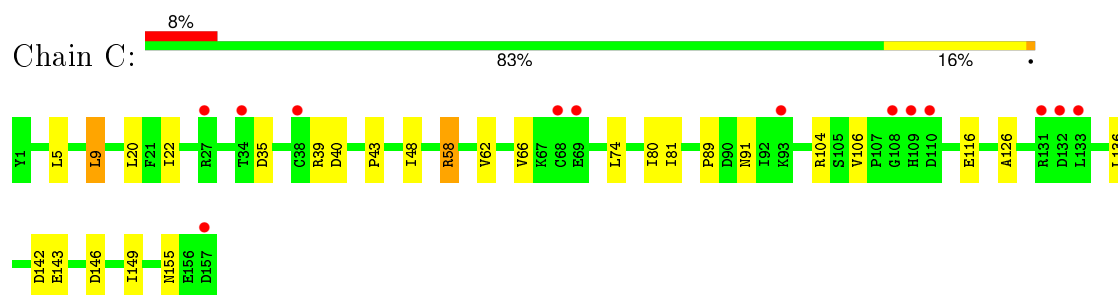
• Molecule 1: Interleukin-18



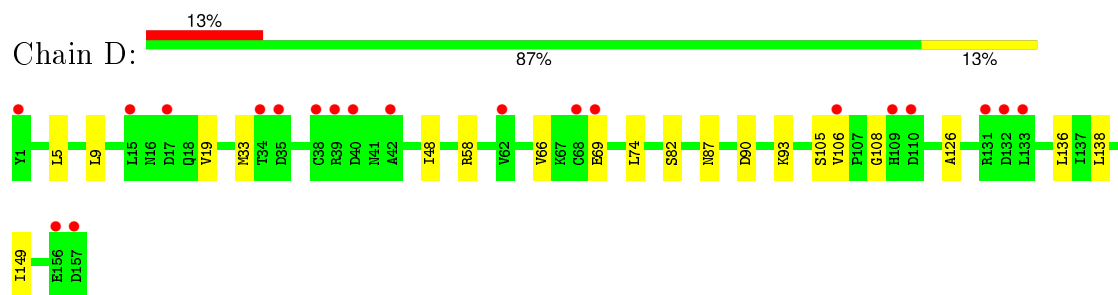
• Molecule 1: Interleukin-18



• Molecule 1: Interleukin-18



• Molecule 1: Interleukin-18



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.15Å 79.51Å 73.46Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	34.82 – 2.33 34.82 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.82-2.33) 97.5 (34.82-2.33)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.271 0.225 , 0.276	Depositor DCC
R_{free} test set	1640 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 32157 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5733	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CPS, 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	0.44	0/1278	0.67	0/1714
1	B	0.43	0/1254	0.70	0/1687
1	C	0.42	0/1287	0.70	0/1726
1	D	0.41	0/1290	0.69	0/1729
All	All	0.42	0/5109	0.69	0/6856

There are no bond length outliers.

There are no bond angle outliers.

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	1257	0	1233	11	0
1	B	1233	0	1194	7	0
1	C	1266	0	1241	12	0
1	D	1266	0	1255	8	0
2	A	86	0	116	5	0
2	B	94	0	128	2	0
2	C	94	0	132	7	0
2	D	107	0	147	6	0
3	A	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	79	0	0	0	0
4	B	93	0	0	0	0
4	C	82	0	0	0	0
4	D	56	0	0	0	0
All	All	5733	0	5446	41	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 4.

All (41) 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:87:ASN:HB3	2:D:203:CPS:H22A	1.68	0.74
1:D:48:ILE:HD11	2:D:201:CPS:H14A	1.74	0.68
1:A:48:ILE:HD11	2:A:201:CPS:H14A	1.77	0.66
1:A:82:SER:HB3	1:C:80:ILE:HD13	1.77	0.65
1:C:58:ARG:O	1:C:104:ARG:NH1	2.35	0.59
1:B:80:ILE:HD13	1:D:82:SER:HB3	1.83	0.59
1:A:109:HIS:HB2	1:A:112:LYS:HE3	1.87	0.56
1:A:22:ILE:HD11	1:A:83:PHE:CE2	2.41	0.56
1:D:90:ASP:H	2:D:203:CPS:H32A	1.72	0.54
1:B:130:GLU:O	1:B:131:ARG:HG3	2.09	0.53
1:A:43:PRO:HG3	2:A:201:CPS:H8	1.93	0.51
1:D:87:ASN:HB2	2:D:203:CPS:H272	1.92	0.51
2:A:201:CPS:H13	2:A:203:CPS:H7	1.92	0.51
1:B:29:LEU:HD21	1:B:133:LEU:HG	1.93	0.50
1:C:89:PRO:HA	2:C:202:CPS:H25A	1.93	0.49
1:A:71:ILE:HD11	2:A:201:CPS:O2	2.14	0.48
1:C:104:ARG:NH2	1:C:116:GLU:OE1	2.46	0.48
1:B:87:ASN:HD21	2:B:203:CPS:H272	1.80	0.47
1:C:48:ILE:HD11	2:C:203:CPS:H14A	1.97	0.46
1:C:91:ASN:HB2	2:C:202:CPS:H32A	1.96	0.46
1:D:106:VAL:HG12	1:D:108:GLY:H	1.80	0.46
1:A:19:VAL:HG13	1:A:33:MET:HB2	1.98	0.45
1:D:19:VAL:HG13	1:D:33:MET:HB2	1.99	0.45
1:A:69:GLU:HG2	1:A:69:GLU:H	1.58	0.45
2:C:201:CPS:H10B	2:C:201:CPS:H21A	1.98	0.45
1:C:126:ALA:HB2	1:C:149:ILE:HG22	1.99	0.44
1:C:74:LEU:HD11	1:C:81:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LEU:HB3	2:C:201:CPS:H14	2.01	0.43
1:A:126:ALA:HB2	1:A:149:ILE:HG22	2.01	0.43
1:B:126:ALA:HB2	1:B:149:ILE:HG22	2.00	0.43
1:A:4:LYS:NZ	1:A:90:ASP:OD1	2.51	0.42
2:D:202:CPS:H1	2:D:202:CPS:H3	1.93	0.42
1:B:131:ARG:HE	1:B:132:ASP:H	1.66	0.42
1:B:88:PRO:HD2	2:B:203:CPS:H21A	2.01	0.42
1:C:35:ASP:HB3	2:C:201:CPS:H22A	2.00	0.42
2:D:201:CPS:H28B	2:D:201:CPS:H262	1.90	0.42
1:C:43:PRO:HG3	2:C:203:CPS:H8	2.01	0.42
2:A:203:CPS:H21A	2:A:203:CPS:O4	2.20	0.41
1:D:126:ALA:HB2	1:D:149:ILE:HG22	2.02	0.41
1:A:74:LEU:HD11	1:A:81:ILE:HG23	2.03	0.41
1:C:143:GLU:HG3	1:C:146:ASP:HB2	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	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
1	B	154/157 (98%)	146 (95%)	8 (5%)	0	100	100
1	C	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
1	D	156/157 (99%)	148 (95%)	8 (5%)	0	100	100
All	All	620/628 (99%)	588 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	143/148 (97%)	132 (92%)	11 (8%)	16	17
1	B	138/148 (93%)	122 (88%)	16 (12%)	7	6
1	C	145/148 (98%)	132 (91%)	13 (9%)	12	11
1	D	144/148 (97%)	134 (93%)	10 (7%)	19	21
All	All	570/592 (96%)	520 (91%)	50 (9%)	12	11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	20	LEU
1	A	36	SER
1	A	44	ARG
1	A	58	ARG
1	A	68	CYS
1	A	69	GLU
1	A	105	SER
1	A	109	HIS
1	A	136	LEU
1	A	155	ASN
1	B	5	LEU
1	B	9	LEU
1	B	19	VAL
1	B	20	LEU
1	B	44	ARG
1	B	58	ARG
1	B	66	VAL
1	B	74	LEU
1	B	106	VAL
1	B	112	LYS
1	B	119	SER
1	B	131	ARG
1	B	133	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	LEU
1	B	144	LEU
1	B	155	ASN
1	C	5	LEU
1	C	9	LEU
1	C	20	LEU
1	C	22	ILE
1	C	39	ARG
1	C	40	ASP
1	C	58	ARG
1	C	62	VAL
1	C	66	VAL
1	C	106	VAL
1	C	136	LEU
1	C	142	ASP
1	C	155	ASN
1	D	5	LEU
1	D	9	LEU
1	D	58	ARG
1	D	66	VAL
1	D	69	GLU
1	D	74	LEU
1	D	93	LYS
1	D	105	SER
1	D	136	LEU
1	D	138	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	C	91	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

16 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	$\# Z > 2$
2	CPS	A	201	-	31,31,45	0.57	0	48,49,70	1.71	12 (25%)
2	CPS	A	202	-	33,33,45	0.59	0	52,52,70	1.94	18 (34%)
2	CPS	A	203	-	31,31,45	0.53	0	48,49,70	3.50	27 (56%)
3	SO4	A	204	-	4,4,4	0.09	0	6,6,6	0.10	0
3	SO4	A	205	-	4,4,4	0.14	0	6,6,6	0.11	0
2	CPS	B	201	-	32,32,45	0.60	0	51,51,70	1.99	14 (27%)
2	CPS	B	202	-	26,26,45	0.63	0	42,43,70	1.88	13 (30%)
2	CPS	B	203	-	44,45,45	0.71	0	67,70,70	1.85	19 (28%)
3	SO4	B	204	-	4,4,4	0.13	0	6,6,6	0.08	0
2	CPS	C	201	-	29,29,45	0.46	0	47,47,70	2.28	17 (36%)
2	CPS	C	202	-	44,45,45	0.69	0	67,70,70	1.89	19 (28%)
2	CPS	C	203	-	29,29,45	0.58	0	47,47,70	1.89	14 (29%)
3	SO4	C	204	-	4,4,4	0.14	0	6,6,6	0.09	0
2	CPS	D	201	-	44,45,45	0.68	0	67,70,70	1.90	15 (22%)
2	CPS	D	202	-	26,26,45	0.58	0	42,43,70	1.95	16 (38%)
2	CPS	D	203	-	44,45,45	0.71	0	67,70,70	1.77	18 (26%)

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
2	CPS	A	201	-	-	0/7/73/90	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPS	A	202	-	-	1/11/76/90	0/4/4/4
2	CPS	A	203	-	-	0/7/73/90	0/4/4/4
3	SO4	A	204	-	-	0/0/0/0	0/0/0/0
3	SO4	A	205	-	-	0/0/0/0	0/0/0/0
2	CPS	B	201	-	-	0/9/74/90	0/4/4/4
2	CPS	B	202	-	-	0/0/65/90	0/4/4/4
2	CPS	B	203	-	-	0/25/90/90	0/4/4/4
3	SO4	B	204	-	-	0/0/0/0	0/0/0/0
2	CPS	C	201	-	-	0/6/71/90	0/4/4/4
2	CPS	C	202	-	-	0/25/90/90	0/4/4/4
2	CPS	C	203	-	-	0/6/71/90	0/4/4/4
3	SO4	C	204	-	-	0/0/0/0	0/0/0/0
2	CPS	D	201	-	-	0/25/90/90	0/4/4/4
2	CPS	D	202	-	-	0/0/65/90	0/4/4/4
2	CPS	D	203	-	-	0/25/90/90	0/4/4/4

There are no bond length outliers.

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	CPS	C9-C5-C6	-12.16	87.77	100.05
2	A	203	CPS	C21-C20-C22	-4.78	102.38	110.35
2	C	201	CPS	C1-C2-C19	-3.86	105.22	111.45
2	C	201	CPS	C9-C5-C6	-3.61	96.40	100.05
2	A	203	CPS	C19-C18-C17	-3.49	107.80	111.92
2	A	203	CPS	C1-C2-C19	-3.40	105.97	111.45
2	A	203	CPS	C8-C7-C6	-3.27	98.55	105.12
2	A	202	CPS	C9-C5-C6	-3.10	96.92	100.05
2	B	203	CPS	C9-C5-C4	-3.08	114.95	117.68
2	D	202	CPS	C11-C2-C1	-2.94	103.25	108.20
2	D	201	CPS	C11-C2-C1	-2.73	103.61	108.20
2	C	202	CPS	C21-C20-C22	-2.70	105.84	110.35
2	C	202	CPS	C9-C5-C6	-2.66	97.36	100.05
2	C	203	CPS	C11-C2-C1	-2.65	103.75	108.20
2	A	202	CPS	C11-C2-C1	-2.50	103.99	108.20
2	A	201	CPS	C11-C2-C1	-2.44	104.11	108.20
2	C	201	CPS	C19-C18-C17	-2.37	109.12	111.92
2	D	202	CPS	C9-C5-C6	-2.36	97.67	100.06
2	B	202	CPS	C11-C2-C1	-2.33	104.28	108.20
2	A	203	CPS	C10-C5-C4	-2.32	106.82	109.09
2	B	203	CPS	C9-C5-C6	-2.32	97.71	100.05
2	C	202	CPS	C11-C2-C1	-2.28	104.36	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	CPS	C9-C5-C4	-2.27	115.66	117.68
2	D	203	CPS	C9-C5-C6	-2.23	97.80	100.05
2	D	202	CPS	C11-C2-C15	-2.17	106.43	110.25
2	D	203	CPS	C11-C2-C1	-2.14	104.60	108.20
2	C	201	CPS	C9-C5-C4	-2.12	115.80	117.68
2	A	203	CPS	C16-C15-C14	-2.07	108.73	111.05
2	B	201	CPS	C16-C15-C14	-2.06	108.74	111.05
2	C	201	CPS	C11-C2-C15	-2.04	106.65	110.25
2	D	203	CPS	C16-C15-C2	2.00	114.86	112.66
2	C	201	CPS	O4-C4-C5	2.03	114.40	111.11
2	A	201	CPS	C5-C6-C18	2.03	117.37	114.75
2	C	202	CPS	O4-C4-C5	2.04	114.43	111.11
2	B	203	CPS	C12-C1-C2	2.05	116.49	112.84
2	D	203	CPS	C28-N2-C27	2.05	114.63	109.43
2	A	202	CPS	C5-C6-C18	2.05	117.39	114.75
2	B	202	CPS	C7-C6-C18	2.05	121.30	118.32
2	C	203	CPS	C1-C2-C15	2.06	111.19	107.81
2	D	203	CPS	C14-C13-C12	2.06	113.15	110.52
2	A	201	CPS	C16-C17-C18	2.07	113.67	111.47
2	D	202	CPS	O4-C4-C5	2.07	114.47	111.11
2	B	203	CPS	C7-C6-C18	2.07	121.33	118.32
2	A	201	CPS	C2-C19-C18	2.09	114.17	111.88
2	A	201	CPS	C15-C14-C13	2.09	116.02	112.91
2	C	203	CPS	C5-C6-C18	2.11	117.47	114.75
2	D	202	CPS	C1-C12-C13	2.11	113.85	110.43
2	D	201	CPS	C25-N1-C24	2.12	126.95	122.79
2	A	202	CPS	C12-C1-C2	2.12	116.62	112.84
2	D	201	CPS	C19-C18-C6	2.14	112.56	109.62
2	B	202	CPS	C10-C5-C6	2.16	114.62	111.22
2	A	202	CPS	O4-C4-C5	2.16	114.62	111.11
2	A	201	CPS	C22-C20-C9	2.17	114.79	110.24
2	B	203	CPS	C16-C15-C2	2.17	115.05	112.66
2	C	203	CPS	C10-C5-C6	2.19	114.66	111.22
2	C	203	CPS	C12-C1-C2	2.19	116.75	112.84
2	D	201	CPS	C12-C1-C2	2.20	116.76	112.84
2	B	203	CPS	C3-C19-C2	2.20	116.08	113.79
2	C	202	CPS	C16-C15-C2	2.21	115.09	112.66
2	B	203	CPS	C21-C20-C22	2.22	114.05	110.35
2	A	203	CPS	C10-C5-C6	2.22	114.72	111.22
2	A	202	CPS	C19-C2-C15	2.23	111.97	108.67
2	C	203	CPS	C19-C18-C6	2.24	112.70	109.62
2	D	203	CPS	C3-C4-C5	2.24	113.48	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	CPS	C10-C5-C6	2.25	114.76	111.22
2	B	203	CPS	C6-C18-C17	2.25	114.86	111.74
2	B	203	CPS	O1S-S-C32	2.26	108.84	106.91
2	D	203	CPS	C8-C9-C20	2.28	116.12	112.05
2	B	202	CPS	C2-C19-C18	2.28	114.39	111.88
2	B	201	CPS	C16-C17-C18	2.29	113.90	111.47
2	C	201	CPS	C15-C14-C13	2.30	116.33	112.91
2	C	202	CPS	C5-C6-C18	2.30	117.72	114.75
2	C	201	CPS	C12-C1-C2	2.33	116.99	112.84
2	B	202	CPS	C15-C14-C13	2.35	116.40	112.91
2	C	202	CPS	C16-C17-C18	2.36	113.97	111.47
2	B	203	CPS	C16-C17-C18	2.38	113.99	111.47
2	B	202	CPS	C6-C18-C17	2.38	115.05	111.74
2	A	202	CPS	C22-C20-C9	2.40	115.29	110.24
2	D	202	CPS	C3-C4-C5	2.41	113.65	111.20
2	C	203	CPS	C21-C20-C9	2.42	116.98	112.96
2	B	203	CPS	C1-C2-C15	2.42	111.79	107.81
2	A	202	CPS	C3-C19-C18	2.44	114.19	110.73
2	C	201	CPS	C14-C15-C2	2.44	115.35	112.66
2	D	203	CPS	C3-C19-C2	2.47	116.36	113.79
2	B	201	CPS	C19-C2-C15	2.51	112.39	108.67
2	A	201	CPS	C16-C15-C2	2.51	115.43	112.66
2	C	202	CPS	C3-C19-C2	2.52	116.41	113.79
2	D	203	CPS	C22-C20-C9	2.52	115.54	110.24
2	D	202	CPS	C10-C5-C6	2.52	115.20	111.22
2	A	202	CPS	C3-C19-C2	2.53	116.42	113.79
2	A	202	CPS	C16-C17-C18	2.54	114.17	111.47
2	D	202	CPS	C2-C19-C18	2.55	114.68	111.88
2	D	201	CPS	C1-C2-C15	2.55	112.00	107.81
2	D	203	CPS	C15-C14-C13	2.58	116.74	112.91
2	B	201	CPS	C3-C19-C18	2.58	114.39	110.73
2	D	202	CPS	C3-C19-C2	2.59	116.48	113.79
2	A	202	CPS	C21-C20-C9	2.60	117.30	112.96
2	C	203	CPS	C14-C15-C2	2.61	115.53	112.66
2	D	201	CPS	C6-C18-C17	2.62	115.37	111.74
2	A	203	CPS	C8-C9-C20	2.63	116.74	112.05
2	B	201	CPS	C8-C9-C5	2.63	106.21	103.60
2	D	202	CPS	C8-C9-C5	2.63	107.69	103.58
2	A	203	CPS	C22-C20-C9	2.65	115.81	110.24
2	A	203	CPS	C23-C22-C20	2.71	119.74	114.52
2	C	202	CPS	C14-C13-C12	2.72	113.99	110.52
2	B	201	CPS	C3-C4-C5	2.73	113.97	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	203	CPS	C3-C19-C18	2.76	114.64	110.73
2	A	203	CPS	C3-C19-C18	2.76	114.65	110.73
2	B	201	CPS	C16-C15-C2	2.77	115.71	112.66
2	C	202	CPS	C5-C9-C20	2.80	122.91	119.50
2	C	202	CPS	C3-C19-C18	2.80	114.71	110.73
2	D	201	CPS	C14-C15-C2	2.83	115.77	112.66
2	A	201	CPS	C6-C18-C17	2.83	115.67	111.74
2	C	202	CPS	C2-C19-C18	2.83	114.99	111.88
2	B	202	CPS	C8-C9-C5	2.85	108.02	103.58
2	C	202	CPS	C15-C14-C13	2.87	117.18	112.91
2	A	203	CPS	C1-C2-C15	2.87	112.52	107.81
2	C	203	CPS	C8-C9-C5	2.87	106.45	103.60
2	D	202	CPS	C12-C1-C2	2.88	117.97	112.84
2	A	203	CPS	C15-C16-C17	2.89	117.67	114.44
2	C	203	CPS	C16-C15-C2	2.95	115.90	112.66
2	A	202	CPS	C16-C15-C2	2.95	115.91	112.66
2	A	203	CPS	C19-C2-C15	2.96	113.05	108.67
2	B	202	CPS	C1-C2-C15	2.96	112.67	107.81
2	B	201	CPS	C6-C18-C17	3.02	115.93	111.74
2	D	202	CPS	C3-C19-C18	3.03	115.03	110.73
2	D	202	CPS	C1-C2-C15	3.04	112.80	107.81
2	A	203	CPS	C12-C1-C2	3.05	118.29	112.84
2	A	203	CPS	C21-C20-C9	3.06	118.05	112.96
2	D	203	CPS	O1S-S-C32	3.06	109.51	106.91
2	B	203	CPS	C3-C19-C18	3.08	115.11	110.73
2	B	202	CPS	C16-C15-C2	3.16	116.14	112.66
2	B	203	CPS	C2-C19-C18	3.17	115.36	111.88
2	C	201	CPS	C2-C19-C18	3.22	115.41	111.88
2	C	201	CPS	C3-C19-C18	3.24	115.33	110.73
2	A	203	CPS	O4-C4-C5	3.32	116.50	111.11
2	A	202	CPS	C2-C19-C18	3.33	115.53	111.88
2	B	201	CPS	C15-C14-C13	3.34	117.89	112.91
2	A	203	CPS	C7-C6-C18	3.35	123.19	118.32
2	D	201	CPS	C16-C15-C2	3.37	116.37	112.66
2	D	203	CPS	C8-C9-C5	3.37	106.95	103.60
2	D	203	CPS	C16-C17-C18	3.37	115.05	111.47
2	B	203	CPS	C8-C9-C5	3.38	106.96	103.60
2	D	203	CPS	C2-C19-C18	3.38	115.59	111.88
2	C	202	CPS	C3-C4-C5	3.40	114.65	111.20
2	D	201	CPS	C22-C20-C9	3.43	117.46	110.24
2	A	201	CPS	C14-C15-C2	3.43	116.44	112.66
2	C	203	CPS	C3-C19-C2	3.45	117.38	113.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	CPS	C2-C19-C18	3.46	115.68	111.88
2	D	203	CPS	O3S-S-C32	3.49	109.89	106.91
2	B	201	CPS	C2-C19-C18	3.52	115.74	111.88
2	A	202	CPS	C8-C9-C5	3.52	107.10	103.60
2	B	201	CPS	C21-C20-C9	3.52	118.83	112.96
2	C	201	CPS	C21-C20-C9	3.59	118.94	112.96
2	C	203	CPS	C5-C9-C20	3.60	123.88	119.50
2	A	202	CPS	C3-C4-C5	3.65	114.91	111.20
2	A	201	CPS	C3-C19-C18	3.68	115.96	110.73
2	D	201	CPS	C21-C20-C22	3.69	116.51	110.35
2	B	203	CPS	C21-C20-C9	3.72	119.15	112.96
2	C	201	CPS	C8-C9-C5	3.74	107.31	103.60
2	C	202	CPS	C8-C9-C5	3.78	107.36	103.60
2	D	202	CPS	C16-C15-C2	3.82	116.87	112.66
2	D	203	CPS	C14-C15-C2	3.86	116.91	112.66
2	D	201	CPS	C8-C9-C20	3.87	118.95	112.05
2	A	203	CPS	C3-C19-C2	3.88	117.82	113.79
2	B	202	CPS	C3-C19-C18	3.88	116.25	110.73
2	C	202	CPS	O3S-S-C32	3.90	110.23	106.91
2	D	201	CPS	C8-C9-C5	3.92	107.50	103.60
2	C	201	CPS	C5-C9-C20	3.92	124.28	119.50
2	A	202	CPS	C5-C9-C20	3.95	124.31	119.50
2	D	202	CPS	C14-C15-C2	4.03	117.09	112.66
2	A	203	CPS	C7-C6-C5	4.07	107.64	103.60
2	D	201	CPS	C3-C19-C18	4.12	116.58	110.73
2	C	201	CPS	C19-C2-C15	4.13	114.78	108.67
2	D	202	CPS	C7-C6-C5	4.20	107.78	103.60
2	B	202	CPS	C7-C6-C5	4.24	107.81	103.60
2	B	203	CPS	C14-C15-C2	4.26	117.34	112.66
2	B	203	CPS	C7-C6-C5	4.27	107.84	103.60
2	A	201	CPS	C7-C6-C5	4.28	107.85	103.60
2	C	202	CPS	O1S-S-C32	4.28	110.56	106.91
2	B	203	CPS	C5-C9-C20	4.30	124.74	119.50
2	B	201	CPS	C5-C9-C20	4.33	124.77	119.50
2	A	202	CPS	C14-C15-C2	4.36	117.46	112.66
2	A	203	CPS	C14-C15-C2	4.39	117.49	112.66
2	D	203	CPS	C7-C6-C5	4.46	108.03	103.60
2	C	203	CPS	C3-C19-C18	4.47	117.08	110.73
2	D	201	CPS	C7-C6-C5	4.48	108.05	103.60
2	B	202	CPS	C14-C15-C2	4.50	117.61	112.66
2	C	202	CPS	C14-C15-C2	4.54	117.65	112.66
2	C	201	CPS	C7-C6-C5	4.54	108.12	103.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	CPS	O3S-S-C32	4.55	110.78	106.91
2	B	201	CPS	C7-C6-C5	4.72	108.29	103.60
2	A	202	CPS	C7-C6-C5	4.75	108.32	103.60
2	B	201	CPS	C14-C15-C2	5.10	118.27	112.66
2	C	202	CPS	C7-C6-C5	5.16	108.73	103.60
2	C	203	CPS	C7-C6-C5	5.18	108.75	103.60
2	D	201	CPS	O1S-S-C32	5.48	111.58	106.91
2	A	203	CPS	C3-C4-C5	5.97	117.27	111.20
2	A	203	CPS	C5-C9-C20	6.33	127.21	119.50
2	C	201	CPS	C16-C15-C2	6.64	119.97	112.66
2	A	203	CPS	C16-C15-C2	6.93	120.30	112.66
2	A	203	CPS	C9-C5-C4	7.60	124.42	117.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	CPS	C23-C24-N1-C25

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	CPS	4	0
2	A	203	CPS	2	0
2	B	203	CPS	2	0
2	C	201	CPS	3	0
2	C	202	CPS	2	0
2	C	203	CPS	2	0
2	D	201	CPS	2	0
2	D	202	CPS	1	0
2	D	203	CPS	3	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, 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	157/157 (100%)	0.62	14 (8%) 12 18	22, 41, 74, 87	0
1	B	156/157 (99%)	0.41	8 (5%) 32 45	19, 40, 72, 98	0
1	C	157/157 (100%)	0.50	13 (8%) 14 22	21, 39, 68, 89	0
1	D	157/157 (100%)	0.88	20 (12%) 5 9	25, 47, 80, 97	0
All	All	627/628 (99%)	0.60	55 (8%) 12 19	19, 42, 76, 98	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ASP	7.3
1	D	133	LEU	7.1
1	A	110	ASP	5.4
1	D	157	ASP	5.0
1	B	69	GLU	4.9
1	D	132	ASP	4.9
1	D	110	ASP	4.9
1	C	131	ARG	4.6
1	C	157	ASP	4.3
1	D	62	VAL	3.9
1	A	68	CYS	3.8
1	C	109	HIS	3.6
1	D	69	GLU	3.6
1	B	38	CYS	3.5
1	D	39	ARG	3.4
1	B	131	ARG	3.3
1	A	133	LEU	3.3
1	C	93	LYS	3.2
1	D	68	CYS	3.2
1	A	69	GLU	3.2
1	D	35	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	156	GLU	3.1
1	A	107	PRO	3.0
1	A	111	ASN	2.9
1	C	69	GLU	2.8
1	B	68	CYS	2.8
1	D	34	THR	2.8
1	D	38	CYS	2.7
1	B	93	LYS	2.7
1	B	110	ASP	2.7
1	C	133	LEU	2.6
1	C	34	THR	2.6
1	D	15	LEU	2.6
1	A	156	GLU	2.5
1	D	1	TYR	2.4
1	B	156	GLU	2.4
1	C	110	ASP	2.4
1	D	42	ALA	2.4
1	D	17	ASP	2.3
1	D	131	ARG	2.3
1	C	132	ASP	2.3
1	A	38	CYS	2.3
1	D	106	VAL	2.3
1	C	68	CYS	2.2
1	D	109	HIS	2.2
1	B	34	THR	2.2
1	D	40	ASP	2.2
1	A	35	ASP	2.1
1	C	108	GLY	2.1
1	C	27	ARG	2.1
1	A	24	GLN	2.1
1	A	109	HIS	2.1
1	A	132	ASP	2.0
1	C	38	CYS	2.0
1	A	106	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
2	CPS	C	202	42/42	0.62	0.35	6.91	57,70,110,111	0
2	CPS	A	203	28/42	0.80	0.29	4.42	71,79,81,81	0
2	CPS	D	203	42/42	0.59	0.32	3.38	58,67,103,105	0
3	SO4	A	204	5/5	0.78	0.37	3.21	108,109,109,109	0
2	CPS	C	201	26/42	0.67	0.35	2.67	90,92,93,94	0
2	CPS	B	203	42/42	0.45	0.40	2.30	54,69,115,116	0
2	CPS	D	201	42/42	0.72	0.29	1.00	53,62,114,116	0
2	CPS	C	203	26/42	0.83	0.22	0.65	63,65,67,68	0
2	CPS	D	202	23/42	0.71	0.31	0.50	81,83,84,85	0
2	CPS	B	201	29/42	0.76	0.24	0.42	65,67,72,75	0
2	CPS	A	202	30/42	0.80	0.26	0.17	58,63,68,71	0
2	CPS	B	202	23/42	0.84	0.18	-0.13	55,59,64,66	0
2	CPS	A	201	28/42	0.88	0.18	-0.26	42,49,58,61	0
3	SO4	A	205	5/5	0.82	0.28	-	111,112,112,112	0
3	SO4	C	204	5/5	0.65	0.29	-	124,124,124,125	0
3	SO4	B	204	5/5	0.73	0.21	-	135,135,135,135	0

6.5 Other polymers ⓘ

There are no such residues in this entry.