



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2016 – 12:49 PM EDT

PDB ID : 5IZ5
Title : Human GIVD cytosolic phospholipase A2
Authors : Wang, H.; Klein, M.G.
Deposited on : 2016-03-24
Resolution : 2.20 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

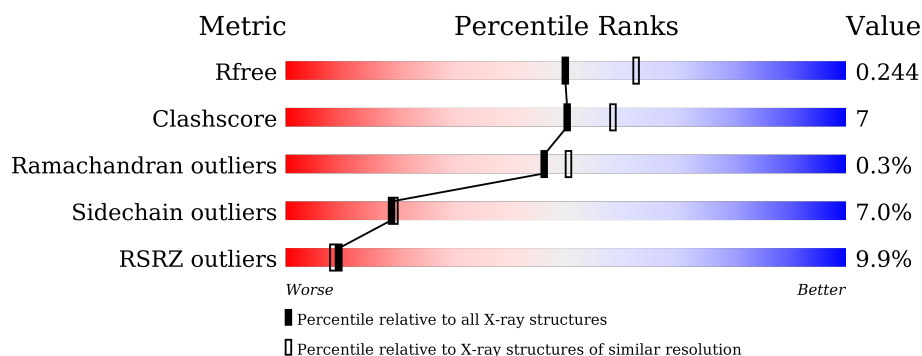
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	814	<div> <div>9%</div> <div>77%</div> <div>14%</div> <div>7%</div> </div>
1	B	814	<div> <div>10%</div> <div>79%</div> <div>11%</div> <div>8%</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	SO4	B	907	-	-	X	X
2	SO4	B	909	-	-	X	X
2	SO4	B	910	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12571 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 Cytosolic phospholipase A2 delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	746	Total	C	N	O	S	0	15	0
			6051	3846	1037	1141	27			
1	A	757	Total	C	N	O	S	0	0	0
			6018	3828	1028	1135	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q86XP0
B	-2	ALA	-	expression tag	UNP Q86XP0
B	-1	MET	-	expression tag	UNP Q86XP0
B	0	GLY	-	expression tag	UNP Q86XP0
B	1	SER	-	expression tag	UNP Q86XP0
B	554	ALA	LYS	engineered mutation	UNP Q86XP0
B	555	ALA	ASP	engineered mutation	UNP Q86XP0
B	556	ALA	LYS	engineered mutation	UNP Q86XP0
A	-3	GLY	-	expression tag	UNP Q86XP0
A	-2	ALA	-	expression tag	UNP Q86XP0
A	-1	MET	-	expression tag	UNP Q86XP0
A	0	GLY	-	expression tag	UNP Q86XP0
A	1	SER	-	expression tag	UNP Q86XP0
A	554	ALA	LYS	engineered mutation	UNP Q86XP0
A	555	ALA	ASP	engineered mutation	UNP Q86XP0
A	556	ALA	LYS	engineered mutation	UNP Q86XP0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

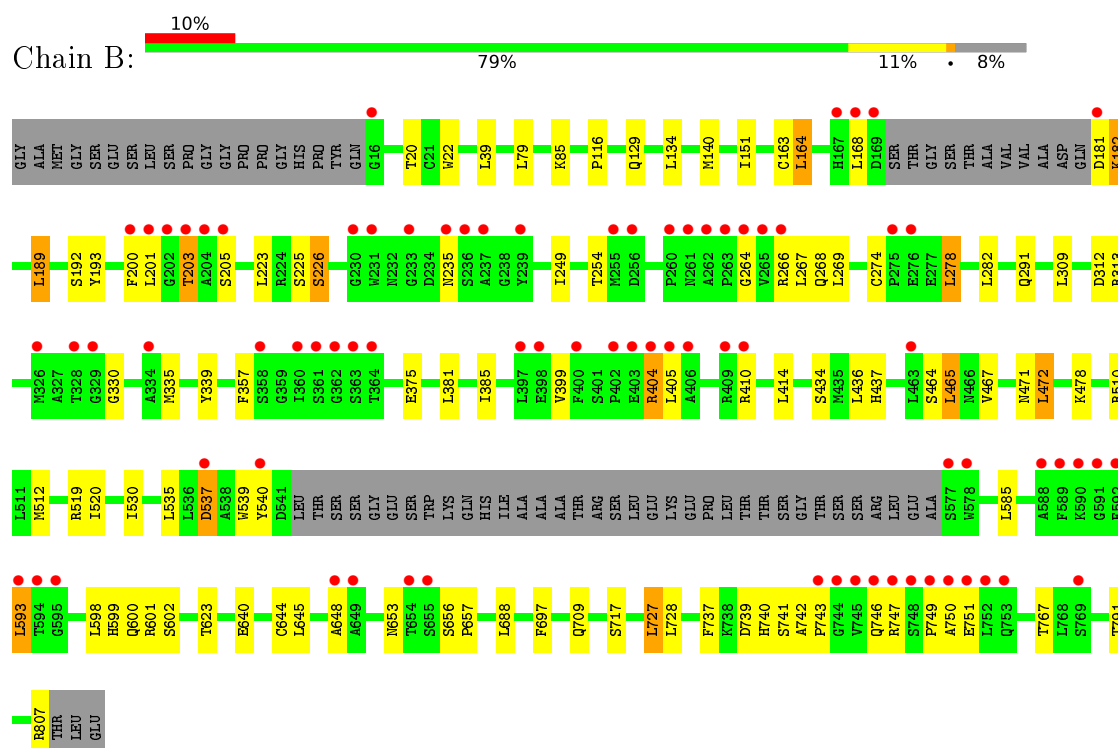
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	257	Total 257	O 257	0	0
3	A	175	Total 175	O 175	0	0

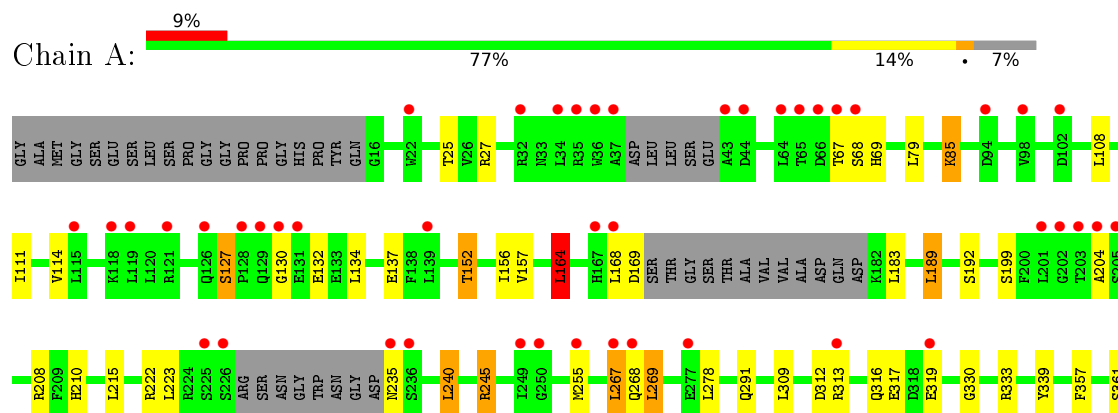
3 Residue-property plots

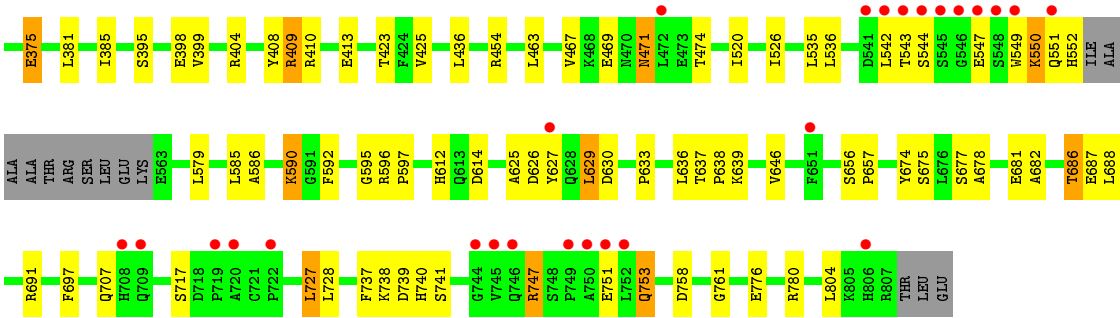
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cytosolic phospholipase A2 delta



• Molecule 1: Cytosolic phospholipase A2 delta





4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	180.78Å 180.78Å 133.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	156.56 – 2.20 45.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (156.56-2.20) 99.7 (45.20-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.223 , 0.238 0.228 , 0.244	Depositor DCC
R_{free} test set	6279 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12571	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.333 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: 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	0.35	0/6160	0.62	2/8358 (0.0%)
1	B	0.35	0/6196	0.62	1/8410 (0.0%)
All	All	0.35	0/12356	0.62	3/16768 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	164	LEU	CA-CB-CG	6.28	129.73	115.30
1	A	269	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	164	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	595	GLY	Peptide
1	B	313	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6018	0	5922	85	0
1	B	6051	0	5946	86	0
2	A	20	0	0	1	0
2	B	50	0	0	12	0
3	A	175	0	0	14	1
3	B	257	0	0	11	0
All	All	12571	0	11868	168	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 7.

All (168) 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:B:740[B]:HIS:CA	1:B:747[B]:ARG:HD2	1.60	1.29
1:B:740[B]:HIS:C	1:B:747[B]:ARG:HD2	1.62	1.19
1:B:740[B]:HIS:C	1:B:747[B]:ARG:CD	2.16	1.14
1:A:333:ARG:NH1	1:A:674:TYR:O	1.86	1.06
1:B:740[B]:HIS:HA	1:B:747[B]:ARG:HD2	1.38	1.06
1:B:740[B]:HIS:CA	1:B:747[B]:ARG:CD	2.36	1.04
1:A:404:ARG:HB3	3:A:1007:HOH:O	1.63	0.97
1:B:540:TYR:OH	1:B:593:LEU:CD1	2.13	0.96
1:B:510:ARG:NH1	3:B:1001:HOH:O	1.82	0.94
1:B:602:SER:N	2:B:909:SO4:O3	2.05	0.88
1:A:737:PHE:O	2:A:904:SO4:O2	1.93	0.86
1:B:767:THR:HG22	3:B:1111:HOH:O	1.75	0.86
1:A:469:GLU:O	1:A:471:ASN:ND2	2.09	0.86
1:B:740[B]:HIS:N	1:B:747[B]:ARG:HD3	1.92	0.84
1:A:761:GLY:N	3:A:1001:HOH:O	2.11	0.83
1:B:737:PHE:O	1:B:747[A]:ARG:NH1	2.11	0.82
1:B:540:TYR:OH	1:B:593:LEU:HD12	1.80	0.81
1:B:740[B]:HIS:N	1:B:747[B]:ARG:CD	2.44	0.80
1:B:274:CYS:SG	3:B:1007:HOH:O	2.41	0.79
1:B:537:ASP:HA	1:B:540:TYR:CE1	2.18	0.78
1:A:758:ASP:OD1	3:A:1001:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:SER:OG	1:A:677:SER:O	2.04	0.76
1:B:140:MET:HG2	3:B:1156:HOH:O	1.84	0.75
1:B:749[A]:PRO:O	1:B:750[A]:ALA:HB3	1.87	0.74
1:A:409:ARG:NH1	1:A:413:GLU:OE2	2.21	0.74
1:A:626:ASP:N	1:A:630:ASP:OD2	2.21	0.74
1:B:540:TYR:OH	1:B:593:LEU:HD11	1.88	0.73
1:B:741[B]:SER:N	1:B:747[B]:ARG:HD2	2.04	0.72
1:A:152:THR:HG21	1:A:612:HIS:HD2	1.55	0.72
1:B:749[A]:PRO:O	1:B:750[A]:ALA:CB	2.39	0.71
1:B:739[B]:ASP:O	1:B:747[B]:ARG:HG2	1.91	0.71
1:A:152:THR:HG23	1:A:157:VAL:HG22	1.74	0.70
1:B:163:CYS:HG	1:B:274:CYS:HG	1.38	0.70
1:B:740[B]:HIS:C	1:B:747[B]:ARG:NE	2.46	0.69
1:B:510:ARG:NH2	3:B:1005:HOH:O	2.26	0.69
1:A:199:SER:OG	1:A:204:ALA:HB3	1.93	0.69
1:A:747:ARG:HG3	1:A:751:GLU:HB2	1.74	0.68
1:B:640:GLU:OE1	3:B:1002:HOH:O	2.09	0.68
2:B:905:SO4:O1	1:A:596:ARG:NH2	2.28	0.67
1:B:200:PHE:O	1:B:203:THR:HG22	1.94	0.67
1:A:592:PHE:O	1:A:596:ARG:NH1	2.29	0.66
1:A:319:GLU:OE2	1:A:804:LEU:O	2.14	0.66
1:B:645:LEU:N	2:B:909:SO4:O2	2.27	0.66
1:A:408:TYR:CZ	3:A:1007:HOH:O	2.47	0.65
1:B:599:HIS:HD2	1:B:600:GLN:O	1.80	0.65
1:A:111:ILE:O	1:A:114:VAL:HG12	1.96	0.65
1:B:742[A]:ALA:HB1	1:B:743[A]:PRO:HD2	1.80	0.64
1:B:339:TYR:OH	2:B:910:SO4:O1	2.13	0.64
1:B:181:ASP:N	1:B:201:LEU:HB2	2.12	0.64
1:A:199:SER:OG	1:A:204:ALA:CB	2.45	0.64
1:A:549:TRP:O	1:A:551:GLN:N	2.31	0.64
1:A:69:HIS:CG	1:A:69:HIS:O	2.51	0.62
1:B:381:LEU:O	1:B:385:ILE:HG12	2.00	0.62
1:B:741[B]:SER:CA	1:B:747[B]:ARG:HE	2.13	0.62
1:A:630:ASP:HA	1:A:636:LEU:HD21	1.80	0.62
1:A:381:LEU:O	1:A:385:ILE:HG12	1.99	0.61
1:B:519:ARG:NH1	2:B:907:SO4:O1	2.29	0.60
1:A:425:VAL:HG11	1:A:526:ILE:HD13	1.83	0.59
1:B:193:TYR:CD2	1:B:512:MET:HE2	2.38	0.59
1:B:168:LEU:O	1:B:266:ARG:O	2.22	0.58
1:B:537:ASP:HA	1:B:540:TYR:CD1	2.38	0.58
1:B:85:LYS:HE3	3:B:1037:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741[B]:SER:N	1:B:747[B]:ARG:NE	2.52	0.57
1:B:741[B]:SER:N	1:B:747[B]:ARG:CD	2.65	0.57
1:A:152:THR:CG2	1:A:157:VAL:HG22	2.34	0.57
1:B:740[A]:HIS:HB3	1:B:742[A]:ALA:O	2.03	0.57
1:B:335:MET:SD	2:B:910:SO4:O2	2.63	0.57
1:A:168:LEU:HD13	1:A:267:LEU:CD1	2.35	0.57
1:B:182:LYS:HD3	1:B:182:LYS:H	1.69	0.56
1:B:741[B]:SER:HB3	1:B:747[B]:ARG:HE	1.71	0.56
1:A:471:ASN:HB3	3:A:1119:HOH:O	2.05	0.56
1:B:741[B]:SER:N	1:B:747[B]:ARG:HE	2.04	0.56
1:B:601:ARG:HB3	2:B:909:SO4:O3	2.07	0.54
1:B:291:GLN:HG2	3:B:1246:HOH:O	2.06	0.54
1:B:478:LYS:NZ	1:A:413:GLU:OE2	2.41	0.53
1:B:697:PHE:CE1	1:B:727:LEU:HD11	2.45	0.52
1:A:395:SER:O	1:A:399:VAL:HG23	2.10	0.52
1:A:586:ALA:O	1:A:590:LYS:HB2	2.10	0.51
1:B:535:LEU:HD12	3:B:1236:HOH:O	2.10	0.51
1:A:682:ALA:O	1:A:686:THR:HG22	2.10	0.51
1:B:339:TYR:HB3	1:B:385:ILE:CD1	2.40	0.51
1:A:27:ARG:HB3	1:A:137:GLU:HG3	1.91	0.51
1:A:535:LEU:HA	1:A:579:LEU:HD11	1.93	0.51
1:B:399:VAL:HA	1:B:404:ARG:HG2	1.93	0.51
1:A:474:THR:HG22	1:A:629:LEU:HD11	1.92	0.50
1:A:678:ALA:HB1	1:A:681:GLU:HB2	1.92	0.50
1:A:152:THR:HG22	1:A:156:ILE:O	2.11	0.50
1:A:375:GLU:HG3	3:A:1148:HOH:O	2.12	0.50
1:A:682:ALA:O	1:A:686:THR:CG2	2.60	0.50
1:A:339:TYR:HB3	1:A:385:ILE:CD1	2.42	0.50
1:B:20:THR:HG23	3:B:1060:HOH:O	2.12	0.50
1:B:225:SER:HB3	1:B:235:ASN:HD22	1.76	0.49
1:B:741[B]:SER:CB	1:B:747[B]:ARG:HE	2.25	0.49
1:B:85:LYS:CE	3:B:1037:HOH:O	2.59	0.49
1:B:602:SER:OG	2:B:909:SO4:O4	2.28	0.49
1:A:152:THR:HG21	1:A:612:HIS:CD2	2.42	0.49
1:B:434:SER:O	1:B:437:HIS:O	2.31	0.49
1:A:67:THR:O	1:A:68:SER:HB3	2.11	0.49
1:B:645:LEU:HD12	2:B:909:SO4:O4	2.13	0.49
1:A:776:GLU:HB2	3:A:1155:HOH:O	2.13	0.48
1:A:423:THR:HG22	1:A:597:PRO:HG2	1.95	0.48
1:A:753:GLN:O	1:A:780:ARG:NH1	2.46	0.48
1:A:168:LEU:HD13	1:A:267:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:THR:OG1	1:B:268:GLN:NE2	2.41	0.47
1:B:519:ARG:HD3	2:B:907:SO4:O1	2.14	0.47
1:B:182:LYS:HD3	1:B:182:LYS:N	2.28	0.47
1:A:550:LYS:NZ	3:A:1005:HOH:O	2.37	0.47
1:B:540:TYR:CZ	1:B:593:LEU:HD11	2.50	0.47
1:A:164:LEU:HD12	1:A:164:LEU:O	2.16	0.46
1:A:268:GLN:OE1	3:A:1002:HOH:O	2.21	0.46
1:B:465:LEU:HD22	1:B:648:ALA:HA	1.97	0.46
1:B:151:ILE:HD13	1:B:278:LEU:HD22	1.98	0.46
1:B:740[B]:HIS:C	1:B:747[B]:ARG:HD3	2.26	0.46
1:A:208:ARG:HG2	1:A:210:HIS:CE1	2.52	0.45
1:A:625:ALA:HA	1:A:630:ASP:OD2	2.16	0.45
1:B:472:LEU:O	1:A:409:ARG:NH2	2.48	0.45
1:A:291:GLN:HG2	3:A:1167:HOH:O	2.15	0.45
1:A:240:LEU:HD12	1:A:255:MET:SD	2.56	0.45
1:A:85:LYS:HG2	1:A:633:PRO:HG3	1.98	0.45
1:B:151:ILE:CD1	1:B:278:LEU:HD22	2.46	0.45
1:B:530:ILE:O	1:B:539:TRP:NE1	2.50	0.45
1:A:189:LEU:HG	1:A:192:SER:HB3	1.98	0.45
1:B:656:SER:N	1:B:657:PRO:CD	2.79	0.45
1:A:542:LEU:HA	1:A:542:LEU:HD23	1.91	0.45
1:A:536:LEU:HD21	1:A:542:LEU:HD12	1.98	0.44
1:A:656:SER:N	1:A:657:PRO:CD	2.81	0.44
1:B:189:LEU:HG	1:B:192:SER:HB3	1.99	0.44
1:A:25:THR:HG23	3:A:1075:HOH:O	2.17	0.44
1:B:163:CYS:SG	1:B:274:CYS:SG	3.02	0.44
1:B:739[B]:ASP:C	1:B:747[B]:ARG:CD	2.86	0.44
1:A:739:ASP:HB2	1:A:740:HIS:ND1	2.33	0.44
1:B:740[B]:HIS:O	1:B:747[B]:ARG:CD	2.63	0.44
1:A:245:ARG:NH1	3:A:1019:HOH:O	2.52	0.43
1:A:596:ARG:HG2	3:A:1079:HOH:O	2.18	0.43
1:A:697:PHE:CE1	1:A:727:LEU:HD11	2.53	0.43
1:B:747[B]:ARG:H	1:B:747[B]:ARG:HG2	1.55	0.43
1:A:474:THR:CG2	1:A:629:LEU:HD11	2.48	0.42
1:A:637:THR:N	1:A:638:PRO:CD	2.83	0.42
1:B:644:CYS:HA	2:B:909:SO4:O2	2.19	0.42
1:A:550:LYS:O	1:A:552:HIS:CD2	2.73	0.42
1:A:687:GLU:OE2	1:A:691:ARG:NH1	2.52	0.42
1:A:164:LEU:C	1:A:164:LEU:HD12	2.39	0.42
1:A:127:SER:OG	1:A:130:GLY:N	2.52	0.42
1:A:469:GLU:C	1:A:471:ASN:ND2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740[B]:HIS:HA	1:B:747[B]:ARG:CD	2.26	0.41
1:A:168:LEU:HD12	1:A:169:ASP:N	2.36	0.41
1:A:549:TRP:HE3	1:A:551:GLN:CB	2.33	0.41
1:A:549:TRP:CE3	1:A:550:LYS:N	2.88	0.41
1:B:601:ARG:CB	2:B:909:SO4:O3	2.67	0.41
1:B:751[B]:GLU:HG2	1:B:751[B]:GLU:O	2.20	0.41
1:A:316:GLN:HG2	1:A:319:GLU:HB2	2.03	0.41
1:A:741:SER:HB3	1:A:747:ARG:HG2	2.02	0.41
1:A:739:ASP:HB2	1:A:740:HIS:CE1	2.55	0.41
1:B:182:LYS:O	1:B:226:SER:OG	2.32	0.41
1:A:398:GLU:HB3	3:A:1107:HOH:O	2.19	0.41
1:A:627:TYR:C	1:A:627:TYR:CD2	2.94	0.41
1:A:747:ARG:HG3	1:A:751:GLU:CB	2.47	0.41
1:A:747:ARG:CZ	1:A:751:GLU:HG3	2.51	0.41
1:A:316:GLN:OE1	1:A:316:GLN:N	2.23	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD12	1.96	0.41
1:B:168:LEU:HD12	1:B:205:SER:HA	2.03	0.41
1:B:653:ASN:HB2	1:A:410:ARG:CD	2.51	0.41
1:B:22:TRP:CZ3	1:B:116:PRO:HB3	2.56	0.40
1:B:539:TRP:HA	1:B:539:TRP:CE3	2.56	0.40
1:B:739[B]:ASP:O	1:B:746[B]:GLN:HG3	2.21	0.40
1:B:739[B]:ASP:C	1:B:747[B]:ARG:HG2	2.40	0.40
1:A:375:GLU:CD	1:A:454:ARG:HH22	2.19	0.40
1:A:111:ILE:O	1:A:114:VAL:CG1	2.67	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)
3:A:1015:HOH:O	3:A:1100:HOH:O[3_455]	1.77	0.43

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	747/814 (92%)	723 (97%)	22 (3%)	2 (0%)	46	50
1	B	755/814 (93%)	733 (97%)	20 (3%)	2 (0%)	46	50
All	All	1502/1628 (92%)	1456 (97%)	42 (3%)	4 (0%)	46	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	GLY
1	A	550	LYS
1	B	330	GLY
1	A	330	GLY

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	659/702 (94%)	610 (93%)	49 (7%)	17	17
1	B	661/702 (94%)	619 (94%)	42 (6%)	22	24
All	All	1320/1404 (94%)	1229 (93%)	91 (7%)	19	20

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	LEU
1	B	79	LEU
1	B	129	GLN
1	B	134	LEU
1	B	164	LEU
1	B	182	LYS
1	B	189	LEU
1	B	203	THR
1	B	223	LEU
1	B	226	SER

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Mol	Chain	Res	Type
1	B	249	ILE
1	B	267	LEU
1	B	269	LEU
1	B	278	LEU
1	B	282	LEU
1	B	309	LEU
1	B	312	ASP
1	B	357	PHE
1	B	375	GLU
1	B	404	ARG
1	B	405	LEU
1	B	410	ARG
1	B	414	LEU
1	B	436	LEU
1	B	464	SER
1	B	465	LEU
1	B	467	VAL
1	B	471	ASN
1	B	472	LEU
1	B	520	ILE
1	B	537	ASP
1	B	585	LEU
1	B	593	LEU
1	B	598	LEU
1	B	623	THR
1	B	688	LEU
1	B	709	GLN
1	B	717	SER
1	B	727	LEU
1	B	728	LEU
1	B	791	THR
1	B	807	ARG
1	A	85	LYS
1	A	108	LEU
1	A	127	SER
1	A	132	GLU
1	A	134	LEU
1	A	152	THR
1	A	164	LEU
1	A	183	LEU
1	A	189	LEU
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	222	ARG
1	A	223	LEU
1	A	235	ASN
1	A	240	LEU
1	A	245	ARG
1	A	267	LEU
1	A	269	LEU
1	A	278	LEU
1	A	309	LEU
1	A	312	ASP
1	A	313	ARG
1	A	317	GLU
1	A	357	PHE
1	A	361	SER
1	A	375	GLU
1	A	409	ARG
1	A	436	LEU
1	A	463	LEU
1	A	467	VAL
1	A	471	ASN
1	A	520	ILE
1	A	543	THR
1	A	544	SER
1	A	547	GLU
1	A	585	LEU
1	A	590	LYS
1	A	614	ASP
1	A	629	LEU
1	A	639	LYS
1	A	646	VAL
1	A	686	THR
1	A	688	LEU
1	A	707	GLN
1	A	717	SER
1	A	727	LEU
1	A	728	LEU
1	A	738	LYS
1	A	747	ARG
1	A	753	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	268	GLN
1	B	281	HIS
1	B	471	ASN
1	B	599	HIS
1	B	628	GLN
1	B	705	GLN
1	A	341	HIS
1	A	471	ASN
1	A	552	HIS
1	A	705	GLN
1	A	708	HIS
1	A	746	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	SO4	A	901	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	A	902	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	A	903	-	4,4,4	0.33	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	904	-	4,4,4	0.40	0	6,6,6	0.26	0
2	SO4	B	901	-	4,4,4	0.32	0	6,6,6	0.16	0
2	SO4	B	902	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	B	903	-	4,4,4	0.35	0	6,6,6	0.19	0
2	SO4	B	904	-	4,4,4	0.32	0	6,6,6	0.06	0
2	SO4	B	905	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	B	906	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	B	907	-	4,4,4	0.42	0	6,6,6	0.17	0
2	SO4	B	908	-	4,4,4	0.48	0	6,6,6	0.21	0
2	SO4	B	909	-	4,4,4	0.56	0	6,6,6	0.22	0
2	SO4	B	910	-	4,4,4	0.35	0	6,6,6	0.16	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
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
2	SO4	A	904	-	-	0/0/0/0	0/0/0/0
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	902	-	-	0/0/0/0	0/0/0/0
2	SO4	B	903	-	-	0/0/0/0	0/0/0/0
2	SO4	B	904	-	-	0/0/0/0	0/0/0/0
2	SO4	B	905	-	-	0/0/0/0	0/0/0/0
2	SO4	B	906	-	-	0/0/0/0	0/0/0/0
2	SO4	B	907	-	-	0/0/0/0	0/0/0/0
2	SO4	B	908	-	-	0/0/0/0	0/0/0/0
2	SO4	B	909	-	-	0/0/0/0	0/0/0/0
2	SO4	B	910	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	904	SO4	1	0
2	B	905	SO4	1	0
2	B	907	SO4	2	0
2	B	909	SO4	7	0
2	B	910	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	757/814 (92%)	0.48	71 (9%) 11 10	34, 56, 94, 131	0
1	B	746/814 (91%)	0.40	78 (10%) 8 7	29, 46, 92, 116	0
All	All	1503/1628 (92%)	0.44	149 (9%) 9 8	29, 51, 93, 131	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	LEU	9.7
1	A	35	ARG	8.8
1	A	37	ALA	8.1
1	A	168	LEU	7.9
1	A	204	ALA	7.6
1	B	593	LEU	7.4
1	A	36	TRP	6.9
1	B	592	PHE	6.8
1	B	540	TYR	6.6
1	B	578	TRP	6.2
1	B	264	GLY	6.0
1	B	400	PHE	6.0
1	B	591	GLY	6.0
1	A	43	ALA	5.5
1	A	749	PRO	5.5
1	A	750	ALA	5.4
1	B	231	TRP	5.4
1	A	202	GLY	5.3
1	A	472	LEU	5.3
1	B	261	ASN	5.1
1	B	201	LEU	5.0
1	A	549	TRP	5.0
1	B	594	THR	4.9
1	A	548	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	129	GLN	4.7
1	A	751	GLU	4.7
1	B	181	ASP	4.6
1	B	203	THR	4.6
1	B	204	ALA	4.4
1	A	543	THR	4.3
1	A	545	SER	4.3
1	B	275	PRO	4.3
1	B	205	SER	4.2
1	A	250	GLY	4.1
1	A	203	THR	4.1
1	B	752[A]	LEU	4.1
1	A	131	GLU	4.1
1	A	119	LEU	3.9
1	A	235	ASN	3.8
1	B	590	LYS	3.8
1	B	749[A]	PRO	3.7
1	B	16	GLY	3.6
1	A	201	LEU	3.6
1	B	751[A]	GLU	3.6
1	B	233	GLY	3.6
1	B	266	ARG	3.6
1	B	265	VAL	3.5
1	A	547	GLU	3.5
1	B	589	PHE	3.4
1	B	202	GLY	3.4
1	B	360	ILE	3.4
1	A	752	LEU	3.4
1	B	406	ALA	3.3
1	A	806	HIS	3.3
1	A	44	ASP	3.3
1	A	544	SER	3.2
1	A	66	ASP	3.2
1	B	263	PRO	3.2
1	A	34	LEU	3.2
1	B	744[A]	GLY	3.2
1	B	537	ASP	3.2
1	A	68	SER	3.1
1	A	722	PRO	3.1
1	A	708	HIS	3.1
1	A	22	TRP	3.1
1	B	402	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	169	ASP	3.0
1	A	130	GLY	3.0
1	A	542	LEU	3.0
1	A	249	ILE	3.0
1	B	230	GLY	2.9
1	B	743[A]	PRO	2.9
1	A	118	LYS	2.9
1	A	98	VAL	2.9
1	A	115	LEU	2.9
1	A	65	THR	2.9
1	B	405	LEU	2.9
1	B	649	ALA	2.9
1	A	546	GLY	2.8
1	B	260	PRO	2.8
1	A	64	LEU	2.8
1	A	541	ASP	2.8
1	B	239	TYR	2.8
1	B	235	ASN	2.8
1	B	577	SER	2.8
1	B	262	ALA	2.7
1	A	319	GLU	2.8
1	A	313	ARG	2.7
1	B	750[A]	ALA	2.7
1	B	595	GLY	2.7
1	A	720	ALA	2.7
1	A	226	SER	2.7
1	A	32	ARG	2.7
1	B	648	ALA	2.7
1	B	747[A]	ARG	2.6
1	A	277	GLU	2.6
1	B	463	LEU	2.6
1	B	410	ARG	2.5
1	A	205	SER	2.5
1	B	255	MET	2.5
1	B	276	GLU	2.5
1	B	409	ARG	2.5
1	B	748[A]	SER	2.5
1	B	746[A]	GLN	2.5
1	B	588	ALA	2.5
1	B	745[A]	VAL	2.4
1	A	128	PRO	2.4
1	A	255	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	362	GLY	2.4
1	A	236	SER	2.4
1	A	719	PRO	2.4
1	B	328	THR	2.4
1	A	126	GLN	2.4
1	A	67	THR	2.4
1	B	361	SER	2.4
1	B	654	THR	2.4
1	B	326	MET	2.3
1	B	753	GLN	2.3
1	B	655	SER	2.3
1	A	102	ASP	2.3
1	B	398	GLU	2.3
1	B	403	GLU	2.3
1	A	225	SER	2.3
1	A	551	GLN	2.3
1	B	237	ALA	2.3
1	B	167	HIS	2.3
1	A	651	PHE	2.3
1	A	709	GLN	2.3
1	A	744	GLY	2.2
1	A	627	TYR	2.2
1	B	334	ALA	2.2
1	B	329	GLY	2.2
1	A	267	LEU	2.2
1	B	200	PHE	2.2
1	B	236	SER	2.2
1	B	364	THR	2.1
1	B	363	SER	2.1
1	A	745	VAL	2.1
1	B	256	ASP	2.1
1	A	167	HIS	2.1
1	A	94	ASP	2.1
1	A	121	ARG	2.1
1	B	397	LEU	2.1
1	A	139	LEU	2.1
1	A	746	GLN	2.0
1	B	769	SER	2.0
1	A	268	GLN	2.0
1	B	404	ARG	2.0
1	B	358	SER	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 carbohydrates 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. 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	SO4	B	910	5/5	0.78	0.61	11.05	64,65,66,66	5
2	SO4	B	909	5/5	0.97	0.34	4.46	26,32,33,34	5
2	SO4	B	907	5/5	0.91	0.23	2.09	66,71,75,77	0
2	SO4	A	904	5/5	0.85	0.37	1.40	98,103,105,107	0
2	SO4	B	904	5/5	0.90	0.15	1.15	91,91,92,95	0
2	SO4	B	906	5/5	0.82	0.21	0.84	120,122,123,124	0
2	SO4	A	901	5/5	0.86	0.28	0.79	120,121,123,123	0
2	SO4	A	903	5/5	0.94	0.16	0.38	83,84,85,85	0
2	SO4	A	902	5/5	0.93	0.14	-0.03	78,80,83,88	0
2	SO4	B	905	5/5	0.95	0.15	-	76,79,80,80	0
2	SO4	B	902	5/5	0.88	0.16	-	89,90,92,93	0
2	SO4	B	903	5/5	0.91	0.20	-	81,89,90,91	0
2	SO4	B	901	5/5	0.94	0.14	-	76,76,78,80	0
2	SO4	B	908	5/5	0.89	0.24	-	71,75,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.