WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:16 PM GMT

PDB ID : 1EV9
Title : RAT GLUTATHIONE S-TRANSFERASE A1-1 MUTANT W21F WITH GSO3 BOUND
Authors : Adman, E.T.; Le Trong, I.; Stenkamp, R.E.; Nieslanik, B.S.; Dietze, E.C.; Tai, G.; Ibarra, C.; Atkins, W.M.
Deposited on : 2000-04-19
Resolution : 2.20 Å(reported)

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 (i)

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	Percentile Ranks	Value
Clashscore		18
Ramachandran outliers		1.9%
Sidechain outliers		7.9%
RSRZ outliers		15.7%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
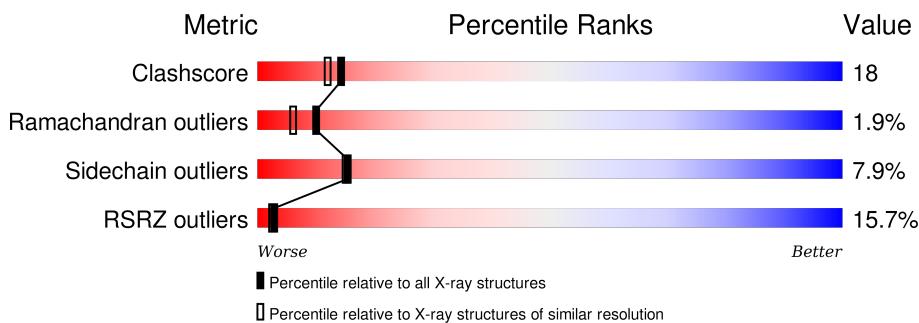
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 <=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	221	10% / 60% / 32% / 6% ·
1	C	221	24% / 61% / 26% / 6% / 6%
1	D	221	11% / 63% / 28% / 6% ·
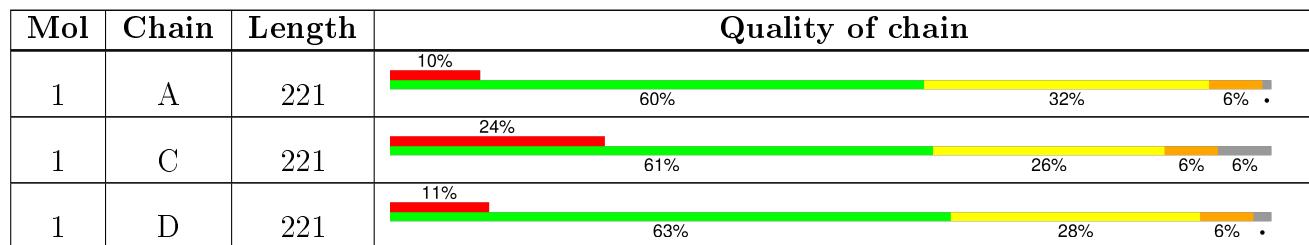
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5388 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 GLUTATHIONE S-TRANSFERASE A1-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total 1765	C 1137	N 296	O 321	S 11	0	0	0
1	C	207	Total 1664	C 1073	N 278	O 302	S 11	0	0	0
1	D	216	Total 1709	C 1100	N 287	O 311	S 11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	TRP	ENGINEERED	UNP P00502
A	96	SER	THR	CONFLICT	UNP P00502
C	21	PHE	TRP	ENGINEERED	UNP P00502
C	96	SER	THR	CONFLICT	UNP P00502
D	21	PHE	TRP	ENGINEERED	UNP P00502
D	96	SER	THR	CONFLICT	UNP P00502

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
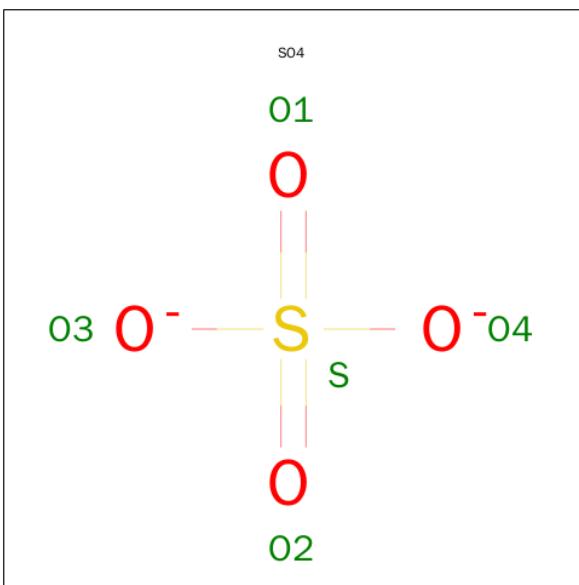
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLUTATHIONE SULFONIC ACID (three-letter code: GTS) (formula: $C_{10}H_{17}N_3O_9S$).
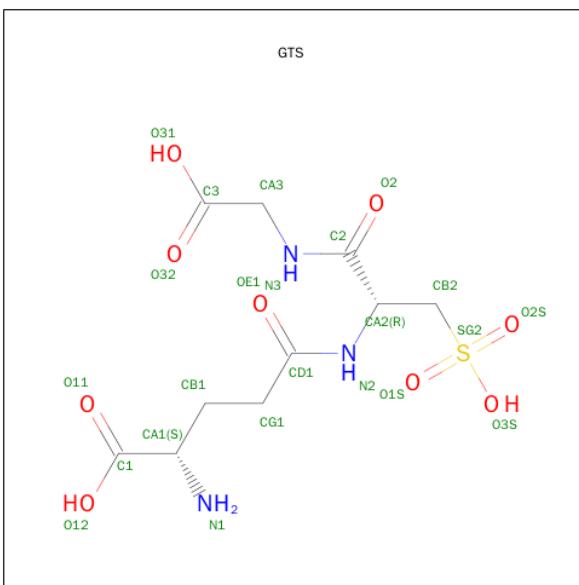
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	10	3	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			23	10	3	9	1		
3	D	1	Total	C	N	O	S	0	0
			23	10	3	9	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	C	20	Total	O	0	0
			20	20		
4	D	28	Total	O	0	0
			28	28		

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: GLUTATHIONE S-TRANSFERASE A1-1

- Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1

- Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1

K205 L206 P207 M208 D209 A210 K211 Q212 I213 E214 E215 A216 R217 LYS ILE PHE LYS PHE
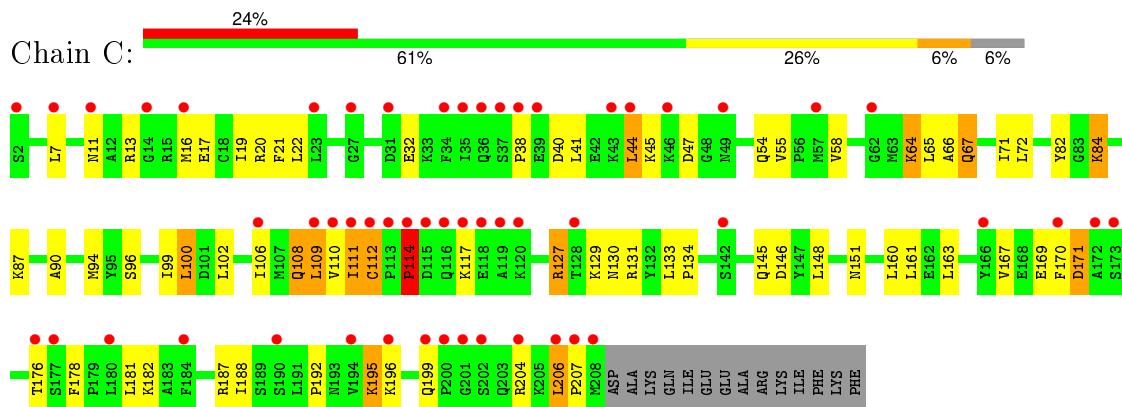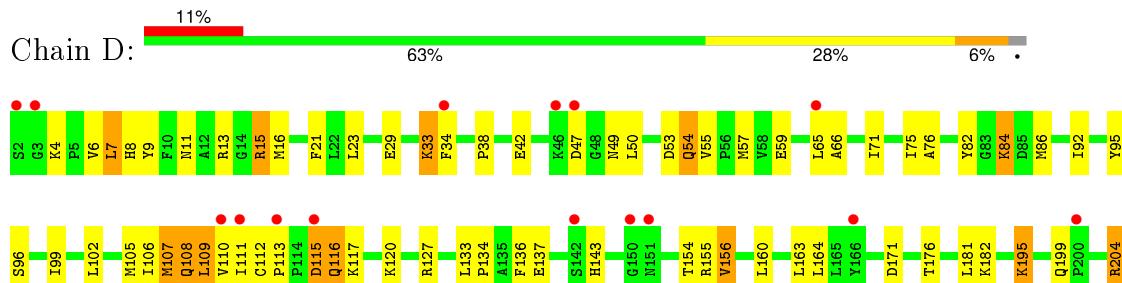
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.70Å 275.10Å 70.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 76.9 (19.83-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.39 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.236 , 0.299 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å²)	25.7	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.30 , 75.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 65590 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: GTS, 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	0.82	1/1796 (0.1%)	1.10	8/2411 (0.3%)
1	C	0.71	0/1694	1.10	11/2276 (0.5%)
1	D	0.69	0/1739	1.08	8/2339 (0.3%)
All	All	0.74	1/5229 (0.0%)	1.09	27/7026 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE1	5.84	1.32	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	CYS	N-CA-CB	-8.72	94.91	110.60
1	D	86	MET	CB-CA-C	-8.17	94.06	110.40
1	D	204	ARG	N-CA-CB	-7.90	96.37	110.60
1	A	141	LYS	CD-CE-NZ	7.71	129.44	111.70
1	A	107	MET	CB-CA-C	-7.50	95.41	110.40
1	C	195	LYS	CG-CD-CE	7.18	133.43	111.90
1	A	4	LYS	N-CA-CB	-6.81	98.34	110.60
1	D	54	GLN	CB-CA-C	-6.29	97.83	110.40
1	C	84	LYS	CB-CG-CD	-6.10	95.73	111.60
1	D	182	LYS	CB-CG-CD	6.02	127.26	111.60
1	D	195	LYS	CB-CG-CD	5.99	127.17	111.60
1	A	32	GLU	CB-CA-C	-5.85	98.70	110.40
1	A	44	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	C	11	ASN	N-CA-CB	5.74	120.93	110.60
1	D	7	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	C	32	GLU	N-CA-CB	-5.65	100.42	110.60
1	C	64	LYS	CB-CG-CD	5.65	126.30	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	105	MET	CB-CA-C	-5.59	99.22	110.40
1	C	206	LEU	N-CA-CB	-5.59	99.23	110.40
1	A	72	LEU	CB-CA-C	-5.51	99.73	110.20
1	C	84	LYS	CD-CE-NZ	-5.44	99.18	111.70
1	C	111	ILE	CG1-CB-CG2	-5.44	99.43	111.40
1	A	218	LYS	CB-CG-CD	5.39	125.62	111.60
1	D	86	MET	N-CA-CB	5.31	120.15	110.60
1	A	214	GLU	N-CA-CB	-5.11	101.41	110.60
1	C	195	LYS	CD-CE-NZ	5.08	123.39	111.70
1	C	169	GLU	CB-CA-C	-5.00	100.39	110.40

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	1765	0	1830	86	0
1	C	1664	0	1726	54	0
1	D	1709	0	1750	54	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	23	0	14	0	0
3	C	23	0	14	5	0
3	D	23	0	14	3	0
4	A	118	0	0	47	0
4	C	20	0	0	2	0
4	D	28	0	0	4	0
All	All	5388	0	5348	191	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 18.

All (191) 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:A:78:LYS:HB3	4:A:681:HOH:O	1.73	0.87
1:A:209:ASP:HA	1:A:213:ILE:HG13	1.57	0.86
1:A:18:CYS:SG	4:A:645:HOH:O	2.36	0.84
1:A:35:ILE:HG13	4:A:660:HOH:O	1.78	0.82
1:D:47:ASP:HB2	1:D:49:ASN:ND2	1.95	0.81
1:D:102:LEU:HD23	1:D:163:LEU:HD21	1.62	0.80
1:A:145:GLN:HB2	4:A:695:HOH:O	1.80	0.80
1:A:160:LEU:HD23	4:A:574:HOH:O	1.82	0.79
1:A:93:ASP:HA	4:A:649:HOH:O	1.83	0.78
1:C:65:LEU:HD13	1:C:71:ILE:HA	1.64	0.78
1:D:71:ILE:HD11	4:D:668:HOH:O	1.83	0.78
1:D:47:ASP:HB2	1:D:49:ASN:HD21	1.49	0.78
1:D:95:TYR:HB2	1:D:156:VAL:HG11	1.66	0.77
1:A:92:ILE:HG23	1:A:156:VAL:HG22	1.68	0.75
1:A:82:TYR:HE2	4:A:522:HOH:O	1.69	0.75
1:A:96:SER:HB2	4:A:649:HOH:O	1.87	0.74
1:D:92:ILE:HG23	1:D:156:VAL:HG22	1.69	0.74
1:A:102:LEU:HB3	4:A:575:HOH:O	1.88	0.72
1:C:127:ARG:O	1:C:131:ARG:HB3	1.89	0.71
1:A:8:HIS:HB2	4:A:595:HOH:O	1.90	0.71
1:A:203:GLN:HG3	4:A:573:HOH:O	1.88	0.71
1:C:54:GLN:HB3	3:C:240:GTS:HG11	1.72	0.71
1:A:82:TYR:HE1	4:A:562:HOH:O	1.74	0.70
1:A:166:TYR:HE1	1:A:204:ARG:HH21	1.37	0.70
1:A:213:ILE:O	1:A:217:ARG:HG3	1.90	0.70
1:C:109:LEU:HD23	1:C:110:VAL:HG22	1.74	0.69
1:A:152:LYS:HB3	4:A:659:HOH:O	1.91	0.68
1:C:90:ALA:HB1	1:D:65:LEU:HD11	1.76	0.68
1:A:97:GLU:HB2	4:A:635:HOH:O	1.92	0.68
1:A:95:TYR:HB2	1:A:156:VAL:HG11	1.76	0.68
1:D:106:ILE:HA	1:D:109:LEU:HD22	1.75	0.67
1:A:215:GLU:O	1:A:218:LYS:HG2	1.94	0.67
1:A:72:LEU:HD21	4:A:645:HOH:O	1.95	0.67
1:A:96:SER:O	1:A:100:LEU:HD22	1.95	0.66
1:D:34:PHE:CE2	1:D:205:LYS:HE3	2.32	0.65
1:A:57:MET:N	4:A:595:HOH:O	2.30	0.64
1:A:208:MET:SD	1:A:208:MET:N	2.70	0.64
1:A:143:HIS:CE1	4:A:695:HOH:O	2.51	0.64
1:A:94:MET:SD	4:A:552:HOH:O	2.55	0.64
1:A:67:GLN:HG2	4:A:509:HOH:O	1.98	0.63
1:D:15:ARG:NH1	3:D:250:GTS:HB11	2.12	0.63
1:A:19:ILE:HG13	4:A:645:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:VAL:O	3:C:240:GTS:HG12	1.99	0.62
1:C:102:LEU:HD23	1:C:163:LEU:HD11	1.81	0.62
1:C:112:CYS:O	1:C:114:PRO:HD3	2.00	0.62
1:A:102:LEU:N	4:A:575:HOH:O	2.33	0.62
1:D:208:MET:SD	1:D:208:MET:N	2.72	0.62
1:A:104:GLU:HA	1:A:107:MET:HG2	1.81	0.62
1:C:129:LYS:HE2	4:C:701:HOH:O	1.99	0.62
1:A:187:ARG:HG3	4:A:607:HOH:O	2.00	0.60
1:C:16:MET:SD	1:C:19:ILE:HD12	2.40	0.60
1:C:13:ARG:HH11	1:C:207:PRO:HA	1.65	0.60
1:A:37:SER:HA	1:A:219:ILE:HD11	1.82	0.60
1:C:41:LEU:HG	1:C:45:LYS:HE2	1.82	0.60
1:C:13:ARG:NH1	1:C:207:PRO:HA	2.17	0.60
1:C:127:ARG:HA	1:C:127:ARG:HE	1.67	0.60
1:D:34:PHE:CZ	1:D:205:LYS:CE	2.86	0.59
1:C:146:ASP:HB3	1:C:187:ARG:HD3	1.84	0.59
1:A:206:LEU:CD2	1:A:207:PRO:HD2	2.34	0.58
1:A:215:GLU:HA	1:A:218:LYS:HE3	1.86	0.58
1:C:65:LEU:HB3	1:C:71:ILE:HG12	1.86	0.58
1:A:206:LEU:HD22	1:A:207:PRO:HD2	1.87	0.57
1:A:179:PRO:HG2	4:A:526:HOH:O	2.04	0.57
1:C:106:ILE:O	1:C:109:LEU:HD22	2.04	0.56
1:A:97:GLU:N	4:A:635:HOH:O	2.38	0.56
1:A:91:LEU:HA	4:A:552:HOH:O	2.05	0.56
1:A:203:GLN:NE2	4:A:514:HOH:O	2.39	0.56
1:D:34:PHE:HE2	1:D:205:LYS:HE3	1.69	0.56
1:C:66:ALA:O	1:C:67:GLN:HB2	2.06	0.56
1:D:76:ALA:HB2	1:D:155:ARG:HD2	1.87	0.56
1:A:11:ASN:HD22	1:A:205:LYS:HE3	1.70	0.56
1:C:90:ALA:HA	4:D:342:HOH:O	2.05	0.55
1:C:99:ILE:HG23	1:C:163:LEU:HD22	1.89	0.55
1:C:17:GLU:HA	1:C:20:ARG:NH1	2.22	0.55
1:D:55:VAL:O	3:D:250:GTS:HG12	2.07	0.55
1:A:182:LYS:HE3	4:A:696:HOH:O	2.07	0.54
1:C:133:LEU:HD22	1:C:181:LEU:HD13	1.88	0.54
1:D:107:MET:O	1:D:110:VAL:HG12	2.07	0.54
1:D:76:ALA:CB	1:D:155:ARG:HD2	2.37	0.54
1:D:23:LEU:HD21	1:D:75:ILE:HD13	1.89	0.53
1:A:86:MET:HG2	1:A:86:MET:O	2.06	0.53
1:D:84:LYS:O	1:D:84:LYS:HG2	2.09	0.53
1:C:58:VAL:HG21	1:C:71:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLU:OE2	1:A:179:PRO:HD2	2.08	0.52
1:C:178:PHE:HB3	1:C:181:LEU:HD12	1.91	0.52
1:A:96:SER:OG	1:A:156:VAL:HG13	2.09	0.52
1:D:107:MET:SD	1:D:107:MET:N	2.82	0.52
1:D:99:ILE:HG13	1:D:136:PHE:CZ	2.45	0.52
1:C:94:MET:SD	1:D:66:ALA:HB3	2.50	0.52
1:A:104:GLU:O	1:A:108:GLN:HG2	2.11	0.51
1:C:170:PHE:O	1:C:171:ASP:HB2	2.10	0.51
1:D:116:GLN:O	1:D:120:LYS:HG3	2.10	0.51
1:C:133:LEU:HB2	1:C:134:PRO:HD3	1.93	0.51
1:D:66:ALA:HA	4:D:668:HOH:O	2.11	0.51
1:D:34:PHE:HZ	1:D:205:LYS:CE	2.23	0.51
1:A:58:VAL:HG23	1:A:71:ILE:HD13	1.93	0.50
1:D:34:PHE:HZ	1:D:205:LYS:HE2	1.76	0.50
1:D:34:PHE:CZ	1:D:205:LYS:HE2	2.46	0.50
1:A:34:PHE:HZ	1:A:205:LYS:HZ1	1.58	0.50
1:A:98:GLY:CA	4:A:508:HOH:O	2.60	0.50
1:D:6:VAL:HB	1:D:59:GLU:HB2	1.94	0.50
1:A:75:ILE:HA	4:A:681:HOH:O	2.12	0.50
1:A:91:LEU:HD23	4:A:552:HOH:O	2.12	0.49
1:C:163:LEU:O	1:C:167:VAL:HG23	2.12	0.49
1:A:13:ARG:NH1	1:A:207:PRO:HB3	2.26	0.49
1:A:44:LEU:HD13	1:A:50:LEU:HD11	1.94	0.49
1:D:195:LYS:O	1:D:199:GLN:HG3	2.13	0.49
1:A:33:LYS:HB2	4:A:301:HOH:O	2.11	0.49
1:A:37:SER:HA	1:A:219:ILE:CD1	2.43	0.49
1:A:148:LEU:HG	4:A:574:HOH:O	2.12	0.49
1:C:96:SER:O	1:C:100:LEU:HB2	2.12	0.48
1:A:92:ILE:HB	4:A:562:HOH:O	2.12	0.48
1:C:206:LEU:HB3	1:C:207:PRO:HD2	1.96	0.48
1:D:208:MET:O	1:D:209:ASP:CB	2.61	0.48
1:A:166:TYR:HE1	1:A:204:ARG:NH2	2.10	0.48
1:A:37:SER:OG	1:A:39:GLU:HB3	2.14	0.48
1:A:96:SER:O	1:A:99:ILE:HB	2.13	0.48
1:A:32:GLU:CD	1:A:34:PHE:HE1	2.17	0.48
1:A:179:PRO:O	1:A:182:LYS:HB3	2.13	0.47
1:A:98:GLY:N	4:A:508:HOH:O	2.47	0.47
1:C:54:GLN:HA	3:C:240:GTS:O2	2.14	0.47
1:D:112:CYS:SG	1:D:117:LYS:HA	2.55	0.47
1:C:196:LYS:HA	1:C:199:GLN:HE21	1.80	0.47
1:C:176:THR:HA	1:C:182:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:O	1:A:109:LEU:HB2	2.14	0.46
1:A:99:ILE:C	4:A:575:HOH:O	2.54	0.46
1:A:183:ALA:HB1	4:A:607:HOH:O	2.16	0.46
1:A:10:PHE:HE1	1:A:219:ILE:HG22	1.79	0.46
1:D:50:LEU:HB2	1:D:53:ASP:HA	1.98	0.46
1:D:212:GLN:HA	1:D:215:GLU:CB	2.46	0.46
1:D:7:LEU:HD13	1:D:16:MET:SD	2.56	0.45
1:A:66:ALA:O	1:A:67:GLN:HB2	2.15	0.45
1:D:57:MET:HA	4:D:668:HOH:O	2.16	0.45
1:A:35:ILE:N	4:A:660:HOH:O	2.49	0.45
1:D:34:PHE:CE2	1:D:205:LYS:CE	3.00	0.45
1:C:146:ASP:HB3	1:C:187:ARG:CD	2.47	0.45
1:A:184:PHE:CZ	1:A:188:ILE:HG13	2.52	0.45
1:C:54:GLN:CB	3:C:240:GTS:HG11	2.44	0.45
1:C:111:ILE:O	1:C:111:ILE:HG22	2.17	0.45
1:D:13:ARG:NH1	1:D:207:PRO:HA	2.32	0.44
1:C:87:LYS:HE2	1:C:87:LYS:HB3	1.79	0.44
1:C:161:LEU:HD22	1:C:188:ILE:HG22	1.99	0.44
1:A:98:GLY:HA3	4:A:508:HOH:O	2.17	0.44
1:C:114:PRO:HA	1:C:117:LYS:HB2	2.00	0.44
1:A:73:ASN:CB	4:A:522:HOH:O	2.65	0.44
1:A:73:ASN:HB3	4:A:522:HOH:O	2.18	0.44
1:D:160:LEU:O	1:D:164:LEU:HG	2.18	0.44
1:D:137:GLU:OE1	1:D:181:LEU:HG	2.18	0.43
1:D:4:LYS:NZ	1:D:29:GLU:HB3	2.34	0.43
1:A:143:HIS:CG	4:A:695:HOH:O	2.71	0.43
1:A:66:ALA:HB3	4:A:509:HOH:O	2.18	0.43
1:A:154:THR:HG22	4:A:312:HOH:O	2.19	0.43
1:A:102:LEU:CB	4:A:575:HOH:O	2.58	0.43
1:C:94:MET:HE2	1:D:65:LEU:HD23	2.00	0.43
1:C:130:ASN:HB3	4:C:682:HOH:O	2.19	0.43
1:A:207:PRO:O	1:A:212:GLN:NE2	2.51	0.42
1:D:106:ILE:O	1:D:109:LEU:HB2	2.19	0.42
1:D:8:HIS:HE2	1:D:59:GLU:HG3	1.84	0.42
1:C:176:THR:HA	1:C:182:LYS:CE	2.49	0.42
1:D:205:LYS:HA	1:D:205:LYS:HD3	1.74	0.42
1:A:141:LYS:HG3	1:A:180:LEU:HD11	2.01	0.42
1:D:9:TYR:O	1:D:34:PHE:HA	2.20	0.42
1:A:19:ILE:N	4:A:645:HOH:O	2.50	0.42
1:A:187:ARG:NH1	4:A:607:HOH:O	2.52	0.42
1:C:99:ILE:HG23	1:C:163:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:THR:HA	1:C:182:LYS:HE2	2.01	0.42
1:C:7:LEU:HD22	1:C:58:VAL:HG22	2.01	0.42
1:D:113:PRO:HB3	1:D:115:ASP:OD2	2.19	0.41
1:C:145:GLN:HB3	1:C:151:ASN:OD1	2.21	0.41
1:A:34:PHE:CD1	1:A:34:PHE:N	2.89	0.41
1:A:110:VAL:C	1:A:111:ILE:HG13	2.41	0.41
1:D:96:SER:OG	1:D:156:VAL:HG13	2.21	0.41
1:C:102:LEU:HD23	1:C:163:LEU:HD21	2.01	0.41
1:C:22:LEU:HD22	1:C:72:LEU:HD22	2.01	0.41
1:C:195:LYS:O	1:C:199:GLN:HG3	2.19	0.41
1:D:154:THR:OG1	1:D:156:VAL:HG23	2.20	0.41
1:C:54:GLN:HB3	3:C:240:GTS:HN2	1.86	0.41
1:D:11:ASN:HA	1:D:34:PHE:CE2	2.55	0.41
1:A:166:TYR:N	1:A:166:TYR:CD1	2.87	0.41
1:D:84:LYS:HE2	1:D:84:LYS:HB3	1.69	0.41
1:D:108:GLN:HE21	1:D:111:ILE:HD12	1.86	0.41
1:C:148:LEU:HD11	1:C:160:LEU:HD22	2.03	0.41
1:D:133:LEU:HB2	1:D:134:PRO:HD3	2.02	0.41
1:A:199:GLN:HA	1:A:200:PRO:HD3	1.96	0.41
1:C:44:LEU:O	1:C:47:ASP:HB2	2.21	0.41
1:C:13:ARG:HB3	1:C:17:GLU:HB2	2.03	0.40
1:A:28:VAL:HG21	1:A:79:TYR:CZ	2.55	0.40
1:D:54:GLN:HB3	3:D:250:GTS:N2	2.36	0.40
1:A:77:THR:HG23	4:A:589:HOH:O	2.21	0.40
1:D:33:LYS:HD2	1:D:33:LYS:HA	1.87	0.40
1:C:19:ILE:HA	1:C:72:LEU:HD21	2.02	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	217/221 (98%)	190 (88%)	24 (11%)	3 (1%)	14	10
1	C	205/221 (93%)	177 (86%)	24 (12%)	4 (2%)	9	5
1	D	214/221 (97%)	194 (91%)	15 (7%)	5 (2%)	8	4
All	All	636/663 (96%)	561 (88%)	63 (10%)	12 (2%)	10	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASP
1	C	114	PRO
1	D	208	MET
1	D	209	ASP
1	D	210	ALA
1	C	171	ASP
1	D	171	ASP
1	A	210	ALA
1	D	176	THR
1	A	217	ARG
1	C	108	GLN
1	C	67	GLN

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	193/195 (99%)	180 (93%)	13 (7%)	20	21
1	C	183/195 (94%)	169 (92%)	14 (8%)	16	16
1	D	183/195 (94%)	166 (91%)	17 (9%)	11	10
All	All	559/585 (96%)	515 (92%)	44 (8%)	15	15

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE

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Mol	Chain	Res	Type
1	A	44	LEU
1	A	65	LEU
1	A	82	TYR
1	A	94	MET
1	A	100	LEU
1	A	114	PRO
1	A	127	ARG
1	A	143	HIS
1	A	156	VAL
1	A	192	PRO
1	A	208	MET
1	A	215	GLU
1	C	21	PHE
1	C	38	PRO
1	C	40	ASP
1	C	44	LEU
1	C	64	LYS
1	C	82	TYR
1	C	84	LYS
1	C	100	LEU
1	C	108	GLN
1	C	109	LEU
1	C	114	PRO
1	C	127	ARG
1	C	192	PRO
1	C	204	ARG
1	D	15	ARG
1	D	21	PHE
1	D	33	LYS
1	D	38	PRO
1	D	42	GLU
1	D	82	TYR
1	D	84	LYS
1	D	107	MET
1	D	108	GLN
1	D	109	LEU
1	D	115	ASP
1	D	116	GLN
1	D	127	ARG
1	D	143	HIS
1	D	156	VAL
1	D	204	ARG

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Mol	Chain	Res	Type
1	D	208	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	36	GLN
1	A	199	GLN
1	C	199	GLN
1	D	36	GLN
1	D	49	ASN
1	D	199	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 ⓘ

There are no carbohydrates in this entry.

5.6　Ligand geometry ⓘ

6 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	$\#|Z| > 2$
3	GTS	A	230	-	15,22,22	0.78	0	19,30,30	1.59	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	260	-	4,4,4	0.69	0	6,6,6	0.34	0
3	GTS	C	240	-	15,22,22	1.02	1 (6%)	19,30,30	1.71	3 (15%)
2	SO4	C	261	-	4,4,4	0.77	0	6,6,6	0.14	0
3	GTS	D	250	-	15,22,22	0.69	0	19,30,30	1.55	4 (21%)
2	SO4	D	262	-	4,4,4	0.28	0	6,6,6	0.23	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
3	GTS	A	230	-	-	0/21/27/27	0/0/0/0
2	SO4	A	260	-	-	0/0/0/0	0/0/0/0
3	GTS	C	240	-	-	0/21/27/27	0/0/0/0
2	SO4	C	261	-	-	0/0/0/0	0/0/0/0
3	GTS	D	250	-	-	0/21/27/27	0/0/0/0
2	SO4	D	262	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	240	GTS	CB2-SG2	2.95	1.82	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	240	GTS	CA3-N3-C2	-3.29	117.82	122.34
3	D	250	GTS	CB2-CA2-C2	-2.76	103.16	109.83
3	C	240	GTS	CG1-CD1-N2	-2.69	111.44	115.83
3	D	250	GTS	CA3-N3-C2	-2.20	119.31	122.34
3	D	250	GTS	CG1-CD1-N2	-2.10	112.41	115.83
3	A	230	GTS	CB2-CA2-C2	-2.08	104.81	109.83
3	D	250	GTS	O1S-SG2-CB2	4.20	110.48	106.94
3	C	240	GTS	O1S-SG2-CB2	5.03	111.18	106.94
3	A	230	GTS	O1S-SG2-CB2	5.11	111.25	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	240	GTS	5	0
3	D	250	GTS	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	219/221 (99%)	0.41	22 (10%)	9	8	20, 35, 93, 100	0
1	C	207/221 (93%)	1.45	54 (26%)	1	1	42, 70, 99, 100	0
1	D	216/221 (97%)	0.59	25 (11%)	6	6	34, 53, 90, 100	0
All	All	642/663 (96%)	0.81	101 (15%)	3	2	20, 53, 96, 100	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	ILE	12.5
1	A	220	PHE	11.0
1	C	115	ASP	10.0
1	C	110	VAL	9.1
1	C	114	PRO	8.3
1	C	112	CYS	7.7
1	C	111	ILE	6.9
1	C	109	LEU	6.4
1	D	216	ALA	6.3
1	A	217	ARG	6.2
1	C	207	PRO	6.0
1	A	212	GLN	5.7
1	D	215	GLU	5.6
1	A	213	ILE	5.5
1	C	206	LEU	5.4
1	C	208	MET	5.4
1	C	2	SER	5.3
1	D	150	GLY	5.2
1	A	211	LYS	5.1
1	A	2	SER	5.1
1	C	113	PRO	4.9
1	C	11	ASN	4.8
1	C	34	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	2	SER	4.6
1	A	215	GLU	4.5
1	A	208	MET	4.5
1	A	210	ALA	4.5
1	C	119	ALA	4.4
1	D	3	GLY	4.4
1	C	173	SER	4.3
1	C	120	LYS	4.2
1	C	176	THR	4.2
1	C	200	PRO	4.1
1	D	166	TYR	3.9
1	C	39	GLU	3.9
1	D	110	VAL	3.8
1	D	211	LYS	3.8
1	D	208	MET	3.7
1	C	117	LYS	3.7
1	C	62	GLY	3.7
1	A	209	ASP	3.6
1	C	204	ARG	3.5
1	C	43	LYS	3.5
1	D	214	GLU	3.4
1	A	214	GLU	3.4
1	D	46	LYS	3.3
1	C	35	ILE	3.3
1	D	210	ALA	3.3
1	C	118	GLU	3.2
1	A	206	LEU	3.1
1	C	16	MET	3.1
1	D	212	GLN	3.1
1	D	113	PRO	3.1
1	C	14	GLY	3.1
1	A	113	PRO	3.1
1	D	213	ILE	3.0
1	C	38	PRO	3.0
1	C	199	GLN	3.0
1	D	115	ASP	2.8
1	D	47	ASP	2.8
1	C	202	SER	2.8
1	C	184	PHE	2.7
1	C	116	GLN	2.7
1	C	49	ASN	2.7
1	D	151	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	31	ASP	2.6
1	C	196	LYS	2.6
1	A	37	SER	2.6
1	A	216	ALA	2.5
1	A	115	ASP	2.5
1	C	180	LEU	2.5
1	C	142	SER	2.4
1	D	111	ILE	2.4
1	C	36	GLN	2.4
1	C	27	GLY	2.3
1	D	65	LEU	2.3
1	C	172	ALA	2.3
1	C	177	SER	2.3
1	D	207	PRO	2.3
1	C	194	VAL	2.2
1	C	166	TYR	2.2
1	A	218	LYS	2.2
1	D	217	ARG	2.2
1	C	128	THR	2.2
1	A	39	GLU	2.2
1	C	106	ILE	2.1
1	C	7	LEU	2.1
1	C	170	PHE	2.1
1	C	44	LEU	2.1
1	C	57	MET	2.1
1	A	200	PRO	2.1
1	D	142	SER	2.1
1	D	34	PHE	2.0
1	A	114	PRO	2.0
1	C	37	SER	2.0
1	D	200	PRO	2.0
1	C	201	GLY	2.0
1	C	46	LYS	2.0
1	A	34	PHE	2.0
1	C	23	LEU	2.0
1	C	190	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
3	GTS	C	240	23/23	0.61	0.24	1.46	63,87,95,98	0
3	GTS	D	250	23/23	0.80	0.18	1.00	52,62,74,76	0
3	GTS	A	230	23/23	0.83	0.16	-0.08	26,54,78,82	0
2	SO4	D	262	5/5	0.80	0.28	-	97,98,100,100	0
2	SO4	A	260	5/5	0.89	0.16	-	64,66,69,72	0
2	SO4	C	261	5/5	0.94	0.18	-	86,86,87,88	0

6.5 Other polymers (i)

There are no such residues in this entry.