



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:52 AM UTC

PDB ID : 2ODF / pdb_00002odf
Title : The crystal structure of gene product Atu2144 from *Agrobacterium tumefaciens*
Authors : Zhang, R.; Xu, X.; Zheng, H.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-12-22
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

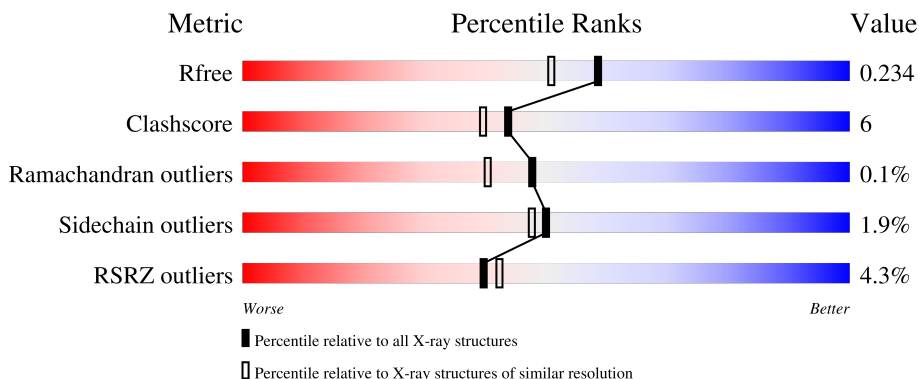
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



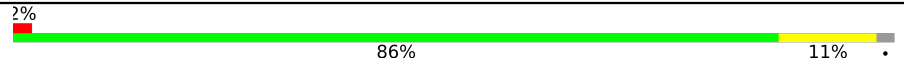


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	257	 86% 10% ..
1	B	257	 4% 87% 11% ..
1	C	257	 % 82% 12% ..
1	D	257	 % 87% 10% ..
1	E	257	 2% 90% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	257	 <p>2% 86% 11% •</p>
1	G	257	 <p>11% 78% 18% ••</p>
1	H	257	 <p>12% 84% 12% ••</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17054 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 Hypothetical protein Atu2144.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1937	1219	343	369	6	0	0	0
1	B	252	1928	1215	338	369	6	0	0	0
1	C	249	1908	1203	337	362	6	0	0	0
1	D	250	1917	1208	338	365	6	0	0	0
1	E	251	1928	1214	342	366	6	0	0	0
1	F	251	1928	1214	342	366	6	0	0	0
1	G	250	1917	1208	338	365	6	0	0	0
1	H	251	1928	1214	342	366	6	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	326	Total O 326 326	0	0
3	B	174	Total O 174 174	0	0

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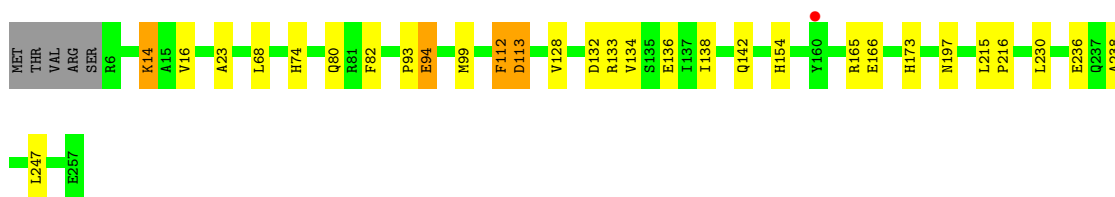
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	216	Total 216	O 216	0	0
3	D	275	Total 275	O 275	0	0
3	E	166	Total 166	O 166	0	0
3	F	171	Total 171	O 171	0	0
3	G	126	Total 126	O 126	0	0
3	H	159	Total 159	O 159	0	0

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.

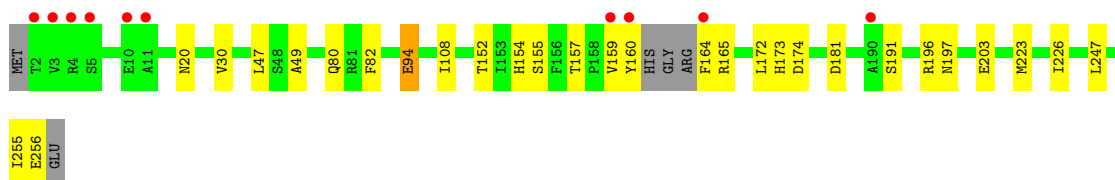
- Molecule 1: Hypothetical protein Atu2144

Chain A: 




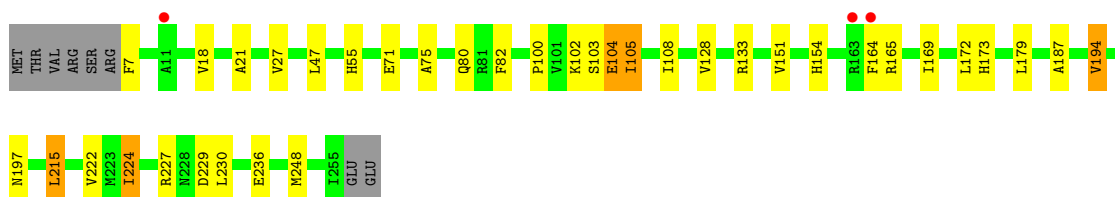
- Molecule 1: Hypothetical protein Atu2144

Chain B: 




- Molecule 1: Hypothetical protein Atu2144

Chain C: 

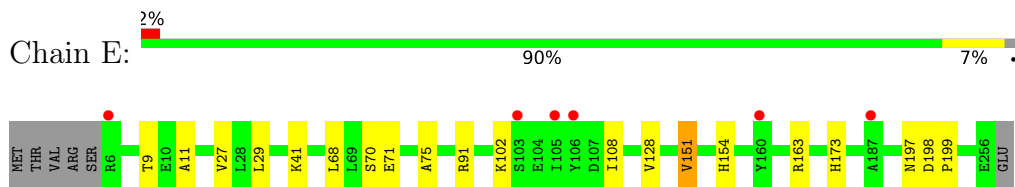


- Molecule 1: Hypothetical protein Atu2144

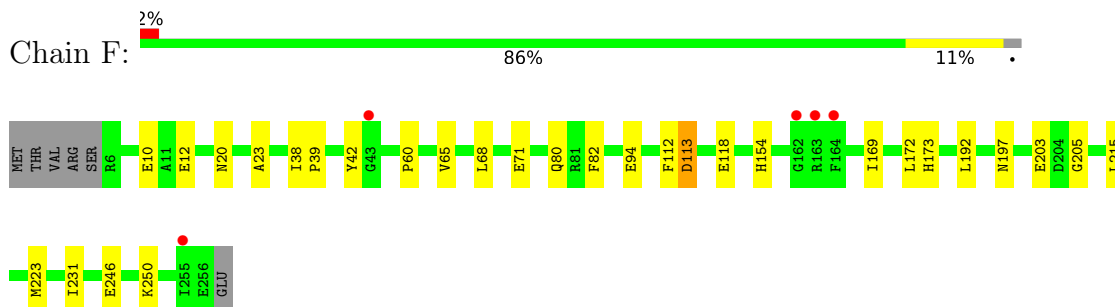
Chain D: 



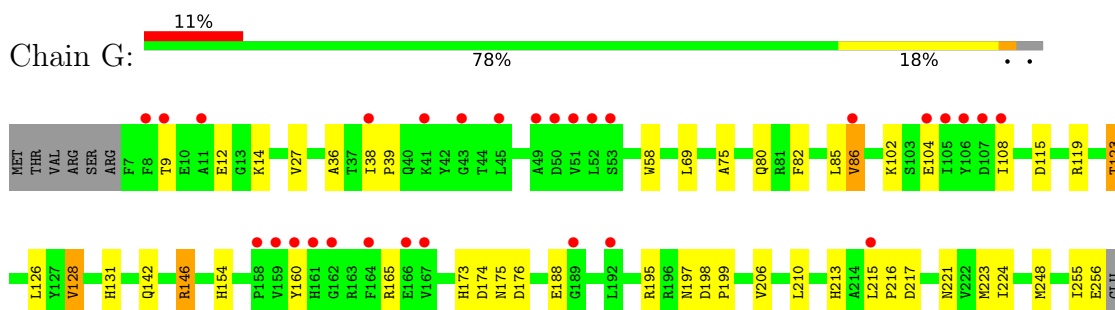
- Molecule 1: Hypothetical protein Atu2144



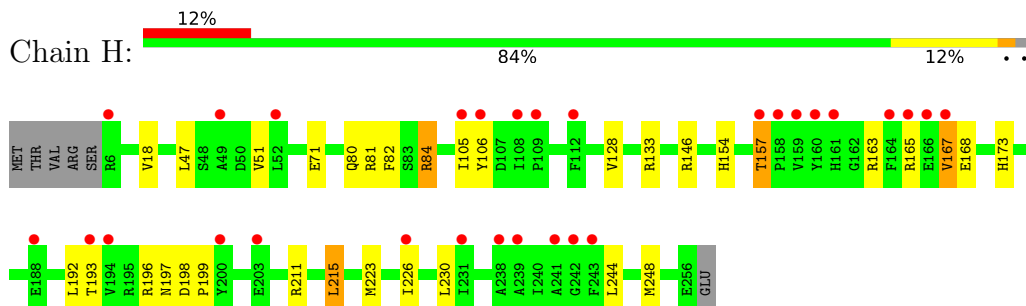
- Molecule 1: Hypothetical protein Atu2144



- Molecule 1: Hypothetical protein Atu2144



- Molecule 1: Hypothetical protein Atu2144



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.52Å 89.77Å 120.36Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	120.00 – 1.90 120.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (120.00-1.90) 99.0 (120.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.234 (Not available) , 0.234	Depositor DCC
R_{free} test set	9148 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtrriage
Anisotropy	0.500	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17054	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.96	6/1977 (0.3%)	0.87	0/2684
1	B	0.75	1/1966 (0.1%)	0.86	0/2670
1	C	0.83	3/1948 (0.2%)	0.88	1/2646 (0.0%)
1	D	0.80	1/1957 (0.1%)	0.88	0/2658
1	E	0.69	0/1968	0.84	0/2672
1	F	0.73	0/1968	0.83	0/2672
1	G	0.68	1/1957 (0.1%)	0.81	0/2658
1	H	0.71	1/1968 (0.1%)	0.83	0/2672
All	All	0.77	13/15709 (0.1%)	0.85	1/21332 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ARG	C-O	-6.59	1.16	1.24
1	A	132	ASP	C-O	-5.99	1.17	1.24
1	C	21	ALA	C-O	-5.80	1.17	1.24
1	D	20	ASN	C-O	-5.79	1.16	1.23
1	A	134	VAL	C-O	-5.62	1.17	1.24
1	A	112	PHE	C-O	-5.54	1.17	1.24
1	A	99	MET	C-O	-5.53	1.17	1.24
1	C	102	LYS	C-O	-5.32	1.17	1.23
1	C	100	PRO	C-O	-5.24	1.18	1.23
1	H	167	VAL	C-O	-5.23	1.18	1.24
1	G	128	VAL	CA-CB	5.15	1.57	1.54
1	B	20	ASN	C-O	-5.05	1.17	1.23
1	A	113	ASP	C-O	-5.02	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105	ILE	CB-CA-C	-5.15	102.84	111.29

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	1937	0	1902	18	0
1	B	1928	0	1895	21	0
1	C	1908	0	1877	38	0
1	D	1917	0	1883	21	0
1	E	1928	0	1896	14	0
1	F	1928	0	1896	21	0
1	G	1917	0	1883	33	0
1	H	1928	0	1896	25	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	1	0
3	A	326	0	0	6	0
3	B	174	0	0	5	0
3	C	216	0	0	6	0
3	D	275	0	0	7	0
3	E	166	0	0	5	0
3	F	171	0	0	6	0
3	G	126	0	0	6	0
3	H	159	0	0	3	0
All	All	17054	0	15128	186	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 (186) 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:C:179:LEU:HD21	1:C:248:MET:HE2	1.32	1.12
1:A:136:GLU:OE1	3:A:539:HOH:O	1.75	1.02
1:F:205:GLY:O	3:F:479:HOH:O	1.76	1.01
1:G:224:ILE:HD11	1:G:248:MET:CE	1.96	0.96
1:C:227:ARG:HD2	1:C:229:ASP:OD1	1.69	0.92
1:B:154:HIS:HD2	3:B:303:HOH:O	1.51	0.91
1:C:215:LEU:HD13	3:C:512:HOH:O	1.75	0.85
1:F:94:GLU:OE1	3:F:478:HOH:O	1.98	0.82
1:G:224:ILE:HD11	1:G:248:MET:HE1	1.60	0.82
1:E:29:LEU:HD23	1:E:151:VAL:HG22	1.62	0.81
1:C:179:LEU:HD21	1:C:248:MET:CE	2.10	0.80
1:G:119:ARG:O	1:G:123:THR:HG23	1.82	0.80
1:E:102:LYS:HA	1:E:108:ILE:HD12	1.65	0.79
1:E:91:ARG:NE	3:E:423:HOH:O	2.17	0.77
1:G:154:HIS:HD2	3:G:335:HOH:O	1.68	0.76
1:D:146:ARG:HD2	3:D:360:HOH:O	1.85	0.75
1:E:68:LEU:O	1:E:71:GLU:HG3	1.87	0.75
1:B:172:LEU:HD22	1:B:197:ASN:HA	1.68	0.74
1:D:154:HIS:HD2	3:D:309:HOH:O	1.71	0.73
1:H:168:GLU:HG3	1:H:193:THR:HB	1.72	0.72
1:C:173:HIS:H	1:C:197:ASN:HD21	1.38	0.71
1:C:222:VAL:CG1	1:C:248:MET:HE1	2.20	0.70
1:B:173:HIS:H	1:B:197:ASN:HD21	1.38	0.70
1:E:9:THR:HG21	3:E:384:HOH:O	1.90	0.70
1:C:80:GLN:HE21	1:C:82:PHE:H	1.39	0.70
1:C:222:VAL:HG12	1:C:248:MET:HE1	1.72	0.70
1:H:154:HIS:HD2	3:H:367:HOH:O	1.74	0.70
1:B:47:LEU:HD21	1:B:108:ILE:HD13	1.73	0.69
1:F:223:MET:SD	3:F:443:HOH:O	2.51	0.68
1:G:80:GLN:HE21	1:G:82:PHE:H	1.40	0.67
1:A:173:HIS:H	1:A:197:ASN:HD21	1.41	0.67
1:A:80:GLN:HE21	1:A:82:PHE:H	1.41	0.67
1:H:71:GLU:HG2	3:H:438:HOH:O	1.96	0.66
1:D:80:GLN:HE21	1:D:82:PHE:H	1.40	0.66
1:G:131:HIS:ND1	1:G:213:HIS:HE1	1.93	0.66
1:H:154:HIS:CE1	1:H:223:MET:HE3	2.31	0.66
1:C:222:VAL:CG1	1:C:248:MET:CE	2.74	0.65
1:G:146:ARG:HD2	3:G:317:HOH:O	1.97	0.65
1:C:222:VAL:HG11	1:C:248:MET:HE3	1.78	0.64
1:F:215:LEU:HD22	3:F:472:HOH:O	1.98	0.64
1:E:128:VAL:HG21	1:G:128:VAL:HG21	1.79	0.63
1:F:80:GLN:HE21	1:F:82:PHE:H	1.44	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LYS:HE3	3:D:524:HOH:O	2.00	0.62
1:E:173:HIS:H	1:E:197:ASN:HD21	1.47	0.62
1:C:227:ARG:CD	1:C:229:ASP:OD1	2.44	0.61
1:A:154:HIS:HD2	3:A:309:HOH:O	1.81	0.61
1:C:222:VAL:HG11	1:C:248:MET:CE	2.31	0.60
1:H:168:GLU:HB3	1:H:230:LEU:HD11	1.82	0.60
1:F:112:PHE:O	1:F:113:ASP:C	2.44	0.60
1:C:222:VAL:HG13	1:C:224:ILE:CD1	2.32	0.59
1:D:41:LYS:NZ	3:D:487:HOH:O	2.35	0.59
1:G:173:HIS:H	1:G:197:ASN:HD21	1.48	0.59
3:E:300:HOH:O	1:G:123:THR:HG21	2.03	0.59
1:B:80:GLN:HE21	1:B:82:PHE:H	1.49	0.59
1:F:68:LEU:O	1:F:71:GLU:HG3	2.04	0.58
1:H:173:HIS:H	1:H:197:ASN:HD21	1.51	0.58
1:A:166:GLU:HG2	3:A:590:HOH:O	2.04	0.57
1:C:47:LEU:HD21	1:C:108:ILE:HD13	1.85	0.57
1:F:173:HIS:H	1:F:197:ASN:HD21	1.54	0.56
1:A:14:LYS:HD2	3:A:347:HOH:O	2.06	0.56
1:F:60:PRO:HD2	3:F:313:HOH:O	2.06	0.55
1:B:173:HIS:HE1	1:B:196:ARG:HE	1.53	0.55
1:B:181:ASP:OD1	1:B:196:ARG:NH2	2.36	0.55
1:E:154:HIS:HD2	3:E:264:HOH:O	1.90	0.55
1:H:226:ILE:HD11	1:H:244:LEU:HD11	1.89	0.55
1:G:213:HIS:HD2	3:G:311:HOH:O	1.90	0.55
1:H:84:ARG:HD3	3:H:339:HOH:O	2.07	0.54
1:H:157:THR:HG22	1:H:165:ARG:HH21	1.73	0.54
1:B:173:HIS:HD2	1:B:174:ASP:O	1.90	0.54
1:G:142:GLN:HE22	1:G:217:ASP:CG	2.15	0.54
1:H:184:LEU:CD1	1:H:196:ARG:HB2	2.38	0.53
1:B:247:LEU:HD12	3:B:325:HOH:O	2.07	0.53
1:C:7:PHE:N	3:C:410:HOH:O	2.41	0.53
1:F:154:HIS:HD2	3:F:328:HOH:O	1.91	0.53
1:E:9:THR:HG23	3:E:286:HOH:O	2.08	0.53
1:C:154:HIS:HE1	3:C:306:HOH:O	1.92	0.53
1:F:203:GLU:CD	1:F:203:GLU:H	2.17	0.53
1:A:14:LYS:HG3	1:A:16:VAL:H	1.74	0.53
1:A:23:ALA:HB1	1:A:74:HIS:O	2.08	0.53
1:C:222:VAL:HG13	1:C:224:ILE:HD11	1.90	0.53
1:D:41:LYS:CE	3:D:524:HOH:O	2.54	0.53
1:C:187:ALA:HB1	1:C:194:VAL:HG13	1.91	0.53
1:C:165:ARG:HD3	3:C:423:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:LEU:HD13	1:G:221:ASN:HD22	1.75	0.51
1:H:157:THR:HG22	1:H:165:ARG:NH2	2.25	0.51
1:D:7:PHE:N	3:D:547:HOH:O	2.44	0.51
1:H:47:LEU:HD22	1:H:51:VAL:HG11	1.93	0.51
1:H:181:ASP:OD1	1:H:196:ARG:NH2	2.43	0.51
1:D:99:MET:HE1	1:D:119:ARG:CB	2.41	0.51
1:B:160:TYR:C	3:B:352:HOH:O	2.54	0.51
1:G:224:ILE:HD11	1:G:248:MET:HE3	1.85	0.51
1:H:81:ARG:NH1	2:H:310:SO4:O2	2.44	0.50
1:G:224:ILE:CD1	1:G:248:MET:HE1	2.38	0.50
1:B:94:GLU:OE2	3:B:322:HOH:O	2.19	0.50
1:H:184:LEU:HD13	1:H:196:ARG:HB2	1.93	0.50
1:G:255:ILE:O	1:G:256:GLU:C	2.54	0.50
1:H:18:VAL:HG21	1:H:133:ARG:CZ	2.41	0.50
1:C:103:SER:O	1:C:103:SER:OG	2.30	0.49
1:D:198:ASP:OD1	1:D:199:PRO:HA	2.12	0.49
1:A:165:ARG:HD3	3:A:504:HOH:O	2.11	0.49
1:D:99:MET:SD	1:D:122:ARG:HD2	2.52	0.49
1:C:222:VAL:HG12	1:C:248:MET:CE	2.38	0.49
1:F:65:VAL:HG21	1:F:231:ILE:HG21	1.95	0.49
1:D:12:GLU:OE2	1:D:40:GLN:N	2.44	0.49
1:B:203:GLU:CD	1:B:203:GLU:H	2.21	0.48
1:E:27:VAL:HG13	1:E:151:VAL:HG13	1.94	0.48
1:G:86:VAL:HG22	1:G:126:LEU:CD1	2.44	0.48
1:C:104:GLU:OE2	2:C:303:SO4:O3	2.30	0.48
1:C:128:VAL:HG21	1:H:128:VAL:HG21	1.95	0.48
1:B:49:ALA:HB3	1:C:164:PHE:HB3	1.96	0.48
1:D:103:SER:HB2	1:D:108:ILE:HD11	1.96	0.48
1:B:159:VAL:O	1:B:160:TYR:HB2	2.14	0.48
1:D:99:MET:HE3	1:D:119:ARG:CZ	2.43	0.47
1:G:38:ILE:HG22	1:G:39:PRO:O	2.13	0.47
1:G:176:ASP:N	3:G:398:HOH:O	2.46	0.47
1:A:93:PRO:HD2	1:A:94:GLU:OE1	2.14	0.47
1:F:246:GLU:HG3	1:F:250:LYS:NZ	2.29	0.47
1:B:255:ILE:O	1:B:256:GLU:CB	2.63	0.47
1:C:105:ILE:HG22	1:C:105:ILE:O	2.13	0.47
1:H:80:GLN:HE21	1:H:82:PHE:H	1.62	0.47
1:A:247:LEU:HD13	3:A:496:HOH:O	2.15	0.47
1:E:9:THR:HG22	1:E:11:ALA:N	2.28	0.47
1:G:27:VAL:O	1:G:75:ALA:HB1	2.15	0.47
1:E:68:LEU:O	1:E:71:GLU:CG	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD13	1:A:238:ALA:HA	1.97	0.46
1:C:103:SER:O	1:C:105:ILE:N	2.49	0.46
1:C:230:LEU:O	1:C:236:GLU:HB3	2.16	0.46
1:D:99:MET:HE1	1:D:119:ARG:HG2	1.97	0.46
1:G:195:ARG:NE	3:G:403:HOH:O	2.48	0.45
1:D:156:PHE:CE2	1:D:227:ARG:HG3	2.50	0.45
1:C:222:VAL:CG1	1:C:224:ILE:HD11	2.47	0.45
1:A:230:LEU:O	1:A:236:GLU:HB3	2.17	0.45
1:H:81:ARG:HG2	1:H:81:ARG:HH11	1.81	0.45
1:A:14:LYS:HE2	1:A:16:VAL:H	1.82	0.44
1:A:138:ILE:O	1:A:142:GLN:HG3	2.17	0.44
1:B:164:PHE:O	1:B:165:ARG:CB	2.65	0.44
1:C:169:ILE:O	1:C:194:VAL:HA	2.17	0.44
1:H:168:GLU:OE1	1:H:192:LEU:HA	2.17	0.44
1:F:20:ASN:HB3	1:F:23:ALA:HB2	1.99	0.44
1:G:80:GLN:HE21	1:G:82:PHE:N	2.13	0.44
1:A:128:VAL:HG21	1:D:128:VAL:HG21	1.99	0.44
1:F:42:TYR:OH	1:F:118:GLU:OE2	2.34	0.44
1:F:172:LEU:HG	1:F:197:ASN:HD22	1.82	0.44
1:H:211:ARG:HA	1:H:215:LEU:HD22	2.00	0.44
1:B:154:HIS:CD2	3:B:303:HOH:O	2.42	0.44
1:G:160:TYR:HB2	1:G:165:ARG:CZ	2.48	0.44
1:G:215:LEU:HD21	3:G:433:HOH:O	2.18	0.44
1:G:215:LEU:N	1:G:216:PRO:CD	2.81	0.43
1:F:80:GLN:HE21	1:F:82:PHE:N	2.14	0.43
1:E:198:ASP:OD1	1:E:199:PRO:HA	2.18	0.43
1:G:210:LEU:HD13	1:G:221:ASN:ND2	2.34	0.43
1:H:105:ILE:HD11	1:H:106:TYR:CZ	2.53	0.43
1:A:112:PHE:O	1:A:113:ASP:C	2.61	0.43
1:F:169:ILE:HD11	1:F:192:LEU:HD13	2.01	0.43
1:C:18:VAL:HG21	1:C:133:ARG:CZ	2.49	0.43
1:D:206:VAL:HB	1:D:223:MET:HE1	2.01	0.42
1:C:151:VAL:HG22	1:C:248:MET:HE1	2.01	0.42
1:G:9:THR:N	1:G:12:GLU:OE1	2.43	0.42
1:G:36:ALA:HB2	1:G:58:TRP:CG	2.54	0.42
1:G:198:ASP:OD1	1:G:199:PRO:HA	2.19	0.42
1:C:7:PHE:N	3:C:493:HOH:O	2.51	0.42
1:G:119:ARG:O	1:G:123:THR:CG2	2.62	0.42
1:B:172:LEU:HB2	1:B:223:MET:HB3	2.01	0.42
1:G:85:LEU:HD22	1:G:108:ILE:CD1	2.50	0.42
1:D:55:HIS:HD2	3:D:396:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:O	1:C:75:ALA:HB1	2.20	0.41
1:C:55:HIS:HE1	1:C:104:GLU:OE1	2.02	0.41
1:B:30:VAL:HB	1:B:152:THR:HG22	2.02	0.41
1:B:49:ALA:HB3	1:C:164:PHE:CB	2.50	0.41
1:C:215:LEU:CD1	3:C:512:HOH:O	2.49	0.41
1:C:224:ILE:CD1	1:C:224:ILE:N	2.84	0.41
1:G:115:ASP:OD1	1:G:115:ASP:C	2.63	0.41
1:H:183:MET:SD	1:H:248:MET:HE2	2.60	0.41
1:D:27:VAL:O	1:D:75:ALA:HB1	2.20	0.41
1:H:183:MET:HE1	1:H:248:MET:HE3	2.03	0.41
1:F:12:GLU:OE2	1:F:39:PRO:HA	2.21	0.41
1:C:172:LEU:HA	1:C:197:ASN:ND2	2.36	0.41
1:D:23:ALA:HB1	1:D:74:HIS:O	2.21	0.41
1:G:206:VAL:HB	1:G:223:MET:HE1	2.02	0.41
1:H:198:ASP:OD1	1:H:199:PRO:HA	2.21	0.41
1:B:155:SER:HA	1:B:226:ILE:O	2.20	0.40
1:A:215:LEU:N	1:A:216:PRO:CD	2.84	0.40
1:F:246:GLU:HG3	1:F:250:LYS:HZ3	1.86	0.40
1:E:70:SER:OG	1:E:75:ALA:O	2.28	0.40
1:F:38:ILE:HG22	1:F:42:TYR:HB2	2.02	0.40
1:D:99:MET:HE1	1:D:119:ARG:CG	2.51	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	250/257 (97%)	245 (98%)	5 (2%)	0	100	100
1	B	248/257 (96%)	244 (98%)	4 (2%)	0	100	100
1	C	247/257 (96%)	239 (97%)	7 (3%)	1 (0%)	30	22
1	D	248/257 (96%)	243 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	249/257 (97%)	243 (98%)	6 (2%)	0	100	100
1	F	249/257 (97%)	238 (96%)	10 (4%)	1 (0%)	30	22
1	G	248/257 (96%)	241 (97%)	7 (3%)	0	100	100
1	H	249/257 (97%)	244 (98%)	5 (2%)	0	100	100
All	All	1988/2056 (97%)	1937 (97%)	49 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	104	GLU
1	F	113	ASP

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	202/207 (98%)	200 (99%)	2 (1%)	68	70
1	B	202/207 (98%)	199 (98%)	3 (2%)	57	56
1	C	199/207 (96%)	195 (98%)	4 (2%)	48	46
1	D	200/207 (97%)	199 (100%)	1 (0%)	81	84
1	E	201/207 (97%)	198 (98%)	3 (2%)	57	56
1	F	201/207 (97%)	200 (100%)	1 (0%)	81	84
1	G	200/207 (97%)	190 (95%)	10 (5%)	22	14
1	H	201/207 (97%)	195 (97%)	6 (3%)	36	30
All	All	1606/1656 (97%)	1576 (98%)	30 (2%)	50	47

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

Mol	Chain	Res	Type
1	A	14	LYS
1	A	94	GLU

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Mol	Chain	Res	Type
1	B	94	GLU
1	B	157	THR
1	B	191	SER
1	C	71	GLU
1	C	194	VAL
1	C	215	LEU
1	C	224	ILE
1	D	146	ARG
1	E	41	LYS
1	E	151	VAL
1	E	163	ARG
1	F	10	GLU
1	G	14	LYS
1	G	69	LEU
1	G	86	VAL
1	G	102	LYS
1	G	104	GLU
1	G	123	THR
1	G	146	ARG
1	G	174	ASP
1	G	175	ASN
1	G	188	GLU
1	H	84	ARG
1	H	146	ARG
1	H	157	THR
1	H	163	ARG
1	H	167	VAL
1	H	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	142	GLN
1	A	154	HIS
1	A	161	HIS
1	A	197	ASN
1	B	80	GLN
1	B	154	HIS
1	B	173	HIS
1	B	197	ASN
1	C	55	HIS

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Mol	Chain	Res	Type
1	C	80	GLN
1	C	154	HIS
1	C	175	ASN
1	C	197	ASN
1	D	80	GLN
1	D	154	HIS
1	E	20	ASN
1	E	154	HIS
1	E	161	HIS
1	E	197	ASN
1	E	245	HIS
1	F	20	ASN
1	F	74	HIS
1	F	80	GLN
1	F	154	HIS
1	F	161	HIS
1	F	175	ASN
1	F	197	ASN
1	G	80	GLN
1	G	154	HIS
1	G	197	ASN
1	G	213	HIS
1	G	221	ASN
1	H	20	ASN
1	H	80	GLN
1	H	154	HIS
1	H	197	ASN
1	H	221	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

10 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	B	302	-	4,4,4	0.18	0	6,6,6	0.34	0
2	SO4	H	310	-	4,4,4	0.31	0	6,6,6	0.44	0
2	SO4	A	301	-	4,4,4	1.69	1 (25%)	6,6,6	0.89	0
2	SO4	C	304	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	D	306	-	4,4,4	0.22	0	6,6,6	0.53	0
2	SO4	C	303	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	F	307	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	F	308	-	4,4,4	0.25	0	6,6,6	0.70	0
2	SO4	G	309	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	D	305	-	4,4,4	0.26	0	6,6,6	0.33	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SO4	O2-S	-2.10	1.32	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	310	SO4	1	0
2	C	303	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, 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	252/257 (98%)	-0.27	1 (0%) 88 90	15, 20, 32, 44	0
1	B	252/257 (98%)	0.18	10 (3%) 42 45	18, 28, 43, 57	0
1	C	249/257 (96%)	0.10	3 (1%) 76 79	18, 27, 36, 46	0
1	D	250/257 (97%)	-0.09	2 (0%) 82 85	15, 24, 33, 48	0
1	E	251/257 (97%)	0.38	6 (2%) 59 63	20, 31, 44, 50	0
1	F	251/257 (97%)	0.28	5 (1%) 65 69	18, 29, 40, 51	0
1	G	250/257 (97%)	0.78	29 (11%) 9 10	21, 33, 53, 63	0
1	H	251/257 (97%)	0.67	30 (11%) 9 9	17, 33, 56, 68	0
All	All	2006/2056 (97%)	0.25	86 (4%) 40 42	15, 28, 47, 68	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	105	ILE	6.4
1	G	106	TYR	4.4
1	B	2	THR	4.3
1	B	3	VAL	4.2
1	G	50	ASP	4.0
1	H	194	VAL	4.0
1	C	163	ARG	3.9
1	B	5	SER	3.7
1	G	41	LYS	3.6
1	B	159	VAL	3.6
1	G	164	PHE	3.5
1	B	160	TYR	3.4
1	H	159	VAL	3.4
1	E	160	TYR	3.3
1	H	160	TYR	3.3
1	H	164	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	51	VAL	3.3
1	E	6	ARG	3.3
1	B	164	PHE	3.2
1	H	167	VAL	3.2
1	H	157	THR	3.2
1	H	112	PHE	3.2
1	G	52	LEU	3.1
1	G	160	TYR	3.0
1	C	164	PHE	2.9
1	F	164	PHE	2.9
1	E	105	ILE	2.9
1	G	45	LEU	2.9
1	G	108	ILE	2.9
1	H	239	ALA	2.8
1	G	215	LEU	2.8
1	G	11	ALA	2.7
1	H	203	GLU	2.7
1	H	108	ILE	2.7
1	G	167	VAL	2.7
1	F	43	GLY	2.6
1	G	49	ALA	2.6
1	G	192	LEU	2.6
1	H	105	ILE	2.6
1	G	189	GLY	2.6
1	G	166	GLU	2.6
1	G	159	VAL	2.6
1	A	160	TYR	2.5
1	H	242	GLY	2.5
1	E	103	SER	2.5
1	D	256	GLU	2.5
1	H	188	GLU	2.5
1	H	200	TYR	2.5
1	H	185	ALA	2.5
1	G	158	PRO	2.5
1	G	38	ILE	2.4
1	G	9	THR	2.4
1	H	158	PRO	2.4
1	B	4	ARG	2.4
1	H	161	HIS	2.4
1	H	49	ALA	2.4
1	H	166	GLU	2.4
1	E	106	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	238	ALA	2.4
1	H	241	ALA	2.4
1	B	10	GLU	2.4
1	G	162	GLY	2.4
1	H	231	ILE	2.3
1	H	6	ARG	2.3
1	G	107	ASP	2.3
1	G	43	GLY	2.2
1	C	11	ALA	2.2
1	G	53	SER	2.2
1	H	109	PRO	2.2
1	G	8	PHE	2.2
1	G	161	HIS	2.2
1	H	226	ILE	2.1
1	D	255	ILE	2.1
1	H	165	ARG	2.1
1	B	11	ALA	2.1
1	B	190	ALA	2.1
1	E	187	ALA	2.1
1	F	255	ILE	2.1
1	H	106	TYR	2.1
1	G	104	GLU	2.1
1	F	162	GLY	2.1
1	H	193	THR	2.0
1	G	86	VAL	2.0
1	H	52	LEU	2.0
1	F	163	ARG	2.0
1	H	243	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	G	309	5/5	0.90	0.10	61,61,61,62	0
2	SO4	F	308	5/5	0.94	0.16	39,41,45,45	0
2	SO4	F	307	5/5	0.94	0.08	52,54,54,55	0
2	SO4	C	304	5/5	0.95	0.14	45,46,46,48	0
2	SO4	B	302	5/5	0.96	0.09	42,44,46,47	0
2	SO4	H	310	5/5	0.96	0.07	45,46,46,48	0
2	SO4	A	301	5/5	0.97	0.17	20,20,20,20	0
2	SO4	D	305	5/5	0.97	0.06	37,41,42,42	0
2	SO4	C	303	5/5	0.97	0.10	33,34,37,37	0
2	SO4	D	306	5/5	0.98	0.06	23,27,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.