



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:21 PM UTC

PDB ID : 1GK3 / pdb_00001gk3
Title : Histidine Ammonia-Lyase (HAL) Mutant D145A from *Pseudomonas putida*
Authors : Baedeker, M.; Schulz, G.E.
Deposited on : 2001-08-07
Resolution : 2.25 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

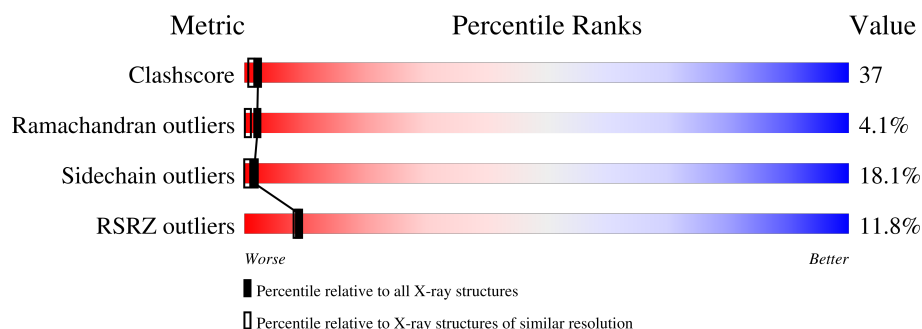
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	509	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1511	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3956 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.

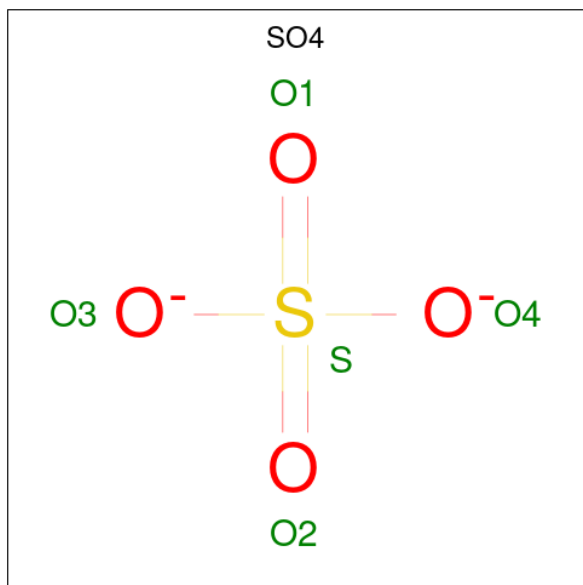
- Molecule 1 is a protein called HISTIDINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	3761	2359	670	716	16	128	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	ASP	engineered mutation	UNP P21310
A	273	ALA	CYS	engineered mutation	UNP P21310

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

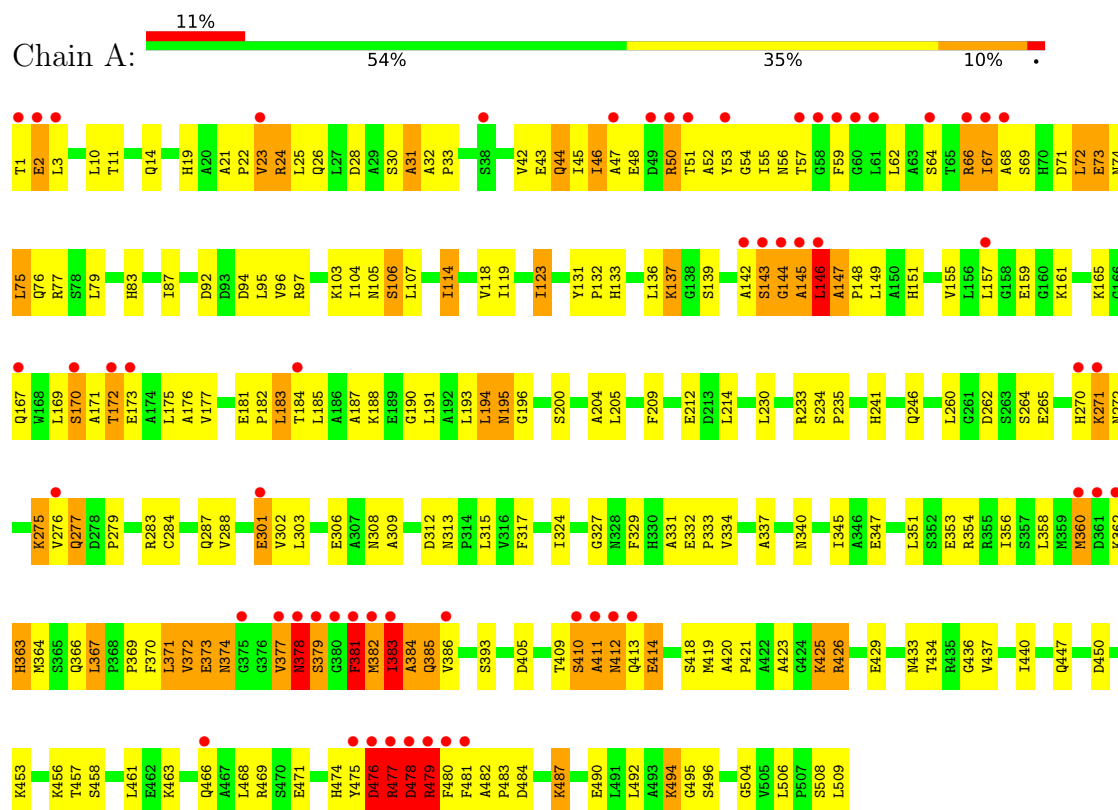
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		

3 Residue-property plots

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: HISTIDINE AMMONIA-LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.81Å 117.11Å 130.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.25 21.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.0 (21.00-2.25) 89.9 (21.00-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.26Å)	Xtriage
Refinement program	SHELX	Depositor
R, R_{free}	0.221 , 0.280 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3956	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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, GOL

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	0.59	5/3819 (0.1%)	1.31	22/5180 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	ALA	N-CA	20.57	1.65	1.46
1	A	386	VAL	N-CA	13.14	1.61	1.46
1	A	384	ALA	N-CA	10.49	1.59	1.46
1	A	144	GLY	C-N	7.21	1.43	1.33
1	A	378	ASN	N-CA	-5.13	1.43	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ALA	N-CA-C	-19.68	87.44	112.23
1	A	146	LEU	CA-C-N	-13.36	102.36	120.26
1	A	146	LEU	C-N-CA	-13.36	102.36	120.26
1	A	386	VAL	N-CA-C	12.75	125.16	110.62
1	A	385	GLN	OE1-CD-NE2	-9.36	113.24	122.60
1	A	385	GLN	CA-C-N	-8.04	109.19	120.53
1	A	385	GLN	C-N-CA	-8.04	109.19	120.53
1	A	386	VAL	N-CA-CB	-7.58	100.99	110.47
1	A	381	PHE	CA-CB-CG	7.34	121.14	113.80
1	A	383	ILE	CA-C-N	-6.90	108.96	120.68
1	A	383	ILE	C-N-CA	-6.90	108.96	120.68
1	A	147	ALA	N-CA-CB	-6.49	100.64	110.30
1	A	385	GLN	CG-CD-NE2	6.37	125.96	116.40
1	A	31	ALA	CA-C-N	6.12	128.66	120.58
1	A	31	ALA	C-N-CA	6.12	128.66	120.58
1	A	241	HIS	CA-CB-CG	-5.89	107.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ASP	CA-C-N	5.83	132.67	121.54
1	A	478	ASP	C-N-CA	5.83	132.67	121.54
1	A	24	ARG	CA-C-N	-5.59	113.81	122.59
1	A	24	ARG	C-N-CA	-5.59	113.81	122.59
1	A	504	GLY	CA-C-N	-5.35	116.26	122.63
1	A	504	GLY	C-N-CA	-5.35	116.26	122.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3761	0	3826	269	1
2	A	5	0	0	1	0
3	A	6	0	8	8	0
4	A	184	0	0	23	0
All	All	3956	0	3834	270	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 37.

All (270) 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:383:ILE:HG12	4:A:2138:HOH:O	1.44	1.13
1:A:59:PHE:CZ	3:A:1511:GOL:H11	1.84	1.12
1:A:145:ALA:HB3	1:A:149:LEU:HG	1.20	1.11
1:A:381:PHE:CZ	1:A:447:GLN:HG2	1.84	1.11
1:A:474:HIS:CD2	1:A:476:ASP:HB3	1.87	1.10
1:A:136:LEU:HD12	1:A:136:LEU:O	1.53	1.08
1:A:381:PHE:HZ	1:A:447:GLN:HG2	0.94	1.06
1:A:145:ALA:HB3	1:A:149:LEU:CG	1.85	1.05
1:A:378:ASN:N	1:A:378:ASN:HD22	1.49	1.01
1:A:144:GLY:C	1:A:146:LEU:H	1.68	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:HIS:HD2	1:A:476:ASP:HB3	1.24	0.99
1:A:146:LEU:HD12	4:A:2033:HOH:O	1.63	0.98
1:A:471:GLU:OE1	1:A:487:LYS:HE2	1.61	0.98
1:A:475:TYR:O	1:A:475:TYR:CD1	2.18	0.96
1:A:145:ALA:CB	1:A:149:LEU:HG	1.96	0.96
1:A:44:GLN:O	1:A:48:GLU:HG3	1.64	0.95
1:A:11:THR:OG1	1:A:14:GLN:HG3	1.66	0.95
1:A:377:VAL:HB	1:A:378:ASN:ND2	1.84	0.93
1:A:83:HIS:HD2	1:A:146:LEU:HD13	1.27	0.93
1:A:59:PHE:HZ	3:A:1511:GOL:H11	1.30	0.91
1:A:479:ARG:HB2	4:A:2173:HOH:O	1.70	0.90
1:A:381:PHE:HZ	1:A:447:GLN:CG	1.82	0.90
1:A:235:PRO:HG2	4:A:2109:HOH:O	1.73	0.89
1:A:377:VAL:HB	1:A:378:ASN:HD22	1.38	0.88
1:A:55:ILE:O	3:A:1511:GOL:H32	1.75	0.86
1:A:378:ASN:HB3	1:A:478:ASP:OD1	1.77	0.84
1:A:474:HIS:CD2	1:A:476:ASP:CB	2.61	0.84
1:A:92:ASP:OD1	1:A:94:ASP:HB2	1.76	0.83
1:A:378:ASN:N	1:A:378:ASN:ND2	2.21	0.81
1:A:214:LEU:HD13	1:A:434:THR:CG2	2.15	0.76
1:A:145:ALA:HB3	1:A:149:LEU:CD1	2.16	0.76
1:A:144:GLY:HA3	1:A:195:ASN:HA	1.68	0.75
1:A:301:GLU:HG3	1:A:302:VAL:N	2.01	0.75
1:A:159:GLU:O	1:A:171:ALA:HB2	1.86	0.75
1:A:378:ASN:HD22	1:A:378:ASN:H	1.35	0.75
1:A:145:ALA:HB2	4:A:2082:HOH:O	1.86	0.74
1:A:48:GLU:HB2	1:A:50:ARG:HG3	1.69	0.74
1:A:83:HIS:CD2	1:A:146:LEU:HD13	2.17	0.73
1:A:144:GLY:O	1:A:146:LEU:N	2.21	0.73
1:A:381:PHE:HB3	1:A:481:PHE:HE1	1.52	0.73
1:A:260:LEU:HD23	1:A:461:LEU:HD11	1.71	0.73
1:A:410:SER:O	1:A:410:SER:OG	2.04	0.73
1:A:382:MET:HE2	1:A:383:ILE:CD1	2.19	0.72
1:A:51:THR:HG22	1:A:66:ARG:HD3	1.73	0.70
1:A:476:ASP:HA	4:A:2171:HOH:O	1.91	0.70
1:A:214:LEU:HD13	1:A:434:THR:HG22	1.73	0.70
1:A:475:TYR:HE2	1:A:479:ARG:O	1.75	0.70
1:A:62:LEU:C	1:A:64:SER:H	1.99	0.69
1:A:382:MET:HE2	1:A:383:ILE:HD13	1.73	0.69
1:A:133:HIS:CD2	1:A:161:LYS:HE2	2.28	0.68
1:A:136:LEU:O	1:A:136:LEU:CD1	2.38	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:C	3:A:1511:GOL:H32	2.17	0.68
1:A:68:ALA:O	1:A:71:ASP:HB2	1.93	0.68
1:A:360:MET:HG3	1:A:385:GLN:HB2	1.75	0.67
1:A:260:LEU:HD23	1:A:461:LEU:CD1	2.25	0.67
1:A:144:GLY:HA2	1:A:196:GLY:H	1.59	0.67
1:A:21:ALA:HB1	1:A:22:PRO:HD2	1.76	0.67
1:A:447:GLN:O	1:A:450:ASP:HB2	1.94	0.67
1:A:409:THR:OG1	1:A:414:GLU:HB2	1.95	0.67
1:A:476:ASP:O	1:A:477:ARG:HB3	1.93	0.67
1:A:67:ILE:HG22	1:A:72:LEU:HD13	1.77	0.66
1:A:420:ALA:N	1:A:421:PRO:CD	2.58	0.66
1:A:317:PHE:CD2	1:A:324:ILE:HD12	2.30	0.66
1:A:381:PHE:C	1:A:383:ILE:N	2.50	0.66
1:A:471:GLU:OE1	1:A:487:LYS:CE	2.43	0.66
1:A:159:GLU:O	1:A:171:ALA:CB	2.43	0.66
1:A:51:THR:CG2	1:A:66:ARG:HD3	2.25	0.65
1:A:144:GLY:CA	1:A:195:ASN:HA	2.27	0.65
1:A:11:THR:H	1:A:14:GLN:HE21	1.46	0.64
1:A:53:TYR:HA	1:A:57:THR:OG1	1.97	0.64
1:A:356:ILE:O	1:A:360:MET:HG2	1.99	0.63
1:A:312:ASP:O	1:A:315:LEU:HD21	1.98	0.63
1:A:155:VAL:HA	1:A:171:ALA:HB1	1.81	0.63
1:A:379:SER:O	1:A:379:SER:OG	2.17	0.63
1:A:377:VAL:C	1:A:378:ASN:HD22	2.06	0.62
1:A:234:SER:N	1:A:235:PRO:CD	2.62	0.62
1:A:475:TYR:CE2	1:A:479:ARG:O	2.52	0.61
1:A:475:TYR:O	1:A:475:TYR:CG	2.54	0.60
1:A:410:SER:HB3	1:A:414:GLU:OE2	2.01	0.60
1:A:69:SER:HA	1:A:72:LEU:HD22	1.83	0.60
1:A:482:ALA:N	1:A:483:PRO:CD	2.65	0.59
1:A:169:LEU:HD22	1:A:173:GLU:OE2	2.02	0.59
1:A:181:GLU:O	1:A:183:LEU:HD23	2.02	0.59
1:A:382:MET:O	1:A:385:GLN:HB3	2.02	0.59
1:A:75:LEU:O	1:A:76:GLN:C	2.46	0.59
1:A:277:GLN:HG3	1:A:283:ARG:NH2	2.18	0.58
1:A:62:LEU:C	1:A:64:SER:N	2.61	0.58
1:A:327:GLY:HA2	1:A:329:PHE:CE2	2.39	0.58
1:A:136:LEU:HD12	1:A:136:LEU:C	2.23	0.58
1:A:381:PHE:CD2	1:A:481:PHE:CE1	2.92	0.58
1:A:436:GLY:O	1:A:440:ILE:HD12	2.04	0.58
1:A:481:PHE:CD2	1:A:484:ASP:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ALA:O	1:A:71:ASP:N	2.36	0.57
1:A:114:ILE:HD11	1:A:118:VAL:CG1	2.34	0.57
1:A:458:SER:OG	1:A:461:LEU:HG	2.05	0.57
1:A:469:ARG:NH2	1:A:474:HIS:HA	2.20	0.57
1:A:264:SER:HA	4:A:2105:HOH:O	2.04	0.57
1:A:317:PHE:HD2	1:A:324:ILE:HD12	1.68	0.57
1:A:332:GLU:N	1:A:333:PRO:HD2	2.19	0.57
1:A:476:ASP:O	1:A:477:ARG:CB	2.51	0.57
1:A:87:ILE:HG23	1:A:137:LYS:HB2	1.86	0.57
1:A:87:ILE:CG2	1:A:137:LYS:HB2	2.35	0.56
1:A:474:HIS:CD2	1:A:476:ASP:H	2.24	0.56
1:A:260:LEU:CD2	1:A:461:LEU:HD11	2.35	0.56
1:A:479:ARG:HG2	1:A:480:PHE:N	2.19	0.56
1:A:490:GLU:HG2	1:A:494:LYS:CD	2.36	0.56
1:A:75:LEU:CD1	1:A:75:LEU:C	2.78	0.56
1:A:143:SER:O	1:A:146:LEU:CD2	2.53	0.56
1:A:360:MET:HG3	1:A:385:GLN:CD	2.30	0.56
1:A:43:GLU:OE1	4:A:2029:HOH:O	2.17	0.56
1:A:474:HIS:NE2	1:A:476:ASP:CB	2.69	0.56
1:A:73:GLU:HG2	4:A:2038:HOH:O	2.05	0.56
1:A:209:PHE:HB3	4:A:2084:HOH:O	2.06	0.55
1:A:67:ILE:CG2	1:A:72:LEU:HD13	2.36	0.55
1:A:183:LEU:HD21	4:A:2078:HOH:O	2.05	0.55
1:A:114:ILE:HD11	1:A:118:VAL:HG11	1.87	0.55
1:A:412:ASN:N	1:A:412:ASN:ND2	2.54	0.55
1:A:474:HIS:CD2	1:A:476:ASP:N	2.74	0.55
1:A:204:ALA:CB	1:A:303:LEU:HD21	2.36	0.55
1:A:169:LEU:HD13	1:A:173:GLU:OE2	2.07	0.54
1:A:2:GLU:HG3	1:A:2:GLU:O	2.03	0.54
1:A:48:GLU:HB2	1:A:50:ARG:CG	2.36	0.54
1:A:190:GLY:O	1:A:194:LEU:HD22	2.08	0.54
1:A:32:ALA:N	1:A:33:PRO:CD	2.71	0.53
1:A:191:LEU:O	1:A:195:ASN:HB2	2.09	0.53
1:A:457:THR:OG1	1:A:458:SER:N	2.41	0.53
1:A:187:ALA:O	1:A:188:LYS:HB3	2.08	0.53
1:A:447:GLN:HE22	1:A:476:ASP:HA	1.72	0.53
1:A:52:ALA:N	1:A:56:ASN:OD1	2.38	0.53
1:A:145:ALA:O	1:A:148:PRO:HD2	2.09	0.53
1:A:264:SER:CA	4:A:2105:HOH:O	2.57	0.53
1:A:277:GLN:HG3	1:A:283:ARG:CZ	2.39	0.53
1:A:381:PHE:C	1:A:383:ILE:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:MET:HA	1:A:385:GLN:OE1	2.09	0.52
1:A:103:LYS:HD2	1:A:107:LEU:HD11	1.90	0.52
1:A:481:PHE:C	1:A:483:PRO:HD2	2.34	0.52
1:A:143:SER:O	1:A:146:LEU:HG	2.09	0.52
1:A:279:PRO:HG2	1:A:358:LEU:CD1	2.40	0.52
1:A:381:PHE:N	1:A:381:PHE:CD1	2.76	0.52
1:A:68:ALA:HB3	1:A:71:ASP:CG	2.35	0.52
1:A:381:PHE:HB3	1:A:481:PHE:CE1	2.40	0.52
1:A:119:ILE:HG22	1:A:123:ILE:HD12	1.90	0.52
1:A:146:LEU:O	1:A:147:ALA:C	2.53	0.52
1:A:270:HIS:O	1:A:271:LYS:C	2.52	0.52
1:A:214:LEU:CD1	1:A:434:THR:HB	2.40	0.52
1:A:381:PHE:HD1	1:A:381:PHE:H	1.58	0.52
1:A:209:PHE:O	1:A:212:GLU:HB2	2.10	0.51
1:A:301:GLU:HG3	1:A:302:VAL:H	1.74	0.51
1:A:418:SER:O	1:A:419:MET:HB2	2.09	0.51
1:A:145:ALA:HB3	1:A:149:LEU:HD12	1.92	0.51
1:A:382:MET:HE2	1:A:383:ILE:HD11	1.90	0.51
1:A:378:ASN:O	1:A:379:SER:CB	2.58	0.51
1:A:68:ALA:HB3	1:A:71:ASP:OD1	2.10	0.51
1:A:96:VAL:HG11	1:A:131:TYR:HB3	1.91	0.51
1:A:46:ILE:HG22	1:A:47:ALA:N	2.26	0.50
1:A:76:GLN:O	1:A:79:LEU:HB2	2.11	0.50
1:A:204:ALA:HB3	1:A:303:LEU:HD21	1.94	0.50
1:A:353:GLU:HA	1:A:356:ILE:HD12	1.93	0.50
1:A:420:ALA:N	1:A:421:PRO:HD3	2.27	0.50
1:A:474:HIS:CD2	1:A:476:ASP:CA	2.94	0.50
1:A:67:ILE:O	1:A:68:ALA:C	2.54	0.50
1:A:381:PHE:O	1:A:382:MET:C	2.51	0.50
1:A:182:PRO:C	1:A:183:LEU:HD23	2.37	0.50
1:A:471:GLU:CD	1:A:487:LYS:HE2	2.35	0.50
1:A:506:LEU:HD13	1:A:509:LEU:HD12	1.94	0.49
1:A:301:GLU:CG	1:A:302:VAL:N	2.72	0.49
1:A:142:ALA:O	1:A:143:SER:CB	2.61	0.49
1:A:51:THR:HG22	1:A:66:ARG:CD	2.41	0.48
1:A:136:LEU:HG	1:A:137:LYS:HG2	1.95	0.48
1:A:353:GLU:OE1	1:A:354:ARG:NE	2.31	0.48
1:A:381:PHE:O	1:A:384:ALA:N	2.35	0.48
1:A:147:ALA:O	1:A:151:HIS:HD2	1.97	0.48
1:A:506:LEU:CD1	1:A:509:LEU:HD12	2.43	0.48
1:A:23:VAL:HG13	1:A:97:ARG:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:O	1:A:146:LEU:HD21	2.14	0.47
1:A:28:ASP:OD2	1:A:30:SER:OG	2.27	0.47
1:A:106:SER:OG	1:A:309:ALA:O	2.31	0.47
1:A:475:TYR:O	1:A:477:ARG:N	2.48	0.47
1:A:360:MET:HG3	1:A:385:GLN:CB	2.44	0.47
1:A:481:PHE:C	1:A:483:PRO:CD	2.87	0.47
1:A:478:ASP:HA	4:A:2172:HOH:O	2.14	0.47
3:A:1511:GOL:O3	3:A:1511:GOL:O1	2.31	0.47
1:A:481:PHE:O	1:A:482:ALA:C	2.57	0.47
1:A:59:PHE:HZ	3:A:1511:GOL:C1	2.14	0.47
1:A:19:HIS:ND1	1:A:209:PHE:HD2	2.13	0.47
1:A:381:PHE:CD2	1:A:481:PHE:HE1	2.33	0.47
1:A:421:PRO:HD2	4:A:2065:HOH:O	2.15	0.47
1:A:433:ASN:O	1:A:437:VAL:HG23	2.16	0.46
1:A:133:HIS:CD2	1:A:161:LYS:CE	2.98	0.46
1:A:412:ASN:N	1:A:412:ASN:HD22	2.13	0.46
1:A:62:LEU:O	1:A:64:SER:N	2.49	0.46
1:A:145:ALA:CB	4:A:2082:HOH:O	2.54	0.46
1:A:317:PHE:CE2	1:A:324:ILE:HD12	2.50	0.46
1:A:28:ASP:O	1:A:31:ALA:HB3	2.16	0.46
1:A:69:SER:O	1:A:72:LEU:HB2	2.16	0.46
1:A:230:LEU:HA	4:A:2087:HOH:O	2.16	0.46
1:A:48:GLU:OE1	1:A:50:ARG:NE	2.49	0.46
1:A:145:ALA:O	1:A:146:LEU:C	2.58	0.45
1:A:317:PHE:CD2	1:A:324:ILE:CD1	2.99	0.45
1:A:360:MET:HA	1:A:360:MET:HE2	1.99	0.45
1:A:136:LEU:CD1	1:A:136:LEU:C	2.88	0.45
1:A:288:VAL:CG1	1:A:351:LEU:HD22	2.47	0.45
1:A:490:GLU:HG2	1:A:494:LYS:HZ2	1.81	0.45
1:A:317:PHE:CE2	1:A:324:ILE:CD1	3.00	0.45
1:A:409:THR:O	1:A:410:SER:C	2.60	0.45
1:A:482:ALA:N	1:A:483:PRO:HD3	2.32	0.45
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.79	0.44
1:A:481:PHE:HD2	1:A:484:ASP:HB2	1.79	0.44
1:A:67:ILE:N	1:A:67:ILE:HD13	2.32	0.44
1:A:149:LEU:HD13	1:A:193:LEU:O	2.17	0.44
1:A:32:ALA:N	1:A:33:PRO:HD3	2.32	0.44
1:A:279:PRO:HG2	1:A:358:LEU:HD11	2.00	0.44
1:A:347:GLU:OE2	1:A:347:GLU:HA	2.17	0.44
1:A:360:MET:CG	1:A:385:GLN:HB2	2.45	0.44
1:A:59:PHE:HE2	1:A:75:LEU:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HA	1:A:171:ALA:CB	2.47	0.44
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.89	0.44
1:A:145:ALA:O	1:A:148:PRO:CD	2.66	0.44
1:A:264:SER:O	1:A:265:GLU:C	2.60	0.43
1:A:378:ASN:HB2	1:A:379:SER:H	1.63	0.43
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.84	0.43
1:A:54:GLY:O	3:A:1511:GOL:H12	2.17	0.43
1:A:67:ILE:CG2	1:A:72:LEU:CD1	2.96	0.43
1:A:188:LYS:N	3:A:1511:GOL:O3	2.42	0.43
1:A:458:SER:OG	1:A:461:LEU:CG	2.66	0.43
1:A:146:LEU:CD1	4:A:2015:HOH:O	2.66	0.43
1:A:284:CYS:HA	1:A:287:GLN:OE1	2.18	0.43
1:A:279:PRO:HG2	1:A:358:LEU:HD13	2.01	0.42
1:A:306:GLU:HG2	1:A:334:VAL:CG2	2.48	0.42
1:A:75:LEU:C	1:A:75:LEU:HD13	2.44	0.42
1:A:139:SER:O	1:A:421:PRO:HG2	2.19	0.42
1:A:495:GLY:O	1:A:496:SER:C	2.63	0.42
1:A:381:PHE:HD2	1:A:481:PHE:CE1	2.34	0.42
1:A:51:THR:HG21	1:A:66:ARG:HD3	2.01	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.82	0.42
1:A:143:SER:O	1:A:146:LEU:CG	2.68	0.42
1:A:105:ASN:ND2	1:A:308:ASN:HA	2.34	0.42
1:A:148:PRO:HB3	4:A:2062:HOH:O	2.20	0.42
1:A:262:ASP:OD1	1:A:262:ASP:N	2.52	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.86	0.42
1:A:104:ILE:HD13	1:A:123:ILE:HG13	2.02	0.42
1:A:170:SER:C	1:A:172:THR:H	2.28	0.42
1:A:423:ALA:O	1:A:426:ARG:NH1	2.49	0.42
1:A:146:LEU:HD12	4:A:2015:HOH:O	2.20	0.42
1:A:155:VAL:HA	1:A:159:GLU:O	2.19	0.42
1:A:313:ASN:ND2	2:A:1510:SO4:O3	2.39	0.42
1:A:490:GLU:HG2	1:A:494:LYS:NZ	2.35	0.42
1:A:76:GLN:OE1	4:A:2039:HOH:O	2.22	0.41
1:A:331:ALA:O	1:A:332:GLU:C	2.63	0.41
1:A:381:PHE:CD2	1:A:481:PHE:CZ	3.08	0.41
1:A:55:ILE:CD1	1:A:188:LYS:HB2	2.50	0.41
1:A:74:ASN:HD22	1:A:74:ASN:HA	1.60	0.41
1:A:312:ASP:O	1:A:315:LEU:CD2	2.67	0.41
1:A:411:ALA:C	1:A:412:ASN:HD22	2.28	0.41
1:A:171:ALA:O	1:A:175:LEU:HG	2.21	0.41
1:A:270:HIS:O	1:A:270:HIS:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:C	1:A:235:PRO:HD2	2.45	0.41
1:A:76:GLN:CB	1:A:185:LEU:HB2	2.51	0.40
1:A:97:ARG:HB2	1:A:131:TYR:CE1	2.56	0.40
1:A:246:GLN:HB2	4:A:2093:HOH:O	2.21	0.40
1:A:131:TYR:HA	1:A:132:PRO:HD3	1.89	0.40
1:A:136:LEU:HD21	1:A:425:LYS:HD2	2.04	0.40
1:A:337:ALA:O	1:A:340:ASN:HB2	2.21	0.40
1:A:475:TYR:O	1:A:475:TYR:HD1	1.93	0.40
1:A:28:ASP:O	1:A:31:ALA:CB	2.69	0.40
1:A:265:GLU:N	4:A:2105:HOH:O	2.29	0.40
1:A:176:ALA:O	1:A:177:VAL:C	2.65	0.40
1:A:381:PHE:O	1:A:383:ILE:N	2.55	0.40
1:A:385:GLN:NE2	4:A:2139:HOH:O	2.51	0.40
1:A:119:ILE:HG22	1:A:123:ILE:CD1	2.52	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)
1:A:393:SER:OG	1:A:405:ASP:OD2[4_555]	2.19	0.01

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	507/509 (100%)	455 (90%)	31 (6%)	21 (4%)	2 0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER
1	A	145	ALA

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Mol	Chain	Res	Type
1	A	146	LEU
1	A	271	LYS
1	A	275	LYS
1	A	363	HIS
1	A	364	MET
1	A	371	LEU
1	A	373	GLU
1	A	374	ASN
1	A	379	SER
1	A	372	VAL
1	A	476	ASP
1	A	411	ALA
1	A	478	ASP
1	A	479	ARG
1	A	366	GLN
1	A	370	PHE
1	A	367	LEU
1	A	477	ARG
1	A	369	PRO

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	387/387 (100%)	317 (82%)	70 (18%)	2 0

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	GLU
1	A	3	LEU
1	A	23	VAL
1	A	24	ARG
1	A	25	LEU
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	42	VAL
1	A	44	GLN
1	A	45	ILE
1	A	46	ILE
1	A	50	ARG
1	A	66	ARG
1	A	67	ILE
1	A	72	LEU
1	A	73	GLU
1	A	75	LEU
1	A	77	ARG
1	A	106	SER
1	A	114	ILE
1	A	123	ILE
1	A	137	LYS
1	A	146	LEU
1	A	157	LEU
1	A	165	LYS
1	A	167	GLN
1	A	170	SER
1	A	172	THR
1	A	183	LEU
1	A	184	THR
1	A	194	LEU
1	A	195	ASN
1	A	200	SER
1	A	272	ASN
1	A	275	LYS
1	A	276	VAL
1	A	277	GLN
1	A	301	GLU
1	A	345	ILE
1	A	360	MET
1	A	362	LYS
1	A	363	HIS
1	A	367	LEU
1	A	371	LEU
1	A	372	VAL
1	A	373	GLU
1	A	374	ASN
1	A	377	VAL
1	A	378	ASN

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Mol	Chain	Res	Type
1	A	381	PHE
1	A	382	MET
1	A	383	ILE
1	A	410	SER
1	A	412	ASN
1	A	413	GLN
1	A	414	GLU
1	A	425	LYS
1	A	426	ARG
1	A	429	GLU
1	A	453	LYS
1	A	456	LYS
1	A	463	LYS
1	A	466	GLN
1	A	468	LEU
1	A	476	ASP
1	A	477	ARG
1	A	479	ARG
1	A	487	LYS
1	A	494	LYS
1	A	508	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	26	GLN
1	A	74	ASN
1	A	83	HIS
1	A	195	ASN
1	A	270	HIS
1	A	277	GLN
1	A	298	GLN
1	A	378	ASN
1	A	412	ASN
1	A	413	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	GOL	A	1511	-	5,5,5	0.67	0	5,5,5	0.40	0
2	SO4	A	1510	-	4,4,4	0.75	0	6,6,6	0.07	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	GOL	A	1511	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1511	GOL	C1-C2-C3-O3
3	A	1511	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1511	GOL	8	0
2	A	1510	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	493/509 (96%)	0.84	58 (11%) 9 8	12, 23, 55, 105	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	PHE	7.4
1	A	382	MET	6.4
1	A	1	THR	6.1
1	A	378	ASN	5.6
1	A	477	ARG	5.6
1	A	476	ASP	5.5
1	A	383	ILE	5.4
1	A	145	ALA	5.3
1	A	143	SER	5.2
1	A	411	ALA	5.0
1	A	146	LEU	5.0
1	A	377	VAL	4.9
1	A	360	MET	4.9
1	A	479	ARG	4.7
1	A	144	GLY	4.6
1	A	271	LYS	4.4
1	A	276	VAL	4.2
1	A	480	PHE	4.2
1	A	375	GLY	4.2
1	A	380	GLY	4.1
1	A	270	HIS	4.1
1	A	410	SER	4.0
1	A	478	ASP	3.8
1	A	362	LYS	3.8
1	A	2	GLU	3.7
1	A	466	GLN	3.7
1	A	64	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	379	SER	3.1
1	A	60	GLY	3.1
1	A	167	GLN	3.1
1	A	61	LEU	3.1
1	A	412	ASN	3.0
1	A	3	LEU	2.9
1	A	38	SER	2.8
1	A	413	GLN	2.7
1	A	47	ALA	2.7
1	A	475	TYR	2.7
1	A	23	VAL	2.7
1	A	58	GLY	2.7
1	A	53	TYR	2.6
1	A	50	ARG	2.6
1	A	49	ASP	2.5
1	A	361	ASP	2.5
1	A	51	THR	2.5
1	A	184	THR	2.5
1	A	68	ALA	2.5
1	A	59	PHE	2.4
1	A	481	PHE	2.3
1	A	142	ALA	2.3
1	A	66	ARG	2.2
1	A	67	ILE	2.2
1	A	170	SER	2.2
1	A	172	THR	2.2
1	A	386	VAL	2.1
1	A	57	THR	2.1
1	A	173	GLU	2.1
1	A	157	LEU	2.1
1	A	301	GLU	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	1510	5/5	0.82	0.26	99,101,109,112	0
3	GOL	A	1511	6/6	0.85	0.15	37,48,54,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.