Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:11 AM GMT

PDB ID	:	3DOH
Title	:	Crystal Structure of a Thermostable Esterase
Authors	:	Levisson, M.; Sun, L.; Hendriks, S.; Dijkstra, B.W.; Van der Oost, J.; Kengen, S.W.M.
Deposited on	:	2008-07-04
Resolution	:	2.60 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 ①) were used in the production of this report:

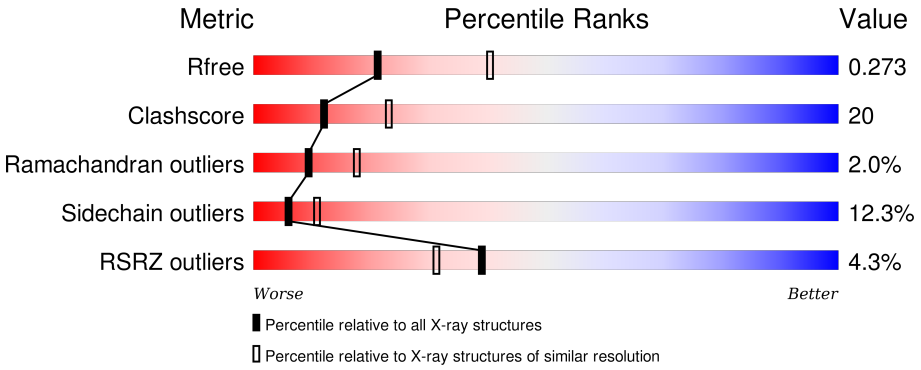
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	380	4% 64% 26% 8% ••
1	B	380	4% 65% 26% 7% •

2 Entry composition

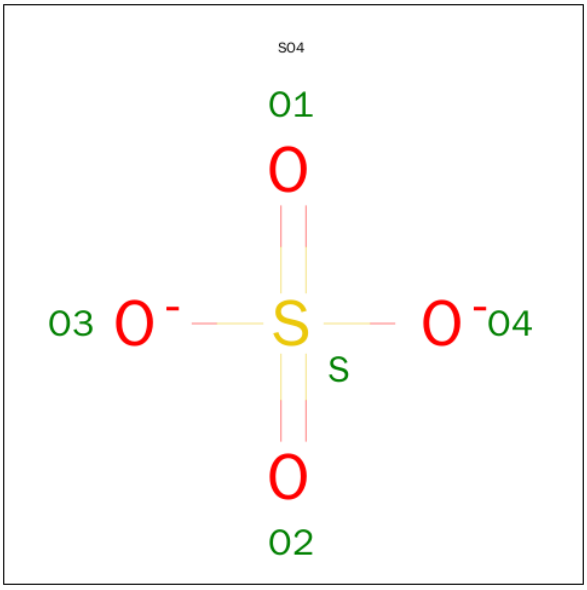
There are 3 unique types of molecules in this entry. The entry contains 6188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			3001	1940	493	560	8			
1	B	373	Total	C	N	O	S	0	0	0
			2981	1929	488	556	8			

- 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	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			

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

- Molecule 3 is water.

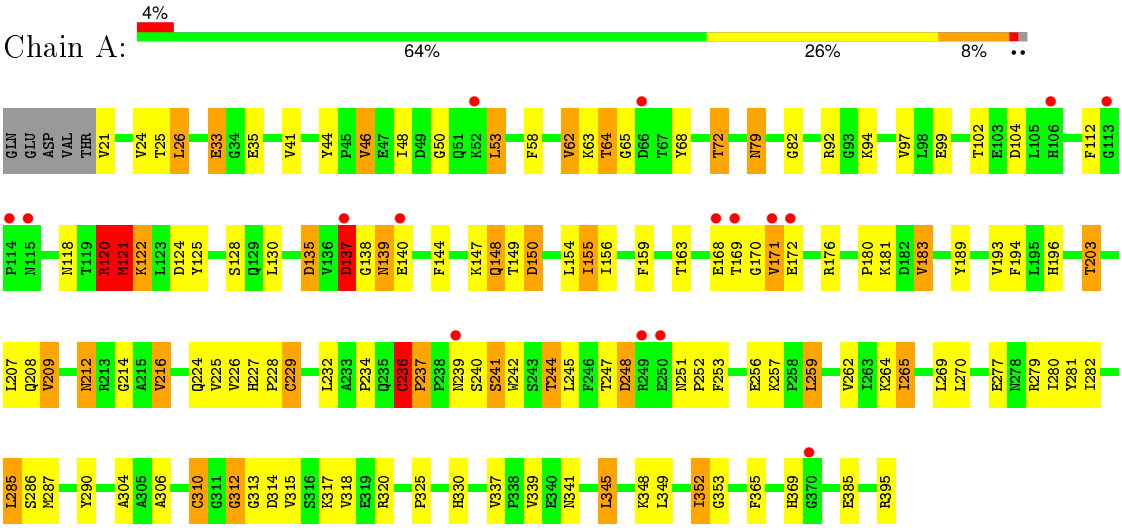
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	88	Total O 88 88	0	0
3	B	68	Total O 68 68	0	0

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.

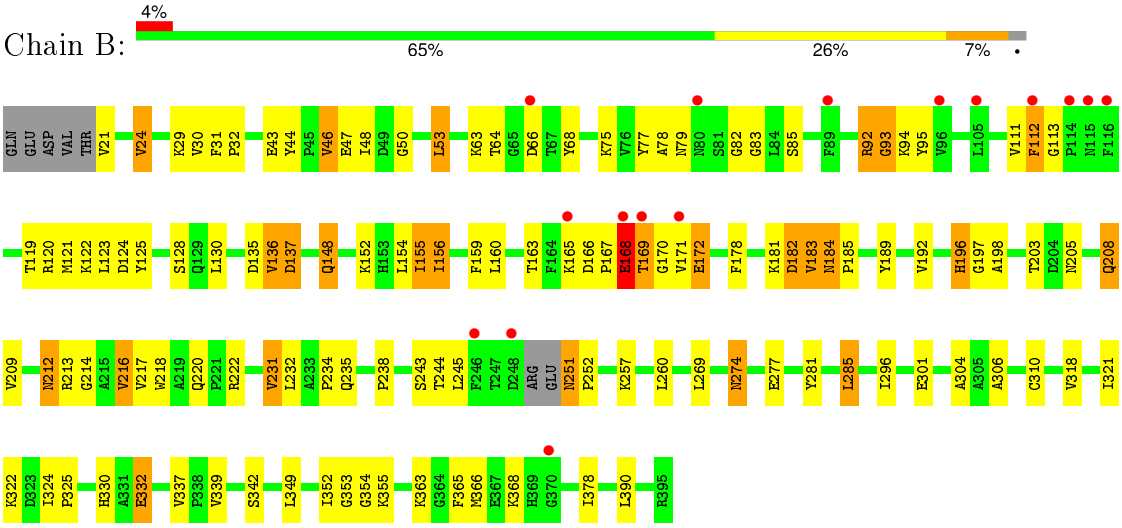
- Molecule 1: esterase

Chain A:



- Molecule 1: esterase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	130.16Å 130.16Å 306.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.60 19.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.96-2.60) 96.4 (19.96-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.268 0.207 , 0.273	Depositor DCC
R_{free} test set	1506 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.6	EDS
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.000 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 29879 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6188	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.98 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.9523e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.83	0/3083	0.80	1/4198 (0.0%)
1	B	0.82	0/3062	0.81	1/4169 (0.0%)
All	All	0.83	0/6145	0.80	2/8367 (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	8
1	B	0	8
All	All	0	16

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	285	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	395	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Peptide
1	A	121	MET	Peptide
1	A	137	ASP	Peptide
1	A	228	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	236	CYS	Peptide
1	A	237	PRO	Peptide
1	A	312	GLY	Peptide
1	A	353	GLY	Peptide
1	B	113	GLY	Peptide
1	B	181	LYS	Peptide
1	B	182	ASP	Peptide
1	B	196	HIS	Peptide
1	B	353	GLY	Peptide
1	B	64	THR	Peptide
1	B	77	TYR	Peptide
1	B	82	GLY	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	3001	0	2956	129	0
1	B	2981	0	2936	109	0
2	A	30	0	0	0	0
2	B	20	0	0	1	0
3	A	88	0	0	2	0
3	B	68	0	0	4	0
All	All	6188	0	5892	237	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 20.

All (237) 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:165:LYS:O	1:B:167:PRO:HD3	1.31	1.23
1:A:244:THR:O	1:A:252:PRO:HA	1.57	1.03
1:A:62:VAL:HG13	1:A:125:TYR:CE1	1.94	1.02
1:A:285:LEU:HD22	1:A:285:LEU:O	1.59	1.02
1:B:79:ASN:HA	1:B:92:ARG:O	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:OD2	1:A:138:GLY:CA	2.16	0.94
1:A:137:ASP:OD2	1:A:138:GLY:HA2	1.66	0.94
1:A:135:ASP:OD1	1:A:138:GLY:HA2	1.66	0.93
1:A:24:VAL:CG2	1:A:148:GLN:HA	1.99	0.91
1:B:365:PHE:HD2	1:B:366:MET:HE2	1.39	0.86
1:A:64:THR:OG1	1:A:121:MET:CE	2.22	0.85
1:A:33:GLU:HG2	3:A:552:HOH:O	1.77	0.84
1:B:208:GLN:HG2	1:B:235:GLN:HB2	1.61	0.83
1:A:64:THR:OG1	1:A:121:MET:HE1	1.80	0.82
1:B:296:ILE:HD11	1:B:306:ALA:CB	2.10	0.82
1:A:125:TYR:H	1:A:148:GLN:HE22	1.26	0.81
1:A:64:THR:O	1:A:64:THR:HG22	1.82	0.80
1:A:149:THR:CG2	1:A:149:THR:O	2.30	0.80
1:A:224:GLN:HE22	1:A:229:CYS:HB3	1.45	0.79
1:B:125:TYR:H	1:B:148:GLN:HE22	1.31	0.79
1:B:212:ASN:HD22	1:B:214:GLY:H	1.29	0.78
1:A:149:THR:HG22	1:A:149:THR:O	1.83	0.78
1:B:167:PRO:HA	1:B:168:GLU:C	2.05	0.78
1:A:148:GLN:H	1:A:148:GLN:HE21	1.32	0.77
1:A:50:GLY:HA2	1:A:53:LEU:HD22	1.65	0.77
1:A:137:ASP:OD2	1:A:138:GLY:O	2.02	0.77
1:B:112:PHE:H	1:B:112:PHE:HD1	1.30	0.75
1:A:62:VAL:CG1	1:A:125:TYR:CE1	2.70	0.75
1:B:274:ASN:H	1:B:274:ASN:HD22	1.33	0.75
1:A:245:LEU:HA	1:A:252:PRO:HB3	1.67	0.74
1:A:62:VAL:HG13	1:A:125:TYR:CZ	2.22	0.74
1:B:296:ILE:HD11	1:B:306:ALA:HB2	1.68	0.74
1:A:24:VAL:HG23	1:A:148:GLN:HA	1.68	0.74
1:A:64:THR:OG1	1:A:121:MET:HE3	1.89	0.73
1:B:330:HIS:HD2	1:B:342:SER:OG	1.71	0.73
1:B:178:PHE:HB3	1:B:231:VAL:HG13	1.71	0.73
1:A:285:LEU:CD2	1:A:285:LEU:O	2.35	0.72
1:A:203:THR:O	1:A:203:THR:HG23	1.89	0.72
1:B:165:LYS:O	1:B:167:PRO:CD	2.24	0.72
1:A:245:LEU:HA	1:A:252:PRO:CB	2.18	0.72
1:A:154:LEU:O	1:A:155:ILE:CB	2.38	0.72
1:A:72:THR:HG23	1:A:104:ASP:OD1	1.90	0.71
1:B:78:ALA:HA	1:B:95:TYR:O	1.90	0.71
1:A:154:LEU:O	1:A:155:ILE:CG1	2.40	0.70
1:A:244:THR:O	1:A:252:PRO:CA	2.38	0.70
1:B:85:SER:HB3	3:B:550:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:PHE:HD2	1:B:366:MET:CE	2.05	0.69
1:A:154:LEU:O	1:A:155:ILE:HG12	1.91	0.69
1:B:296:ILE:HG22	1:B:321:ILE:CG2	2.22	0.69
1:A:224:GLN:NE2	1:A:229:CYS:HB3	2.07	0.69
1:A:314:ASP:OD2	1:A:317:LYS:HD2	1.92	0.69
1:B:79:ASN:O	1:B:95:TYR:HB2	1.94	0.68
1:B:196:HIS:CD2	1:B:208:GLN:HB3	2.28	0.68
1:B:220:GLN:NE2	1:B:222:ARG:HH11	1.91	0.68
1:A:79:ASN:HD22	1:A:79:ASN:C	1.97	0.68
1:A:169:THR:OG1	1:A:171:VAL:HG23	1.92	0.68
1:A:241:SER:HB2	1:A:287:MET:SD	2.33	0.68
1:A:226:VAL:HG23	1:A:227:HIS:ND1	2.08	0.68
1:B:47:GLU:O	1:B:136:VAL:HG22	1.94	0.67
1:B:183:VAL:CG1	1:B:183:VAL:O	2.43	0.67
1:B:296:ILE:CG2	1:B:324:ILE:HD12	2.24	0.67
1:A:154:LEU:O	1:A:155:ILE:HB	1.95	0.66
1:A:270:LEU:HD21	1:A:280:ILE:HD11	1.77	0.66
1:B:79:ASN:CA	1:B:92:ARG:O	2.40	0.66
1:B:155:ILE:HG22	1:B:155:ILE:O	1.96	0.66
1:A:148:GLN:H	1:A:148:GLN:NE2	1.94	0.66
1:A:154:LEU:C	1:A:155:ILE:HG12	2.17	0.65
1:A:46:VAL:HG21	1:A:135:ASP:OD2	1.97	0.65
1:B:365:PHE:CD2	1:B:366:MET:HE2	2.27	0.64
1:A:330:HIS:HE1	1:A:337:VAL:O	1.81	0.64
1:B:296:ILE:HG23	1:B:324:ILE:HD12	1.79	0.64
1:B:274:ASN:N	1:B:274:ASN:HD22	1.95	0.64
1:A:137:ASP:OD2	1:A:138:GLY:C	2.35	0.64
1:B:318:VAL:HG13	1:B:349:LEU:CD1	2.28	0.64
1:B:43:GLU:OE2	1:B:94:LYS:HD3	1.98	0.63
1:A:135:ASP:OD1	1:A:138:GLY:CA	2.45	0.63
1:A:193:VAL:HG22	1:A:282:ILE:HG13	1.80	0.63
1:A:79:ASN:HD21	1:A:82:GLY:H	1.46	0.63
1:B:24:VAL:HG22	1:B:148:GLN:HA	1.80	0.62
1:B:318:VAL:HG13	1:B:349:LEU:HD13	1.80	0.62
1:B:63:LYS:HB3	1:B:124:ASP:HB3	1.80	0.62
1:B:296:ILE:CD1	1:B:306:ALA:CB	2.77	0.62
1:A:212:ASN:HD22	1:A:214:GLY:H	1.48	0.62
1:A:64:THR:CG2	1:A:64:THR:O	2.48	0.61
1:B:50:GLY:HA2	1:B:53:LEU:HD22	1.81	0.61
1:B:183:VAL:HG13	1:B:189:TYR:CZ	2.35	0.61
1:B:365:PHE:CD2	1:B:366:MET:CE	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:H	1:A:285:LEU:HD13	1.66	0.60
1:B:156:ILE:HG12	1:B:209:VAL:CG1	2.32	0.60
1:B:137:ASP:N	1:B:137:ASP:OD1	2.35	0.60
1:A:226:VAL:HG23	1:A:227:HIS:CE1	2.37	0.59
1:B:148:GLN:H	1:B:148:GLN:HE21	1.48	0.59
1:A:41:VAL:HG22	1:A:97:VAL:HG22	1.84	0.59
1:B:44:TYR:CD1	1:B:48:ILE:HD11	2.37	0.59
1:A:156:ILE:HG12	1:A:209:VAL:HG13	1.85	0.59
1:A:247:THR:O	1:A:248:ASP:HB2	2.03	0.59
1:A:279:ARG:HD2	1:A:281:TYR:OH	2.03	0.59
1:A:35:GLU:OE1	1:A:120:ARG:NH1	2.35	0.58
1:B:296:ILE:CD1	1:B:306:ALA:HB2	2.33	0.58
1:B:296:ILE:HG22	1:B:321:ILE:HG22	1.84	0.58
1:A:285:LEU:N	1:A:285:LEU:HD13	2.18	0.58
1:A:149:THR:HG22	1:A:150:ASP:OD2	2.03	0.58
1:A:227:HIS:O	1:A:229:CYS:HB2	2.04	0.58
1:B:94:LYS:HD2	1:B:95:TYR:CE2	2.39	0.58
1:B:296:ILE:HG22	1:B:321:ILE:HG21	1.84	0.58
1:B:245:LEU:HA	1:B:252:PRO:CB	2.33	0.58
1:A:203:THR:O	1:A:203:THR:CG2	2.52	0.57
1:A:72:THR:CG2	1:A:104:ASP:OD1	2.52	0.57
1:A:330:HIS:CE1	1:A:337:VAL:O	2.57	0.57
1:B:156:ILE:HG12	1:B:209:VAL:HG13	1.86	0.57
1:A:262:VAL:HA	1:A:265:ILE:HG23	1.85	0.57
1:A:79:ASN:ND2	1:A:82:GLY:H	2.04	0.56
1:B:167:PRO:HA	1:B:169:THR:N	2.21	0.56
1:A:139:ASN:O	1:A:140:GLU:HG2	2.06	0.56
1:A:242:TRP:O	1:A:259:LEU:HB2	2.07	0.55
1:B:330:HIS:CD2	1:B:342:SER:OG	2.57	0.55
1:A:232:LEU:HG	1:A:234:PRO:HD3	1.89	0.55
1:B:183:VAL:O	1:B:183:VAL:HG13	2.07	0.55
1:B:198:ALA:HB3	2:B:500:SO4:O4	2.06	0.55
1:B:212:ASN:ND2	1:B:214:GLY:H	2.04	0.55
1:A:154:LEU:HD13	3:A:545:HOH:O	2.07	0.54
1:A:240:SER:O	1:A:241:SER:HB3	2.06	0.54
1:B:330:HIS:HE1	1:B:337:VAL:O	1.91	0.54
1:B:304:ALA:O	1:B:325:PRO:HD2	2.07	0.54
1:A:286:SER:HA	1:A:310:CYS:O	2.08	0.54
1:A:317:LYS:O	1:A:320:ARG:HG3	2.08	0.53
1:A:149:THR:O	1:A:150:ASP:OD2	2.27	0.53
1:B:310:CYS:HA	1:B:330:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:HG22	1:A:216:VAL:HG22	1.91	0.52
1:B:155:ILE:O	1:B:155:ILE:CG2	2.57	0.52
1:B:156:ILE:O	1:B:156:ILE:CG2	2.56	0.52
1:A:318:VAL:HG21	1:A:348:LYS:HG3	1.91	0.52
1:B:155:ILE:HG22	1:B:216:VAL:HG22	1.90	0.52
1:B:196:HIS:HB2	1:B:197:GLY:HA3	1.91	0.52
1:B:296:ILE:HD11	1:B:306:ALA:HB1	1.91	0.51
1:B:168:GLU:O	1:B:169:THR:HB	2.11	0.51
1:B:152:LYS:HE3	1:B:154:LEU:CD2	2.41	0.51
1:B:171:VAL:O	1:B:171:VAL:HG13	2.10	0.51
1:A:62:VAL:O	1:A:68:TYR:HA	2.10	0.51
1:A:148:GLN:N	1:A:148:GLN:HE21	2.06	0.51
1:A:25:THR:HG23	1:A:150:ASP:HB3	1.92	0.51
1:A:285:LEU:CD2	1:A:285:LEU:C	2.79	0.50
1:A:341:ASN:O	1:A:345:LEU:HD22	2.11	0.50
1:A:236:CYS:SG	1:A:241:SER:HA	2.51	0.50
1:A:112:PHE:HD1	1:A:118:ASN:ND2	2.08	0.50
1:B:163:THR:CG2	1:B:172:GLU:HG2	2.42	0.50
1:B:232:LEU:HG	1:B:234:PRO:HD3	1.93	0.50
1:A:193:VAL:HG22	1:A:193:VAL:O	2.11	0.49
1:B:83:GLY:HA3	3:B:556:HOH:O	2.12	0.49
1:A:236:CYS:SG	1:A:237:PRO:HD2	2.52	0.49
1:A:193:VAL:HG13	1:A:281:TYR:O	2.11	0.49
1:A:194:PHE:CE1	1:A:285:LEU:CD1	2.95	0.49
1:B:24:VAL:CG2	1:B:148:GLN:HA	2.41	0.49
1:B:93:GLY:O	1:B:94:LYS:C	2.51	0.48
1:B:281:TYR:HB3	1:B:390:LEU:HD11	1.95	0.48
1:B:32:PRO:HB3	1:B:378:ILE:HG23	1.95	0.48
1:B:354:GLY:O	1:B:355:LYS:HB2	2.12	0.48
1:B:183:VAL:HG13	1:B:189:TYR:OH	2.12	0.48
1:A:193:VAL:HG21	1:A:282:ILE:HD12	1.94	0.48
1:A:193:VAL:CG2	1:A:193:VAL:O	2.59	0.48
1:B:184:ASN:C	1:B:184:ASN:OD1	2.52	0.48
1:A:26:LEU:HD22	1:A:148:GLN:HG3	1.95	0.48
1:B:183:VAL:HG13	1:B:189:TYR:CE2	2.49	0.47
1:B:43:GLU:HG3	1:B:95:TYR:CE1	2.48	0.47
1:A:245:LEU:HA	1:A:252:PRO:HB2	1.94	0.47
1:B:238:PRO:O	3:B:536:HOH:O	2.20	0.47
1:B:192:VAL:O	1:B:231:VAL:HA	2.15	0.47
1:A:130:LEU:HD21	1:B:130:LEU:HD21	1.95	0.47
1:A:138:GLY:HA3	1:A:139:ASN:HA	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:CZ	1:A:313:GLY:O	2.67	0.47
1:A:135:ASP:C	1:A:135:ASP:OD1	2.52	0.47
1:A:194:PHE:HZ	1:A:285:LEU:HD11	1.80	0.47
1:A:125:TYR:O	1:A:147:LYS:HA	2.16	0.46
1:B:159:PHE:HE1	1:B:231:VAL:HG22	1.80	0.46
1:B:163:THR:HG22	1:B:172:GLU:HG2	1.97	0.46
1:B:232:LEU:HD13	1:B:269:LEU:HD11	1.97	0.46
1:B:208:GLN:H	1:B:208:GLN:HG3	1.23	0.46
1:A:330:HIS:CE1	1:A:339:VAL:HA	2.51	0.46
1:B:205:ASN:N	1:B:235:GLN:OE1	2.38	0.46
1:B:184:ASN:HA	1:B:185:PRO:HD3	1.82	0.46
1:B:29:LYS:NZ	1:B:213:ARG:NH2	2.64	0.46
1:A:79:ASN:ND2	1:A:79:ASN:C	2.67	0.45
1:B:30:VAL:HG21	1:B:156:ILE:HD11	1.98	0.45
1:B:296:ILE:HG23	1:B:324:ILE:CD1	2.44	0.45
1:B:217:VAL:HG13	1:B:218:TRP:N	2.31	0.45
1:A:194:PHE:CZ	1:A:285:LEU:HD11	2.51	0.45
1:A:241:SER:CB	1:A:287:MET:SD	3.04	0.45
1:A:194:PHE:HE1	1:A:285:LEU:CD1	2.30	0.45
1:A:313:GLY:HA3	1:A:345:LEU:HD11	1.99	0.45
1:A:304:ALA:O	1:A:325:PRO:HD2	2.16	0.45
1:A:193:VAL:HG22	1:A:282:ILE:CG1	2.44	0.45
1:B:244:THR:O	1:B:252:PRO:HA	2.17	0.45
1:A:196:HIS:CD2	1:A:208:GLN:HB2	2.52	0.45
1:A:122:LYS:NZ	1:A:122:LYS:HB3	2.32	0.45
1:A:159:PHE:HB3	1:A:176:ARG:HB3	1.99	0.44
1:A:24:VAL:O	1:A:24:VAL:HG23	2.16	0.44
1:B:245:LEU:HA	1:B:252:PRO:HB2	1.98	0.44
1:A:21:VAL:HG21	1:A:144:PHE:CE2	2.52	0.44
1:B:243:SER:C	1:B:245:LEU:H	2.20	0.44
1:B:31:PHE:O	1:B:32:PRO:C	2.56	0.44
1:A:64:THR:HA	1:A:65:GLY:HA2	1.59	0.44
1:B:183:VAL:CG1	1:B:189:TYR:CZ	3.01	0.44
1:B:332:GLU:HG2	1:B:363:LYS:HB2	1.99	0.44
1:A:352:ILE:HA	1:A:352:ILE:HD13	1.91	0.43
1:A:365:PHE:CD2	1:A:365:PHE:C	2.92	0.43
1:B:183:VAL:O	1:B:184:ASN:C	2.56	0.43
1:A:365:PHE:O	1:A:369:HIS:HD2	2.02	0.43
1:B:330:HIS:CE1	1:B:337:VAL:O	2.71	0.43
1:A:282:ILE:O	1:A:306:ALA:HA	2.19	0.43
1:A:125:TYR:H	1:A:148:GLN:NE2	2.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:N	1:B:274:ASN:ND2	2.65	0.43
1:B:330:HIS:CE1	1:B:339:VAL:HA	2.54	0.42
1:A:237:PRO:O	1:A:239:ASN:N	2.53	0.42
1:A:58:PHE:HA	1:A:128:SER:O	2.19	0.42
1:B:29:LYS:HZ3	1:B:213:ARG:HH21	1.67	0.42
1:B:30:VAL:CG2	1:B:156:ILE:CD1	2.97	0.42
1:A:163:THR:CG2	1:A:172:GLU:HG2	2.49	0.42
1:A:247:THR:OG1	1:A:256:GLU:OE1	2.26	0.42
1:A:44:TYR:CG	1:A:48:ILE:HD11	2.55	0.41
1:B:47:GLU:O	1:B:135:ASP:HB2	2.20	0.41
1:A:313:GLY:HA3	1:A:345:LEU:HD21	2.02	0.41
1:A:120:ARG:O	1:A:121:MET:C	2.59	0.41
1:B:125:TYR:H	1:B:148:GLN:NE2	2.07	0.41
1:A:290:TYR:CE1	1:A:312:GLY:HA3	2.55	0.41
1:A:24:VAL:O	1:A:24:VAL:CG2	2.67	0.41
1:B:368:LYS:NZ	3:B:567:HOH:O	2.53	0.41
1:A:24:VAL:HG21	1:A:148:GLN:HA	1.94	0.41
1:A:183:VAL:HG13	1:A:189:TYR:CE2	2.56	0.41
1:B:30:VAL:CG2	1:B:156:ILE:HD11	2.51	0.41
1:A:183:VAL:HG22	1:A:189:TYR:CZ	2.55	0.41
1:B:63:LYS:HD3	1:B:68:TYR:CZ	2.56	0.40
1:A:170:GLY:O	1:A:171:VAL:C	2.59	0.40
1:A:168:GLU:HB3	1:A:264:LYS:NZ	2.36	0.40
1:B:46:VAL:HG13	1:B:47:GLU:N	2.36	0.40
1:B:318:VAL:HG13	1:B:349:LEU:HD12	2.03	0.40
1:B:251:ASN:HA	1:B:252:PRO:HD3	1.80	0.40
1:A:171:VAL:HG21	1:A:257:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	373/380 (98%)	339 (91%)	26 (7%)	8 (2%)	9 16
1	B	369/380 (97%)	335 (91%)	27 (7%)	7 (2%)	10 19
All	All	742/760 (98%)	674 (91%)	53 (7%)	15 (2%)	9 18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	B	66	ASP
1	B	166	ASP
1	B	169	THR
1	A	121	MET
1	A	248	ASP
1	A	229	CYS
1	A	244	THR
1	B	93	GLY
1	A	171	VAL
1	A	241	SER
1	A	310	CYS
1	B	155	ILE
1	B	168	GLU
1	B	170	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	333/338 (98%)	290 (87%)	43 (13%)	5 9
1	B	331/338 (98%)	292 (88%)	39 (12%)	6 12
All	All	664/676 (98%)	582 (88%)	82 (12%)	6 11

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU

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Mol	Chain	Res	Type
1	A	33	GLU
1	A	46	VAL
1	A	53	LEU
1	A	62	VAL
1	A	63	LYS
1	A	64	THR
1	A	72	THR
1	A	79	ASN
1	A	92	ARG
1	A	94	LYS
1	A	99	GLU
1	A	102	THR
1	A	120	ARG
1	A	121	MET
1	A	122	LYS
1	A	124	ASP
1	A	135	ASP
1	A	137	ASP
1	A	139	ASN
1	A	148	GLN
1	A	150	ASP
1	A	180	PRO
1	A	181	LYS
1	A	183	VAL
1	A	203	THR
1	A	207	LEU
1	A	209	VAL
1	A	212	ASN
1	A	216	VAL
1	A	225	VAL
1	A	236	CYS
1	A	251	ASN
1	A	259	LEU
1	A	265	ILE
1	A	269	LEU
1	A	277	GLU
1	A	285	LEU
1	A	315	VAL
1	A	345	LEU
1	A	349	LEU
1	A	352	ILE
1	A	385	GLU

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Mol	Chain	Res	Type
1	B	21	VAL
1	B	24	VAL
1	B	46	VAL
1	B	53	LEU
1	B	75	LYS
1	B	92	ARG
1	B	111	VAL
1	B	112	PHE
1	B	119	THR
1	B	120	ARG
1	B	121	MET
1	B	122	LYS
1	B	123	LEU
1	B	128	SER
1	B	136	VAL
1	B	137	ASP
1	B	148	GLN
1	B	156	ILE
1	B	160	LEU
1	B	168	GLU
1	B	172	GLU
1	B	182	ASP
1	B	183	VAL
1	B	184	ASN
1	B	203	THR
1	B	208	GLN
1	B	212	ASN
1	B	216	VAL
1	B	231	VAL
1	B	251	ASN
1	B	257	LYS
1	B	260	LEU
1	B	274	ASN
1	B	277	GLU
1	B	285	LEU
1	B	301	GLU
1	B	322	LYS
1	B	332	GLU
1	B	352	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	148	GLN
1	A	212	ASN
1	A	220	GLN
1	A	251	ASN
1	A	330	HIS
1	A	369	HIS
1	B	148	GLN
1	B	212	ASN
1	B	220	GLN
1	B	274	ASN
1	B	330	HIS
1	B	341	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	400	-	4,4,4	0.50	0	6,6,6	0.45	0
2	SO4	A	401	-	4,4,4	0.43	0	6,6,6	1.18	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	402	-	4,4,4	0.32	0	6,6,6	0.33	0
2	SO4	A	403	-	4,4,4	0.51	0	6,6,6	0.27	0
2	SO4	A	404	-	4,4,4	0.07	0	6,6,6	0.37	0
2	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SO4	B	500	-	4,4,4	0.36	0	6,6,6	0.44	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.47	0
2	SO4	B	503	-	4,4,4	0.21	0	6,6,6	0.41	0
2	SO4	B	504	-	4,4,4	0.19	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
2	SO4	A	400	-	-	0/0/0/0	0/0/0/0
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	SO4	O2-S-O1	2.57	117.63	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	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, 95^{th} 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	375/380 (98%)	-0.16	16 (4%)	39	31	21, 34, 59, 75	0
1	B	373/380 (98%)	-0.18	16 (4%)	39	31	22, 34, 56, 73	0
All	All	748/760 (98%)	-0.17	32 (4%)	39	31	21, 34, 58, 75	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	PHE	4.2
1	B	169	THR	4.1
1	A	169	THR	3.8
1	B	115	ASN	3.8
1	A	249	ARG	3.7
1	A	250	GLU	3.6
1	A	114	PRO	3.5
1	B	116	PHE	3.4
1	A	171	VAL	3.4
1	B	114	PRO	3.3
1	B	168	GLU	3.3
1	A	113	GLY	3.2
1	B	171	VAL	3.0
1	A	115	ASN	2.8
1	B	80	ASN	2.8
1	B	66	ASP	2.7
1	B	248	ASP	2.7
1	A	168	GLU	2.6
1	B	96	VAL	2.6
1	B	246	PHE	2.6
1	A	52	LYS	2.5
1	A	66	ASP	2.4
1	A	106	HIS	2.3
1	B	105	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	370	GLY	2.2
1	B	165	LYS	2.2
1	B	89	PHE	2.1
1	A	172	GLU	2.1
1	A	370	GLY	2.1
1	A	137	ASP	2.1
1	A	140	GLU	2.1
1	A	239	ASN	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, 95^{th} 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	503	5/5	0.99	0.14	-0.39	46,48,49,51	0
2	SO4	B	500	5/5	0.97	0.10	-0.57	50,51,51,52	0
2	SO4	A	400	5/5	0.98	0.07	-0.94	37,37,38,39	0
2	SO4	A	403	5/5	0.98	0.12	-1.12	43,43,44,44	0
2	SO4	B	504	5/5	0.97	0.08	-1.39	62,64,65,65	0
2	SO4	A	404	5/5	0.98	0.10	-1.95	48,49,50,50	0
2	SO4	A	401	5/5	0.98	0.08	-2.17	44,45,46,47	0
2	SO4	B	501	5/5	0.97	0.08	-3.55	52,54,54,55	0
2	SO4	A	502	5/5	0.98	0.16	-	51,51,54,54	0
2	SO4	A	402	5/5	0.99	0.14	-	44,45,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.