



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 PM GMT

PDB ID : 4HU8  
Title : Crystal Structure of a Bacterial Ig-like Domain Containing GH10 Xylanase from Termite Gut  
Authors : Han, Q.; Liu, N.; Robinson, H.; Cao, L.; Qian, C.; Wang, Q.; Xie, L.; Ding, H.; Wang, Q.; Huang, Y.; Li, J.; Zhou, Z.  
Deposited on : 2012-11-02  
Resolution : 2.00 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](mailto: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.

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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

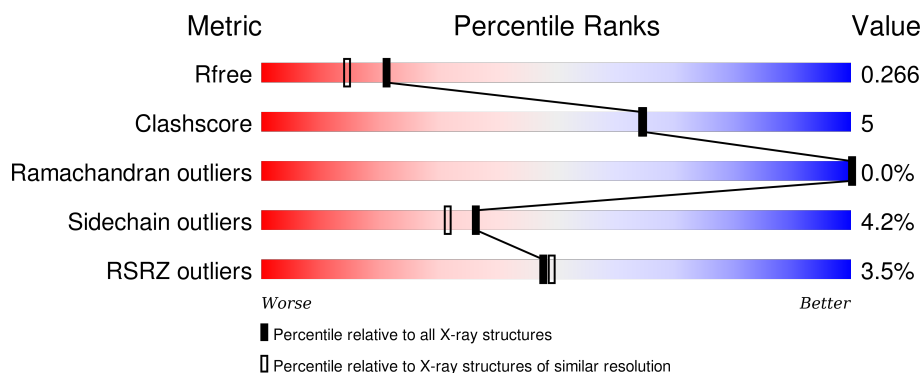
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	456	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 84%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>14%</span> <span>..</span> </div> </div>
1	B	456	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 12%, green 86%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>86%</span> <span>12%</span> <span>..</span> </div> </div>
1	C	456	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 87%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>11%</span> <span>..</span> </div> </div>
1	D	456	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 89%, yellow 9%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>89%</span> <span>9%</span> <span>.</span> </div> </div>
1	E	456	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 12%, green 86%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>86%</span> <span>12%</span> <span>..</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	456	
1	G	456	
1	H	456	

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	502	-	-	-	X
3	GOL	C	504	-	-	-	X
3	GOL	H	503	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30836 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 GH10 Xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3558	2248	613	679	18			
1	B	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	C	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	D	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	E	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	F	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	G	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	H	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		

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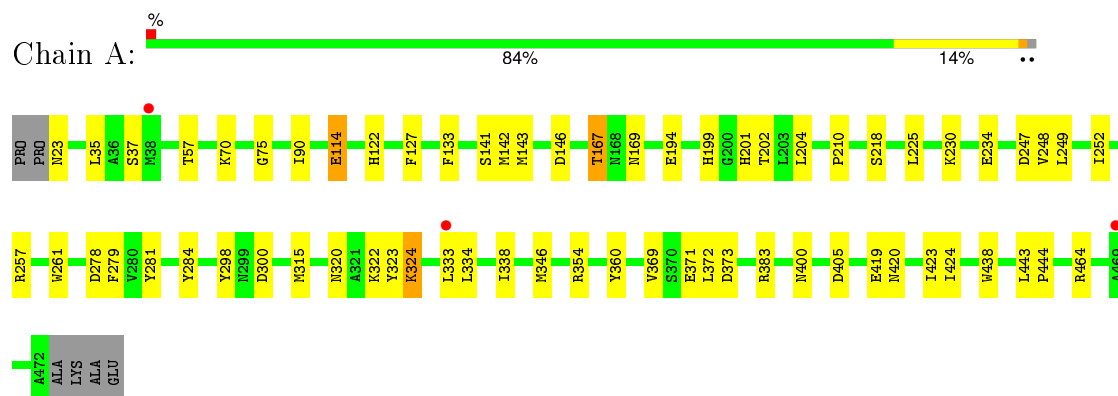
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	216	Total 216	O 216	0	0
4	C	457	Total 457	O 457	0	0
4	D	412	Total 412	O 412	0	0
4	E	207	Total 207	O 207	0	0
4	F	177	Total 177	O 177	0	0
4	G	134	Total 134	O 134	0	0
4	H	297	Total 297	O 297	0	0

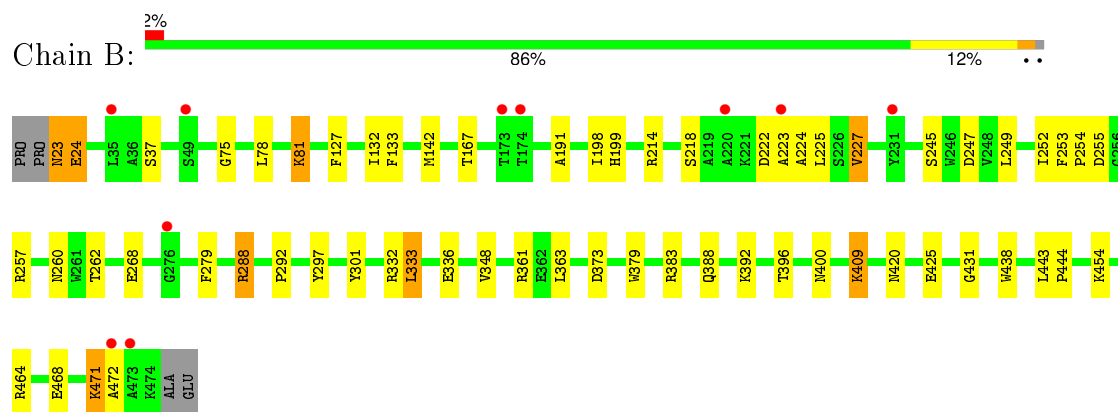
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

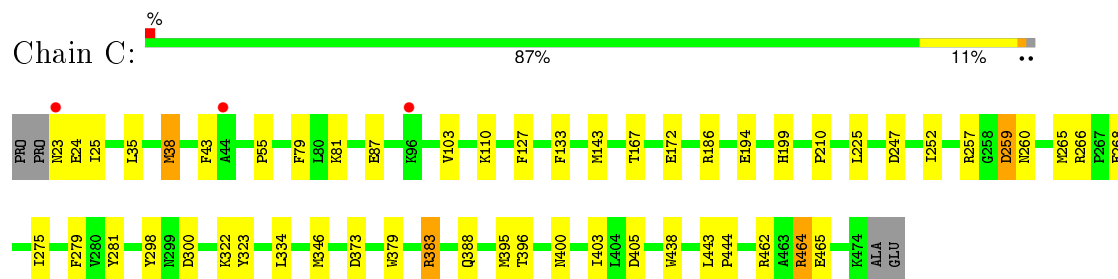
#### • Molecule 1: GH10 Xylanase



#### • Molecule 1: GH10 Xylanase

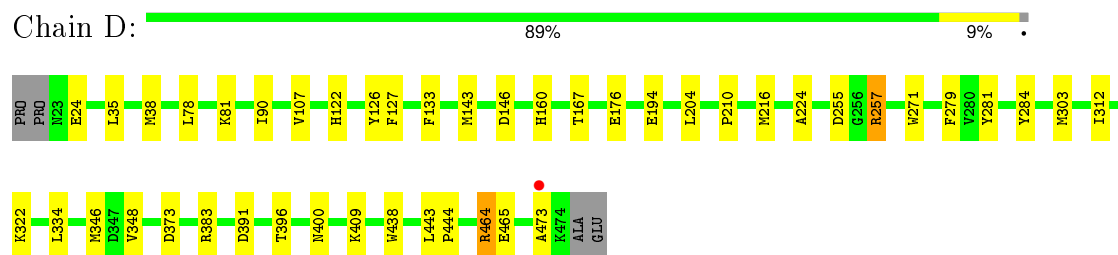


#### • Molecule 1: GH10 Xylanase

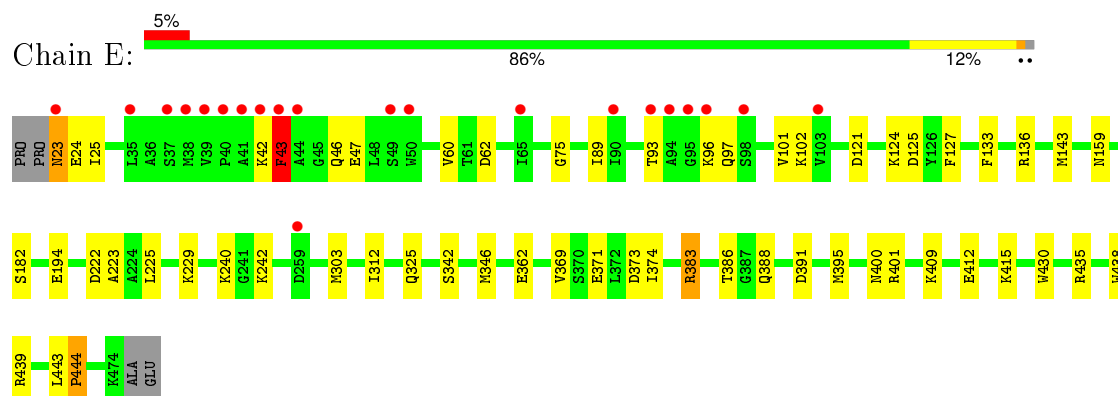


#### • Molecule 1: GH10 Xylanase

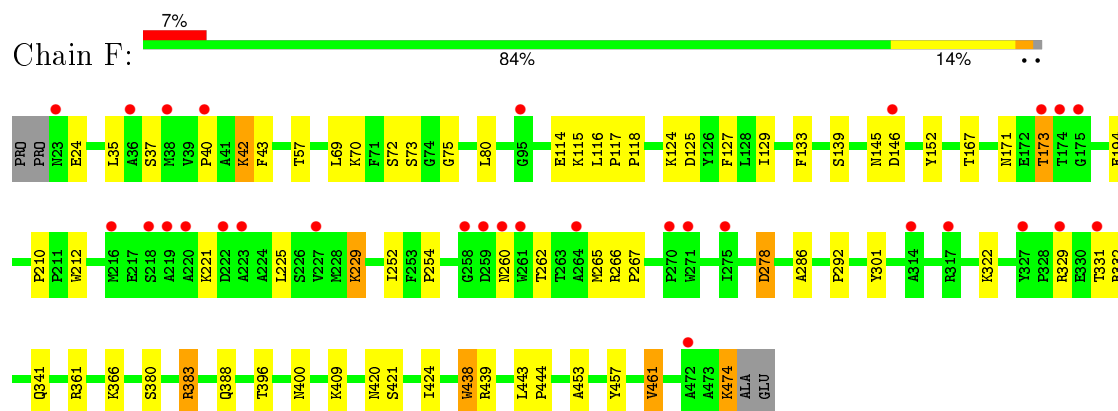




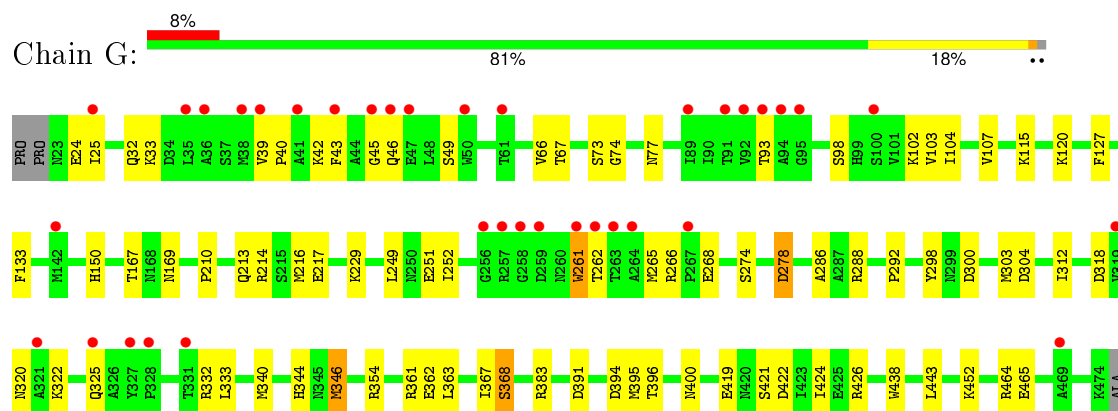
• Molecule 1: GH10 Xylanase



• Molecule 1: GH10 Xylanase



• Molecule 1: GH10 Xylanase



Chain H:

5% 89% 10%

L235 L226 V227 T233 T237 I252 E257 G258 I259 M265 R266 R267 E268 M269 P270 K273 G276 F279 Y284 K377 Q325 A326 Y327 P328 R329 E330 T331 L334 W379 R383 D391 S437 W438 L443 P444 L445 A473 K474 ALA GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.69 Å 86.96 Å 246.43 Å 92.96° 90.86° 108.56°	Depositor
Resolution (Å)	49.08 – 2.00 49.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.08-2.00) 95.5 (49.08-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.219 , 0.266 0.218 , 0.266	Depositor DCC
$R_{free}$ test set	14946 reflections (5.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.8	EDS
Estimated twinning fraction	0.129 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 286977 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: GOL, 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	0.46	0/3640	0.59	0/4932
1	B	0.41	0/3654	0.57	0/4950
1	C	0.52	0/3654	0.63	0/4950
1	D	0.51	0/3654	0.62	0/4950
1	E	0.45	0/3654	0.58	0/4950
1	F	0.40	0/3654	0.54	0/4950
1	G	0.41	0/3654	0.57	1/4950 (0.0%)
1	H	0.43	0/3654	0.59	1/4950 (0.0%)
All	All	0.45	0/29218	0.59	2/39582 (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	C	0	1
1	D	0	1
1	E	0	1
1	H	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	225	LEU	CA-CB-CG	5.91	128.88	115.30
1	G	45	GLY	N-CA-C	-5.89	98.39	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	43	PHE	Peptide
1	D	473	ALA	Peptide
1	E	46	GLN	Peptide
1	H	220	ALA	Peptide
1	H	473	ALA	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	3558	0	3474	40	0
1	B	3572	0	3492	38	0
1	C	3572	0	3492	34	0
1	D	3572	0	3492	23	0
1	E	3572	0	3492	38	0
1	F	3572	0	3492	41	0
1	G	3572	0	3492	64	0
1	H	3572	0	3492	16	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	1	0
2	E	5	0	0	1	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	18	0	24	3	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	G	12	0	16	0	0
3	H	12	0	16	2	0
4	A	248	0	0	4	0
4	B	216	0	0	3	0
4	C	457	0	0	6	0
4	D	412	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	207	0	0	4	0
4	F	177	0	0	5	0
4	G	134	0	0	4	0
4	H	297	0	0	0	0
All	All	30836	0	28006	291	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 5.

All (291) 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:G:24:GLU:CG	1:G:102:LYS:HE2	1.77	1.14
1:G:24:GLU:CG	1:G:102:LYS:CE	2.26	1.13
1:G:24:GLU:HG3	1:G:102:LYS:HE2	1.20	1.10
1:G:24:GLU:HG2	1:G:102:LYS:HE3	1.40	1.03
1:F:75:GLY:HA2	1:F:400:ASN:HB2	1.43	1.00
1:B:75:GLY:HA2	1:B:400:ASN:HB2	1.44	0.98
1:C:395:MET:SD	4:C:1040:HOH:O	2.22	0.97
1:G:24:GLU:HG2	1:G:102:LYS:CE	1.93	0.94
1:A:75:GLY:HA2	1:A:400:ASN:HB2	1.49	0.93
1:H:167:THR:HG23	1:H:210:PRO:HG3	1.50	0.91
1:E:42:LYS:HG3	1:E:43:PHE:CD2	2.05	0.91
1:B:471:LYS:HG2	1:B:472:ALA:N	1.84	0.90
1:F:474:LYS:H	1:F:474:LYS:HE3	1.38	0.89
1:G:24:GLU:CG	1:G:102:LYS:HE3	1.98	0.89
1:C:464:ARG:NH1	1:C:465:GLU:OE2	2.06	0.88
1:F:361:ARG:HH21	1:F:420:ASN:HD22	1.22	0.87
1:E:75:GLY:HA2	1:E:400:ASN:HB2	1.56	0.85
1:A:324:LYS:HE2	1:A:324:LYS:HA	1.59	0.84
1:E:42:LYS:HG3	1:E:43:PHE:HD2	1.46	0.78
1:G:24:GLU:HG3	1:G:102:LYS:CE	2.00	0.78
1:B:223:ALA:O	1:B:227:VAL:HG12	1.85	0.77
1:C:464:ARG:HH11	1:C:464:ARG:HG2	1.51	0.76
1:F:260:ASN:ND2	1:F:262:THR:OG1	2.20	0.75
1:A:202:THR:HG22	1:A:247:ASP:HB2	1.67	0.74
1:G:251:GLU:O	1:G:266:ARG:NH1	2.21	0.73
1:F:388:GLN:NE2	4:F:627:HOH:O	2.21	0.73
1:G:229:LYS:HG3	1:G:286:ALA:CB	2.20	0.71
3:C:504:GOL:C1	4:C:940:HOH:O	2.38	0.71
3:C:504:GOL:H12	4:C:940:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:NH1	4:D:672:HOH:O	2.24	0.70
1:B:199:HIS:NE2	1:B:247:ASP:OD1	2.24	0.70
1:G:229:LYS:HG3	1:G:286:ALA:HB2	1.74	0.69
1:E:42:LYS:HG3	1:E:43:PHE:CE2	2.27	0.69
1:B:361:ARG:HH21	1:B:420:ASN:HD22	1.41	0.69
1:G:93:THR:HG22	1:G:98:SER:HB3	1.75	0.68
1:G:288:ARG:NH2	1:G:333:LEU:O	2.27	0.67
1:G:320:ASN:HB3	1:G:333:LEU:HD11	1.76	0.67
1:C:464:ARG:NH1	1:C:464:ARG:HG2	2.08	0.67
1:E:371:GLU:HG2	1:E:430:TRP:CE3	2.31	0.66
1:H:143:MET:HG3	1:H:194:GLU:HG3	1.78	0.66
1:B:23:ASN:OD1	1:B:23:ASN:C	2.33	0.66
1:D:464:ARG:HG3	1:D:465:GLU:N	2.09	0.66
1:A:143:MET:HG3	1:A:194:GLU:HG3	1.78	0.66
1:B:333:LEU:H	1:B:333:LEU:HD12	1.59	0.65
1:A:324:LYS:CE	1:A:324:LYS:HA	2.25	0.65
1:D:78:LEU:HB2	1:D:81:LYS:HD3	1.77	0.65
1:C:395:MET:HE2	4:C:942:HOH:O	1.95	0.65
1:C:464:ARG:HH11	1:C:464:ARG:CG	2.09	0.65
1:E:23:ASN:O	1:E:23:ASN:ND2	2.30	0.65
1:D:346:MET:SD	4:D:946:HOH:O	2.54	0.64
1:F:396:THR:HG21	1:F:443:LEU:HD11	1.78	0.64
1:A:324:LYS:HE2	1:A:324:LYS:CA	2.21	0.63
1:D:143:MET:HG3	1:D:194:GLU:HG3	1.80	0.63
1:F:221:LYS:NZ	1:F:278:ASP:OD2	2.32	0.62
1:B:75:GLY:CA	1:B:400:ASN:HB2	2.26	0.62
1:F:383:ARG:NH2	4:F:627:HOH:O	2.31	0.62
1:G:367:ILE:HB	1:G:424:ILE:HG12	1.82	0.62
1:A:383:ARG:NH2	4:A:750:HOH:O	2.32	0.61
1:B:292:PRO:O	1:B:332:ARG:NH1	2.23	0.60
1:A:423:ILE:HD12	1:A:424:ILE:HG13	1.83	0.60
1:B:23:ASN:ND2	4:B:732:HOH:O	2.34	0.60
1:H:214:ARG:NH2	1:H:268:GLU:O	2.29	0.60
1:F:457:TYR:O	1:F:461:VAL:HG12	2.00	0.60
1:B:78:LEU:HB2	1:B:81:LYS:HD3	1.83	0.60
1:B:191:ALA:HB3	1:B:198:ILE:HD11	1.84	0.60
1:F:329:ARG:HH11	1:F:329:ARG:HG2	1.66	0.60
1:B:224:ALA:HA	1:B:227:VAL:CG1	2.32	0.60
1:E:401:ARG:NH2	2:E:501:SO4:O3	2.33	0.60
1:A:141:SER:HB3	4:A:837:HOH:O	2.01	0.60
1:G:261:TRP:HZ3	1:G:318:ASP:OD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASP:OD2	1:C:259:ASP:N	2.32	0.59
1:D:122:HIS:NE2	1:D:464:ARG:HG2	2.17	0.59
1:B:348:VAL:O	1:B:409:LYS:NZ	2.28	0.58
1:F:388:GLN:OE1	1:F:439:ARG:NH1	2.36	0.58
1:A:249:LEU:HD11	1:A:252:ILE:HD12	1.84	0.58
1:C:143:MET:HG3	1:C:194:GLU:HG3	1.85	0.58
1:B:443:LEU:N	1:B:444:PRO:HD3	2.18	0.58
1:C:388:GLN:HG3	3:C:502:GOL:H2	1.85	0.58
1:F:438:TRP:CD1	1:F:439:ARG:HG2	2.39	0.57
1:G:24:GLU:CD	1:G:102:LYS:CE	2.72	0.57
1:F:361:ARG:HH21	1:F:420:ASN:ND2	2.00	0.57
1:F:114:GLU:OE1	1:F:146:ASP:HB2	2.05	0.57
1:D:303:MET:HE2	1:D:312:ILE:HD13	1.87	0.57
1:B:468:GLU:HA	1:B:471:LYS:HD3	1.86	0.57
1:B:255:ASP:OD2	1:B:257:ARG:NE	2.36	0.57
1:A:354:ARG:NH2	1:A:419:GLU:OE1	2.38	0.56
1:H:252:ILE:HG13	1:H:265:MET:HG2	1.86	0.56
1:G:452:LYS:NZ	4:G:675:HOH:O	2.38	0.56
1:A:278:ASP:OD1	1:A:322:LYS:NZ	2.38	0.56
1:A:354:ARG:NH1	4:A:606:HOH:O	2.37	0.56
1:F:443:LEU:N	1:F:444:PRO:HD3	2.21	0.56
1:C:167:THR:HG23	1:C:210:PRO:HG3	1.87	0.55
1:A:320:ASN:HB3	1:A:333:LEU:HD11	1.89	0.55
1:B:388:GLN:O	1:B:392:LYS:NZ	2.31	0.55
1:A:323:TYR:CD1	1:A:334:LEU:HD22	2.42	0.55
1:B:249:LEU:HD11	1:B:252:ILE:HD13	1.88	0.55
1:E:342:SER:OG	1:E:369:VAL:HG13	2.07	0.55
1:A:201:HIS:ND1	1:A:202:THR:HG23	2.21	0.54
1:G:261:TRP:CD1	1:G:261:TRP:C	2.79	0.54
1:E:443:LEU:N	1:E:444:PRO:HD3	2.22	0.54
1:F:278:ASP:OD1	1:F:278:ASP:N	2.41	0.54
1:G:304:ASP:N	4:G:601:HOH:O	2.40	0.54
1:F:474:LYS:N	1:F:474:LYS:HE3	2.17	0.54
1:D:348:VAL:O	1:D:409:LYS:NZ	2.40	0.54
1:E:42:LYS:C	1:E:43:PHE:CD2	2.81	0.53
1:H:437:SER:HB2	1:H:445:LEU:HD11	1.91	0.53
1:G:249:LEU:HD11	1:G:252:ILE:HD13	1.90	0.53
1:H:233:THR:O	1:H:237:THR:OG1	2.24	0.53
1:B:199:HIS:ND1	1:B:245:SER:OG	2.30	0.52
1:C:186:ARG:NE	3:H:503:GOL:O1	2.34	0.52
1:A:298:TYR:OH	1:A:300:ASP:OD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LYS:NZ	2:D:501:SO4:O3	2.31	0.52
1:G:25:ILE:HD11	1:G:33:LYS:HE3	1.91	0.52
1:A:373:ASP:HB2	1:A:444:PRO:HB2	1.91	0.52
1:E:346:MET:O	1:E:409:LYS:NZ	2.42	0.52
1:F:72:SER:OG	1:F:73:SER:N	2.43	0.52
1:A:114:GLU:OE1	1:A:146:ASP:HB2	2.10	0.51
1:F:145:ASN:ND2	4:F:766:HOH:O	2.32	0.51
1:H:443:LEU:N	1:H:444:PRO:HD3	2.25	0.51
1:F:116:LEU:HD11	1:F:453:ALA:HB2	1.93	0.51
1:B:255:ASP:OD1	1:B:255:ASP:N	2.43	0.51
1:G:24:GLU:CD	1:G:102:LYS:HE3	2.32	0.51
1:F:254:PRO:HG3	1:F:266:ARG:HG2	1.93	0.51
1:A:57:THR:HA	1:A:70:LYS:HG2	1.93	0.50
1:A:167:THR:HG23	1:A:210:PRO:HG3	1.92	0.50
1:A:122:HIS:CE1	1:A:464:ARG:HE	2.29	0.50
1:C:79:PHE:HB2	1:C:403:ILE:HD11	1.93	0.50
1:H:379:TRP:HE1	1:H:383:ARG:NH2	2.09	0.50
1:E:42:LYS:O	1:E:43:PHE:CD2	2.64	0.50
1:B:199:HIS:CE1	1:B:245:SER:HG	2.26	0.50
1:G:368:SER:OG	1:G:426:ARG:HB3	2.12	0.49
1:C:55:PRO:HG2	1:E:182:SER:HB2	1.94	0.49
1:F:420:ASN:O	1:F:424:ILE:HG22	2.13	0.49
1:A:443:LEU:N	1:A:444:PRO:HD3	2.27	0.49
1:C:87:GLU:OE2	1:G:73:SER:HB2	2.11	0.49
1:G:229:LYS:HG3	1:G:286:ALA:HB1	1.92	0.49
1:B:23:ASN:OD1	1:B:23:ASN:O	2.30	0.49
1:G:278:ASP:N	1:G:278:ASP:OD1	2.46	0.49
1:H:55:PRO:HG3	3:H:503:GOL:H2	1.95	0.49
1:F:229:LYS:HE2	1:F:286:ALA:HB2	1.94	0.49
1:C:462:ARG:NH1	4:C:955:HOH:O	2.31	0.48
1:B:361:ARG:HH21	1:B:420:ASN:ND2	2.08	0.48
1:B:288:ARG:NH2	1:B:336:GLU:OE2	2.46	0.48
1:C:35:LEU:HG	1:C:38:MET:HE3	1.95	0.48
1:G:354:ARG:NH2	1:G:419:GLU:OE1	2.45	0.48
1:F:80:LEU:HD11	1:F:396:THR:HG22	1.96	0.48
1:A:75:GLY:CA	1:A:400:ASN:HB2	2.32	0.48
1:G:43:PHE:O	1:G:46:GLN:HB2	2.14	0.48
1:D:126:TYR:O	4:D:894:HOH:O	2.20	0.48
1:F:57:THR:HA	1:F:70:LYS:HG2	1.95	0.48
1:D:443:LEU:N	1:D:444:PRO:HD3	2.29	0.48
1:E:242:LYS:NZ	4:E:616:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:PHE:HZ	1:E:97:GLN:OE1	1.97	0.47
1:E:75:GLY:CA	1:E:400:ASN:HB2	2.37	0.47
1:H:284:TYR:HB3	1:H:334:LEU:HG	1.96	0.47
1:D:167:THR:HG23	1:D:210:PRO:HG3	1.96	0.47
1:G:396:THR:HG21	1:G:443:LEU:HD11	1.95	0.47
1:D:107:VAL:HG21	1:D:400:ASN:OD1	2.15	0.47
1:C:396:THR:HG21	1:C:443:LEU:HD11	1.97	0.47
1:C:25:ILE:HD11	1:C:103:VAL:HG22	1.95	0.47
1:C:298:TYR:OH	1:C:300:ASP:OD2	2.27	0.47
1:G:322:LYS:HG3	1:G:325:GLN:NE2	2.30	0.47
1:A:261:TRP:CE2	1:A:315:MET:HA	2.50	0.47
1:A:199:HIS:HE2	1:A:247:ASP:CG	2.17	0.47
1:G:210:PRO:HG2	1:G:213:GLN:HG3	1.97	0.47
1:E:371:GLU:HG2	1:E:430:TRP:CZ3	2.50	0.47
1:A:252:ILE:CD1	1:A:279:PHE:HZ	2.28	0.46
1:H:214:ARG:HE	1:H:214:ARG:HA	1.79	0.46
1:G:167:THR:HG23	1:G:210:PRO:HG3	1.96	0.46
1:C:379:TRP:O	1:C:383:ARG:HB2	2.15	0.46
1:E:240:LYS:HE2	4:E:788:HOH:O	2.16	0.46
1:F:40:PRO:HB3	1:F:42:LYS:HD2	1.97	0.46
1:C:252:ILE:HG13	1:C:265:MET:HB3	1.96	0.46
1:G:346:MET:HE2	1:G:346:MET:HA	1.98	0.46
1:A:230:LYS:NZ	1:A:234:GLU:OE2	2.45	0.46
1:D:255:ASP:OD2	1:D:257:ARG:NE	2.45	0.46
1:E:388:GLN:OE1	1:E:439:ARG:NH2	2.48	0.46
1:B:297:TYR:OH	1:B:425:GLU:OE2	2.20	0.46
1:B:199:HIS:HE2	1:B:247:ASP:CG	2.17	0.46
1:F:292:PRO:O	1:F:332:ARG:NH1	2.45	0.46
1:A:420:ASN:HB3	1:A:423:ILE:HD11	1.97	0.46
1:G:74:GLY:O	1:G:77:ASN:HB2	2.15	0.46
1:B:260:ASN:OD1	1:B:262:THR:OG1	2.34	0.46
1:F:421:SER:HA	1:F:424:ILE:HG23	1.98	0.45
1:G:115:LYS:HA	1:G:115:LYS:HD3	1.69	0.45
1:A:333:LEU:HA	1:A:333:LEU:HD12	1.63	0.45
1:F:171:ASN:OD1	1:F:173:THR:HG23	2.16	0.45
1:E:225:LEU:O	1:E:229:LYS:HG3	2.16	0.45
1:D:284:TYR:HB3	1:D:334:LEU:HG	1.98	0.45
1:D:35:LEU:HD12	1:D:90:ILE:HG21	1.98	0.45
1:C:281:TYR:CD2	1:C:322:LYS:HE3	2.51	0.45
1:G:32:GLN:HG2	1:G:67:THR:OG1	2.17	0.45
1:E:222:ASP:OD1	1:E:223:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:TYR:OH	4:B:705:HOH:O	2.21	0.45
1:G:107:VAL:HG21	1:G:400:ASN:OD1	2.16	0.45
1:C:373:ASP:HB2	1:C:444:PRO:HB2	1.99	0.44
1:A:281:TYR:CG	1:A:322:LYS:HD3	2.52	0.44
1:E:143:MET:HG3	1:E:194:GLU:HG3	1.99	0.44
1:H:210:PRO:HG2	1:H:213:GLN:HG3	2.00	0.44
1:A:202:THR:HG22	1:A:247:ASP:CB	2.41	0.44
1:A:249:LEU:HD21	1:A:252:ILE:HD13	1.99	0.44
1:B:132:ILE:HG12	1:B:431:GLY:HA2	1.99	0.44
1:F:322:LYS:NZ	4:F:631:HOH:O	2.50	0.44
1:A:338:ILE:HG21	1:A:360:TYR:CE2	2.53	0.44
1:A:248:VAL:HB	1:A:284:TYR:CZ	2.53	0.44
1:G:229:LYS:NZ	1:G:229:LYS:HB2	2.32	0.44
1:G:361:ARG:HH22	1:G:422:ASP:CG	2.21	0.44
1:B:443:LEU:O	1:B:454:LYS:NZ	2.50	0.44
1:F:42:LYS:O	1:F:43:PHE:C	2.55	0.44
1:E:374:ILE:O	1:E:444:PRO:HA	2.18	0.44
1:G:344:HIS:HE1	4:G:601:HOH:O	2.01	0.44
1:E:303:MET:HE2	1:E:312:ILE:HD13	2.00	0.44
1:C:55:PRO:HG2	1:E:182:SER:CB	2.48	0.43
1:D:373:ASP:HB2	1:D:444:PRO:HB2	1.99	0.43
1:E:386:THR:HG22	1:E:395:MET:HB2	2.00	0.43
1:A:323:TYR:CG	1:A:334:LEU:HB2	2.53	0.43
1:G:383:ARG:HA	1:G:383:ARG:HD3	1.95	0.43
1:E:23:ASN:ND2	1:E:23:ASN:C	2.70	0.43
1:F:117:PRO:HA	1:F:118:PRO:HD3	1.92	0.43
1:E:62:ASP:OD2	1:E:62:ASP:N	2.37	0.43
1:B:214:ARG:NH1	1:B:268:GLU:O	2.39	0.43
1:C:199:HIS:HE2	1:C:247:ASP:CG	2.22	0.43
1:G:346:MET:CE	1:G:346:MET:HA	2.49	0.43
1:C:225:LEU:HD23	1:C:275:ILE:HD13	2.00	0.43
1:B:420:ASN:ND2	4:B:772:HOH:O	2.46	0.43
1:A:204:LEU:HA	4:A:668:HOH:O	2.18	0.43
1:G:303:MET:HE2	1:G:312:ILE:HD13	2.00	0.43
1:G:24:GLU:HG2	1:G:104:ILE:HD11	2.01	0.43
1:G:49:SER:N	1:G:93:THR:O	2.49	0.43
1:E:373:ASP:HB2	1:E:444:PRO:HB2	2.01	0.43
1:C:323:TYR:CG	1:C:334:LEU:HB2	2.53	0.43
1:G:24:GLU:CD	1:G:102:LYS:HE2	2.33	0.42
1:G:24:GLU:HG3	1:G:102:LYS:HB3	2.01	0.42
1:B:396:THR:HG21	1:B:443:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:VAL:HA	1:G:40:PRO:HD3	1.90	0.42
1:E:383:ARG:NH2	4:E:602:HOH:O	2.38	0.42
1:E:121:ASP:O	1:E:124:LYS:HG2	2.19	0.42
1:G:66:VAL:HG21	1:G:103:VAL:HG21	2.01	0.42
1:G:422:ASP:N	1:G:422:ASP:OD1	2.52	0.42
1:F:212:TRP:HB3	4:F:722:HOH:O	2.19	0.42
1:D:204:LEU:HD22	1:D:271:TRP:CD1	2.55	0.42
1:F:301:TYR:HB3	1:F:341:GLN:OE1	2.19	0.42
1:F:167:THR:HG23	1:F:210:PRO:HG3	2.02	0.42
1:B:373:ASP:HB2	1:B:444:PRO:HB2	2.02	0.42
1:C:172:GLU:OE2	4:C:1014:HOH:O	2.22	0.42
1:H:115:LYS:HD3	1:H:115:LYS:HA	1.84	0.42
1:D:122:HIS:HE2	1:D:464:ARG:HG2	1.84	0.42
1:C:400:ASN:HA	1:C:403:ILE:HD12	2.01	0.42
1:F:124:LYS:HG3	1:F:125:ASP:N	2.35	0.42
1:E:159:ASN:HB3	1:G:395:MET:SD	2.60	0.42
1:G:49:SER:HB2	1:G:93:THR:OG1	2.19	0.41
1:G:261:TRP:CG	1:G:262:THR:N	2.87	0.41
1:D:281:TYR:CE1	1:D:322:LYS:HG2	2.55	0.41
1:F:229:LYS:HE2	1:F:286:ALA:CB	2.50	0.41
1:B:24:GLU:HG2	1:B:24:GLU:H	1.59	0.41
1:D:346:MET:O	1:D:409:LYS:HE3	2.19	0.41
1:H:188:VAL:O	1:H:192:ILE:HG12	2.20	0.41
1:A:346:MET:HE2	1:A:405:ASP:HB3	2.03	0.41
1:E:23:ASN:O	1:E:101:VAL:HG23	2.21	0.41
1:F:266:ARG:HA	1:F:267:PRO:HD2	1.92	0.41
1:E:412:GLU:HA	1:E:415:LYS:HE2	2.02	0.41
1:G:120:LYS:HE2	1:G:150:HIS:O	2.20	0.41
1:G:252:ILE:HG13	1:G:265:MET:HB3	2.03	0.41
1:G:292:PRO:O	1:G:332:ARG:NH1	2.49	0.41
1:G:24:GLU:OE2	1:G:102:LYS:CE	2.68	0.41
1:G:303:MET:SD	1:G:340:MET:HG2	2.61	0.41
1:A:371:GLU:OE2	3:A:502:GOL:O1	2.37	0.41
1:E:435:ARG:NH1	4:E:770:HOH:O	2.38	0.41
1:E:89:ILE:HD13	1:E:102:LYS:HA	2.02	0.41
1:C:298:TYR:CE2	1:C:300:ASP:HB2	2.55	0.41
1:D:216:MET:CE	1:D:224:ALA:HA	2.51	0.41
1:F:252:ILE:HG13	1:F:265:MET:HG2	2.02	0.41
1:E:136:ARG:NH1	1:G:394:ASP:HB2	2.36	0.41
1:B:253:PHE:HA	1:B:254:PRO:HD3	1.85	0.41
1:G:93:THR:HG22	1:G:98:SER:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:THR:HG21	1:D:443:LEU:HD11	2.03	0.41
1:A:369:VAL:CG1	1:A:372:LEU:HB2	2.50	0.41
1:C:266:ARG:HD3	1:C:268:GLU:OE1	2.19	0.41
1:G:216:MET:O	1:G:274:SER:HB3	2.21	0.41
1:C:346:MET:HE1	1:C:405:ASP:HB3	2.02	0.41
1:G:421:SER:O	4:G:692:HOH:O	2.22	0.40
1:E:23:ASN:N	1:E:23:ASN:HD22	2.18	0.40
1:C:383:ARG:HB3	1:C:383:ARG:HE	1.65	0.40
1:G:298:TYR:CE2	1:G:300:ASP:HB2	2.56	0.40
1:B:379:TRP:HE1	1:B:383:ARG:CZ	2.35	0.40
1:H:117:PRO:HA	1:H:118:PRO:HD3	1.95	0.40
1:G:214:ARG:NH1	1:G:217:GLU:OE1	2.55	0.40
1:F:129:ILE:HG22	1:F:152:TYR:HD1	1.86	0.40
1:D:24:GLU:HG2	1:D:24:GLU:H	1.67	0.40
1:F:35:LEU:O	1:F:37:SER:O	2.39	0.40
1:H:212:TRP:O	1:H:216:MET:HG2	2.22	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	448/456 (98%)	441 (98%)	7 (2%)	0	100	100
1	B	450/456 (99%)	438 (97%)	12 (3%)	0	100	100
1	C	450/456 (99%)	442 (98%)	8 (2%)	0	100	100
1	D	450/456 (99%)	439 (98%)	11 (2%)	0	100	100
1	E	450/456 (99%)	438 (97%)	11 (2%)	1 (0%)	52	48
1	F	450/456 (99%)	442 (98%)	8 (2%)	0	100	100
1	G	450/456 (99%)	436 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	450/456 (99%)	443 (98%)	7 (2%)	0	100	100
All	All	3598/3648 (99%)	3519 (98%)	78 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	43	PHE

### 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	377/381 (99%)	362 (96%)	15 (4%)	38	33
1	B	378/381 (99%)	358 (95%)	20 (5%)	28	22
1	C	378/381 (99%)	365 (97%)	13 (3%)	44	41
1	D	378/381 (99%)	367 (97%)	11 (3%)	50	49
1	E	378/381 (99%)	361 (96%)	17 (4%)	34	29
1	F	378/381 (99%)	358 (95%)	20 (5%)	28	22
1	G	378/381 (99%)	363 (96%)	15 (4%)	38	33
1	H	378/381 (99%)	362 (96%)	16 (4%)	36	31
All	All	3023/3048 (99%)	2896 (96%)	127 (4%)	36	31

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	35	LEU
1	A	37	SER
1	A	90	ILE
1	A	114	GLU
1	A	127	PHE
1	A	133	PHE

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Mol	Chain	Res	Type
1	A	142	MET
1	A	167	THR
1	A	169	ASN
1	A	218	SER
1	A	225	LEU
1	A	257	ARG
1	A	324	LYS
1	A	438	TRP
1	B	23	ASN
1	B	24	GLU
1	B	37	SER
1	B	81	LYS
1	B	127	PHE
1	B	133	PHE
1	B	142	MET
1	B	167	THR
1	B	218	SER
1	B	222	ASP
1	B	225	LEU
1	B	227	VAL
1	B	279	PHE
1	B	288	ARG
1	B	333	LEU
1	B	363	LEU
1	B	409	LYS
1	B	438	TRP
1	B	464	ARG
1	B	471	LYS
1	C	23	ASN
1	C	24	GLU
1	C	38	MET
1	C	110	LYS
1	C	127	PHE
1	C	133	PHE
1	C	257	ARG
1	C	259	ASP
1	C	260	ASN
1	C	279	PHE
1	C	383	ARG
1	C	438	TRP
1	C	464	ARG
1	D	38	MET

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Mol	Chain	Res	Type
1	D	127	PHE
1	D	133	PHE
1	D	146	ASP
1	D	160	HIS
1	D	176	GLU
1	D	257	ARG
1	D	279	PHE
1	D	391	ASP
1	D	438	TRP
1	D	464	ARG
1	E	23	ASN
1	E	24	GLU
1	E	25	ILE
1	E	43	PHE
1	E	47	GLU
1	E	60	VAL
1	E	93	THR
1	E	96	LYS
1	E	125	ASP
1	E	127	PHE
1	E	133	PHE
1	E	325	GLN
1	E	362	GLU
1	E	383	ARG
1	E	391	ASP
1	E	438	TRP
1	E	444	PRO
1	F	24	GLU
1	F	42	LYS
1	F	69	LEU
1	F	115	LYS
1	F	127	PHE
1	F	133	PHE
1	F	139	SER
1	F	173	THR
1	F	194	GLU
1	F	225	LEU
1	F	229	LYS
1	F	278	ASP
1	F	331	THR
1	F	366	LYS
1	F	380	SER

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Mol	Chain	Res	Type
1	F	383	ARG
1	F	409	LYS
1	F	438	TRP
1	F	461	VAL
1	F	474	LYS
1	G	42	LYS
1	G	127	PHE
1	G	133	PHE
1	G	169	ASN
1	G	261	TRP
1	G	268	GLU
1	G	278	ASP
1	G	346	MET
1	G	362	GLU
1	G	363	LEU
1	G	368	SER
1	G	391	ASP
1	G	438	TRP
1	G	464	ARG
1	G	465	GLU
1	H	24	GLU
1	H	42	LYS
1	H	63	LYS
1	H	91	THR
1	H	127	PHE
1	H	133	PHE
1	H	160	HIS
1	H	225	LEU
1	H	273	LYS
1	H	279	PHE
1	H	325	GLN
1	H	329	ARG
1	H	331	THR
1	H	391	ASP
1	H	438	TRP
1	H	474	LYS

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

Mol	Chain	Res	Type
1	B	420	ASN
1	C	169	ASN

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Mol	Chain	Res	Type
1	E	325	GLN
1	F	165	ASN
1	F	206	HIS
1	F	260	ASN
1	F	420	ASN
1	G	320	ASN
1	G	325	GLN
1	G	420	ASN
1	H	299	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

23 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	501	-	4,4,4	0.14	0	6,6,6	0.31	0
3	GOL	A	502	-	5,5,5	0.34	0	5,5,5	1.11	1 (20%)
2	SO4	B	501	-	4,4,4	0.20	0	6,6,6	0.14	0
2	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.07	0
3	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.17	0
3	GOL	C	502	-	5,5,5	0.91	1 (20%)	5,5,5	0.51	0
3	GOL	C	503	-	5,5,5	0.22	0	5,5,5	0.44	0
3	GOL	C	504	-	5,5,5	0.78	0	5,5,5	1.12	0
2	SO4	D	501	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	D	502	-	4,4,4	0.22	0	6,6,6	0.14	0
3	GOL	D	503	-	5,5,5	0.52	0	5,5,5	1.12	0
2	SO4	E	501	-	4,4,4	0.15	0	6,6,6	0.07	0
3	GOL	E	502	-	5,5,5	0.32	0	5,5,5	0.29	0
2	SO4	F	501	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	F	502	-	4,4,4	0.10	0	6,6,6	0.25	0
2	SO4	G	501	-	4,4,4	0.18	0	6,6,6	0.18	0
3	GOL	G	502	-	5,5,5	0.26	0	5,5,5	0.74	0
3	GOL	G	503	-	5,5,5	0.31	0	5,5,5	0.24	0
2	SO4	H	501	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	H	502	-	4,4,4	0.15	0	6,6,6	0.13	0
3	GOL	H	503	-	5,5,5	0.80	0	5,5,5	1.16	0
3	GOL	H	504	-	5,5,5	0.31	0	5,5,5	0.44	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	501	-	-	0/0/0/0	0/0/0/0
3	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
3	GOL	C	502	-	-	0/4/4/4	0/0/0/0
3	GOL	C	503	-	-	0/4/4/4	0/0/0/0
3	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
3	GOL	D	503	-	-	0/4/4/4	0/0/0/0
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
3	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	SO4	F	501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	501	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	502	-	-	0/4/4/4	0/0/0/0
3	GOL	G	503	-	-	0/4/4/4	0/0/0/0
2	SO4	H	501	-	-	0/0/0/0	0/0/0/0
2	SO4	H	502	-	-	0/0/0/0	0/0/0/0
3	GOL	H	503	-	-	0/4/4/4	0/0/0/0
3	GOL	H	504	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	GOL	O2-C2	-2.01	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	GOL	O3-C3-C2	-2.01	100.45	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
3	C	502	GOL	1	0
3	C	504	GOL	2	0
2	D	501	SO4	1	0
2	E	501	SO4	1	0
3	H	503	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/456 (98%)	-0.03	3 (0%) 89 89	14, 28, 45, 56	0
1	B	452/456 (99%)	0.17	10 (2%) 65 66	19, 35, 52, 74	0
1	C	452/456 (99%)	-0.18	3 (0%) 89 89	10, 18, 34, 57	0
1	D	452/456 (99%)	-0.24	1 (0%) 95 95	10, 20, 33, 51	0
1	E	452/456 (99%)	0.22	21 (4%) 36 38	16, 29, 62, 96	0
1	F	452/456 (99%)	0.33	30 (6%) 22 22	20, 35, 56, 76	0
1	G	452/456 (99%)	0.51	36 (7%) 15 16	19, 36, 61, 82	0
1	H	452/456 (99%)	0.17	23 (5%) 32 33	16, 29, 53, 65	0
All	All	3614/3648 (99%)	0.12	127 (3%) 48 49	10, 28, 52, 96	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	PRO	6.5
1	E	38	MET	5.2
1	E	43	PHE	4.6
1	G	261	TRP	4.3
1	E	94	ALA	4.2
1	E	44	ALA	4.1
1	F	218	SER	4.1
1	G	39	VAL	4.0
1	G	257	ARG	3.9
1	G	43	PHE	3.9
1	G	263	THR	3.9
1	B	220	ALA	3.9
1	G	331	THR	3.9
1	F	258	GLY	3.9
1	E	49	SER	3.8
1	D	473	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	220	ALA	3.7
1	E	39	VAL	3.7
1	H	270	PRO	3.6
1	F	95	GLY	3.6
1	F	219	ALA	3.6
1	H	174	THR	3.6
1	F	174	THR	3.6
1	G	95	GLY	3.5
1	F	173	THR	3.5
1	G	259	ASP	3.4
1	E	35	LEU	3.4
1	B	473	ALA	3.4
1	F	264	ALA	3.3
1	F	270	PRO	3.3
1	E	95	GLY	3.3
1	E	98	SER	3.3
1	H	220	ALA	3.2
1	F	216	MET	3.2
1	B	174	THR	3.2
1	G	38	MET	3.2
1	F	38	MET	3.1
1	F	223	ALA	3.1
1	F	261	TRP	3.1
1	E	50	TRP	3.0
1	G	41	ALA	3.0
1	G	325	GLN	3.0
1	F	175	GLY	3.0
1	E	103	VAL	3.0
1	G	91	THR	2.9
1	G	93	THR	2.9
1	E	65	ILE	2.9
1	F	314	ALA	2.9
1	G	94	ALA	2.9
1	H	258	GLY	2.9
1	C	23	ASN	2.9
1	H	267	PRO	2.9
1	G	262	THR	2.9
1	G	469	ALA	2.9
1	G	258	GLY	2.8
1	F	329	ARG	2.8
1	G	35	LEU	2.8
1	F	327	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	331	THR	2.8
1	E	259	ASP	2.8
1	E	37	SER	2.7
1	E	96	LYS	2.7
1	F	222	ASP	2.7
1	G	45	GLY	2.7
1	H	172	GLU	2.7
1	A	38	MET	2.7
1	H	257	ARG	2.7
1	E	93	THR	2.7
1	G	25	ILE	2.7
1	H	327	TYR	2.7
1	E	41	ALA	2.6
1	B	231	TYR	2.6
1	F	227	VAL	2.6
1	G	50	TRP	2.6
1	F	260	ASN	2.6
1	F	275	ILE	2.6
1	G	89	ILE	2.6
1	H	218	SER	2.6
1	H	173	THR	2.6
1	C	44	ALA	2.6
1	F	472	ALA	2.6
1	G	264	ALA	2.6
1	E	90	ILE	2.6
1	B	49	SER	2.5
1	B	173	THR	2.5
1	F	259	ASP	2.5
1	G	321	ALA	2.5
1	E	23	ASN	2.5
1	G	100	SER	2.4
1	G	328	PRO	2.4
1	H	225	LEU	2.4
1	G	47	GLU	2.4
1	G	61	THR	2.4
1	H	227	VAL	2.4
1	B	472	ALA	2.4
1	B	276	GLY	2.4
1	F	271	TRP	2.4
1	H	175	GLY	2.4
1	A	469	ALA	2.4
1	F	23	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	40	PRO	2.3
1	H	95	GLY	2.3
1	H	223	ALA	2.3
1	G	319	VAL	2.3
1	G	256	GLY	2.3
1	C	96	LYS	2.3
1	E	42	LYS	2.3
1	A	333	LEU	2.2
1	H	177	ILE	2.2
1	G	92	VAL	2.2
1	H	222	ASP	2.2
1	H	211	PRO	2.2
1	G	327	TYR	2.2
1	G	267	PRO	2.2
1	F	317	ARG	2.2
1	H	276	GLY	2.2
1	F	146	ASP	2.1
1	G	36	ALA	2.1
1	H	171	ASN	2.1
1	F	36	ALA	2.1
1	H	317	ARG	2.1
1	G	142	MET	2.1
1	G	46	GLN	2.0
1	B	35	LEU	2.0
1	B	223	ALA	2.0
1	H	259	ASP	2.0
1	H	96	LYS	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	H	503	6/6	0.86	0.18	4.13	21,25,32,35	0
3	GOL	C	504	6/6	0.84	0.18	3.34	12,21,25,30	0
3	GOL	A	502	6/6	0.87	0.15	2.05	20,21,25,26	0
3	GOL	D	503	6/6	0.93	0.14	1.31	13,17,17,22	0
3	GOL	C	503	6/6	0.82	0.13	1.26	24,29,31,39	0
3	GOL	E	502	6/6	0.96	0.15	0.92	22,23,24,25	0
3	GOL	B	503	6/6	0.93	0.12	0.92	25,29,30,32	0
3	GOL	G	502	6/6	0.94	0.14	0.57	24,30,31,38	0
3	GOL	G	503	6/6	0.87	0.18	0.23	43,49,50,51	0
3	GOL	H	504	6/6	0.94	0.12	0.10	23,29,32,33	0
2	SO4	A	501	5/5	0.94	0.12	-0.99	39,39,47,50	0
2	SO4	H	502	5/5	0.96	0.08	-1.51	35,35,39,41	0
2	SO4	F	501	5/5	0.98	0.08	-1.73	30,30,32,35	0
2	SO4	D	501	5/5	0.96	0.08	-1.94	23,27,29,33	0
2	SO4	E	501	5/5	0.96	0.10	-2.58	38,48,49,57	0
2	SO4	B	501	5/5	0.99	0.06	-3.07	31,35,38,43	0
2	SO4	B	502	5/5	0.98	0.07	-	32,40,40,42	0
2	SO4	H	501	5/5	0.96	0.09	-	38,40,45,46	0
2	SO4	F	502	5/5	0.85	0.11	-	41,45,57,61	0
2	SO4	G	501	5/5	0.97	0.08	-	45,51,51,55	0
2	SO4	D	502	5/5	0.98	0.09	-	29,32,36,38	0
3	GOL	C	502	6/6	0.76	0.21	-	24,36,38,47	0
2	SO4	C	501	5/5	0.98	0.09	-	30,36,45,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.