



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2017 – 02:15 PM EDT

PDB ID : 5WWP  
Title : Crystal structure of Middle East respiratory syndrome coronavirus helicase (MERS-CoV nsp13)  
Authors : Hao, W.; Wojdyla, J.A.; Zhao, R.; Han, R.; Das, R.; Zlatev, I.; Manoharan, M.; Wang, M.; Cui, S.  
Deposited on : 2017-01-03  
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029077

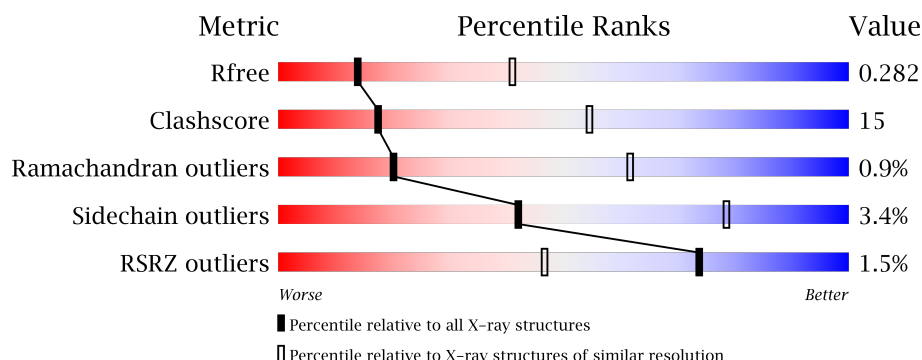
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	600	<div> <div>0.5%</div> <div>58%</div> <div>26%</div> <div>•</div> <div>14%</div> </div>
1	B	600	<div> <div>2%</div> <div>65%</div> <div>32%</div> <div>••</div> </div>

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
2	ZN	A	602	-	-	X	-
2	ZN	B	602	-	-	X	-
3	SO4	A	604	-	-	-	X
3	SO4	A	605	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8571 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 ORF1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	591	Total	C	N	O	S	0	0	0
			4579	2917	767	861	34			
1	A	515	Total	C	N	O	S	0	0	0
			3961	2514	669	744	34			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP K0BWD0
B	0	PRO	-	expression tag	UNP K0BWD0
A	-1	GLY	-	expression tag	UNP K0BWD0
A	0	PRO	-	expression tag	UNP K0BWD0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

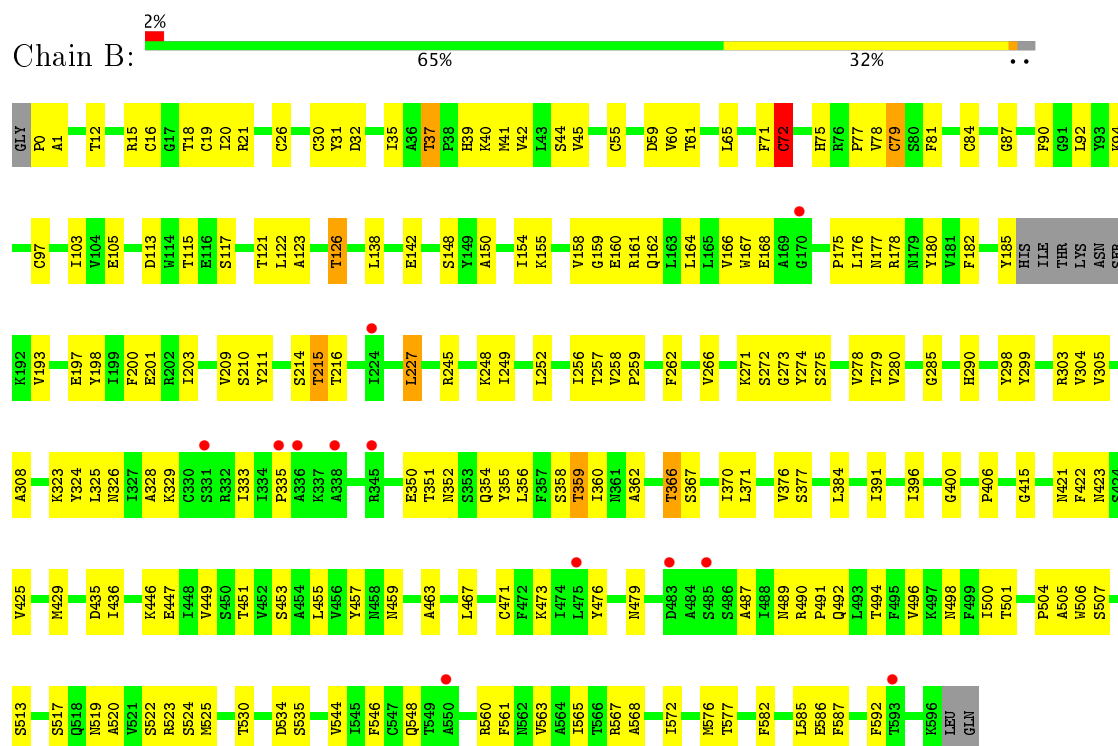


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

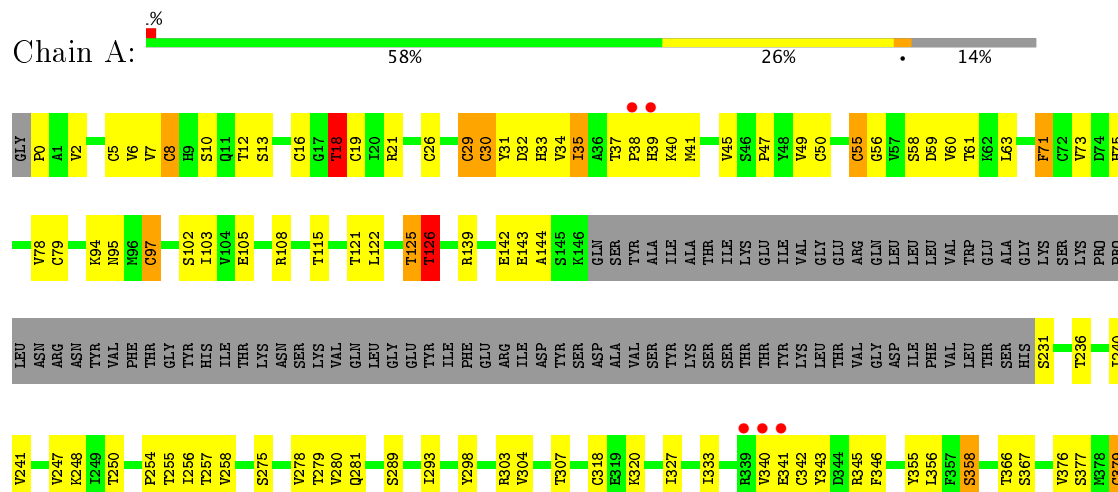
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ORF1ab



#### • Molecule 1: ORF1ab



I488	I489	Q492	K497	I506	S513	P514	P515	I516	S517	Q518	I519	Q531	T532	S535	S536	Q537	E540	V544	T549	T552	N556	N559	R560	F561	F562	P563	A564	I565	Q569	I572	L581	L585	F586	F587	F592	Q598
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.68Å 185.68Å 185.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.95 – 3.00 48.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.95-3.00) 99.6 (48.95-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.232 , 0.277 0.233 , 0.282	Depositor DCC
$R_{free}$ test set	1828 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, 0.333 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: ZN, 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	0.81	6/4046 (0.1%)	0.62	1/5504 (0.0%)
1	B	0.65	2/4679 (0.0%)	0.57	1/6364 (0.0%)
All	All	0.73	8/8725 (0.1%)	0.59	2/11868 (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	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	CYS	CB-SG	-8.26	1.68	1.82
1	A	8	CYS	CB-SG	-7.18	1.70	1.82
1	A	97	CYS	CB-SG	-7.02	1.70	1.82
1	A	30	CYS	CB-SG	-6.00	1.72	1.81
1	A	379	CYS	CB-SG	-5.47	1.72	1.81
1	A	236	THR	C-N	-5.17	1.22	1.34
1	B	30	CYS	CB-SG	-5.11	1.73	1.81
1	A	29	CYS	CB-SG	-5.04	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	PRO	N-CA-CB	5.97	110.46	103.30
1	B	0	PRO	N-CA-CB	5.90	110.38	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	THR	Peptide
1	A	71	PHE	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	3961	0	3939	122	1
1	B	4579	0	4564	142	1
2	A	3	0	0	3	0
2	B	3	0	0	3	0
3	A	20	0	0	1	0
3	B	5	0	0	1	0
All	All	8571	0	8503	263	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 15.

All (263) 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:55:CYS:HG	2:B:603:ZN:ZN	0.69	1.01
1:B:19:CYS:HG	2:B:602:ZN:ZN	0.66	0.97
1:A:19:CYS:HG	2:A:602:ZN:ZN	0.63	0.93
1:B:534:ASP:OD2	1:B:560:ARG:NH2	2.05	0.89
1:A:94:LYS:NZ	1:A:95:ASN:OD1	2.11	0.84
1:A:513:SER:OG	1:A:519:ASN:OD1	1.97	0.80
1:A:486:SER:OG	1:A:517:SER:OG	1.97	0.78
1:B:19:CYS:SG	2:B:602:ZN:ZN	1.71	0.76
1:B:20:ILE:HG23	1:B:21:ARG:HG2	1.68	0.74
1:B:285:GLY:N	3:B:604:SO4:O1	2.17	0.74
1:A:405:LEU:HB2	1:A:537:GLN:OE1	1.88	0.72
1:A:8:CYS:SG	2:A:601:ZN:ZN	1.77	0.72
1:B:177:ASN:OD1	1:B:178:ARG:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:O	1:A:423:ASN:ND2	2.23	0.71
1:A:531:GLN:OE1	1:A:535:SER:OG	2.09	0.70
1:A:19:CYS:SG	2:A:602:ZN:ZN	1.77	0.70
1:A:257:THR:OG1	1:A:258:VAL:N	2.24	0.69
1:A:49:VAL:HG12	1:A:58:SER:HB3	1.75	0.69
1:A:532:THR:HB	1:A:535:SER:H	1.58	0.68
1:B:113:ASP:OD2	1:B:115:THR:OG1	2.10	0.68
1:A:8:CYS:HB2	1:A:10:SER:H	1.56	0.67
1:B:329:LYS:HG2	1:B:354:GLN:H	1.59	0.67
1:B:167:TRP:HZ2	1:B:176:LEU:HD21	1.60	0.67
1:B:513:SER:OG	1:B:519:ASN:OD1	2.11	0.66
1:A:380:THR:OG1	1:A:383:ASP:OD2	2.11	0.66
1:B:366:THR:OG1	1:B:367:SER:N	2.27	0.66
1:A:59:ASP:OD1	1:A:61:THR:N	2.28	0.66
1:B:333:ILE:HD11	1:B:356:LEU:HD13	1.78	0.65
1:A:404:GLN:O	1:A:559:ASN:ND2	2.29	0.64
1:B:451:THR:HG22	1:B:586:GLU:H	1.63	0.64
1:B:490:ARG:NH1	1:B:525:MET:SD	2.71	0.64
1:B:258:VAL:HG22	1:B:259:PRO:O	1.99	0.63
1:A:60:VAL:HA	1:A:63:LEU:HD12	1.82	0.62
1:B:201:GLU:O	1:B:210:SER:N	2.28	0.62
1:B:329:LYS:HD3	1:B:354:GLN:HB2	1.81	0.62
1:A:18:THR:OG1	1:A:18:THR:O	2.16	0.62
1:A:304:VAL:HG22	1:A:355:TYR:CD1	2.35	0.62
1:A:55:CYS:SG	1:A:56:GLY:HA3	2.40	0.61
1:B:257:THR:HG22	1:B:258:VAL:H	1.65	0.61
1:A:405:LEU:HD21	1:A:560:ARG:HG2	1.82	0.61
1:B:159:GLY:O	1:B:162:GLN:N	2.24	0.61
1:B:180:TYR:HD2	1:B:227:LEU:HD11	1.65	0.61
1:B:376:VAL:O	1:B:423:ASN:ND2	2.32	0.61
1:B:257:THR:HG22	1:B:258:VAL:HG12	1.83	0.61
1:A:18:THR:HG23	1:A:39:HIS:HB3	1.83	0.61
1:B:19:CYS:SG	1:B:39:HIS:ND1	2.74	0.60
1:A:515:TYR:O	1:A:519:ASN:ND2	2.33	0.60
1:B:197:GLU:N	1:B:214:SER:OG	2.32	0.60
1:B:335:PRO:HG3	1:B:362:ALA:HB2	1.82	0.60
1:A:448:ILE:HG22	1:A:587:PHE:CE1	2.35	0.60
1:A:279:THR:HG23	1:A:435:ASP:H	1.67	0.60
1:A:532:THR:H	1:A:535:SER:HB3	1.66	0.60
1:A:552:THR:O	1:A:556:ASN:ND2	2.34	0.60
1:B:519:ASN:O	1:B:522:SER:OG	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HB	1:A:358:SER:HB2	1.85	0.59
1:B:333:ILE:HB	1:B:358:SER:HB2	1.84	0.59
1:A:32:ASP:HA	1:A:35:ILE:HD12	1.85	0.59
1:A:420:GLU:OE1	1:A:431:ASN:ND2	2.34	0.59
1:A:489:ASN:HB2	1:A:549:THR:HG23	1.85	0.59
1:B:161:ARG:HB2	1:B:211:TYR:HD2	1.68	0.58
1:B:180:TYR:CD2	1:B:227:LEU:HD11	2.38	0.58
1:A:516:ASN:ND2	3:A:605:SO4:S	2.74	0.58
1:A:12:THR:HB	1:A:26:CYS:HA	1.84	0.58
1:B:37:THR:HG23	1:B:39:HIS:H	1.69	0.57
1:A:12:THR:OG1	1:A:13:SER:N	2.38	0.57
1:B:308:ALA:O	1:B:360:ILE:HG13	2.05	0.57
1:B:519:ASN:HD22	1:B:530:THR:HG1	1.53	0.57
1:A:448:ILE:HG22	1:A:587:PHE:CZ	2.40	0.56
1:A:31:TYR:O	1:A:35:ILE:HG13	2.05	0.56
1:A:303:ARG:HH12	1:A:356:LEU:HD13	1.70	0.56
1:A:447:GLU:O	1:A:451:THR:OG1	2.22	0.56
1:B:117:SER:HB3	1:B:415:GLY:HA3	1.88	0.56
1:A:449:VAL:HG11	1:A:463:ALA:HB2	1.88	0.56
1:B:561:PHE:CZ	1:B:565:ILE:HD11	2.41	0.55
1:B:544:VAL:HG23	1:B:572:ILE:HG13	1.88	0.55
1:B:371:LEU:HB3	1:B:396:ILE:HG12	1.88	0.55
1:B:18:THR:HG23	1:B:41:MET:HB3	1.87	0.55
1:A:32:ASP:HB2	1:A:103:ILE:HG12	1.89	0.55
1:A:30:CYS:O	1:A:34:VAL:HG22	2.07	0.55
1:A:8:CYS:SG	1:A:29:CYS:SG	3.04	0.54
1:A:247:VAL:HG23	1:A:248:LYS:HG3	1.88	0.54
1:B:90:PHE:HA	1:B:94:LYS:NZ	2.22	0.54
1:A:366:THR:OG1	1:A:367:SER:N	2.40	0.54
1:B:305:VAL:HG22	1:B:356:LEU:HB2	1.90	0.54
1:B:453:SER:O	1:B:459:ASN:N	2.31	0.54
1:A:281:GLN:HG3	1:A:402:PRO:HD2	1.89	0.54
1:B:249:ILE:HG13	1:B:274:TYR:CZ	2.43	0.53
1:B:406:PRO:HB3	1:B:422:PHE:CZ	2.44	0.53
1:B:40:LYS:O	1:B:60:VAL:HG23	2.09	0.53
1:A:71:PHE:HD1	1:A:75:HIS:HB2	1.72	0.53
1:A:19:CYS:SG	1:A:33:HIS:NE2	2.81	0.53
1:B:489:ASN:OD1	1:B:492:GLN:HG2	2.09	0.53
1:A:405:LEU:HG	1:A:563:VAL:HG21	1.91	0.53
1:A:451:THR:HG21	1:A:585:LEU:HD23	1.91	0.53
1:B:473:LYS:HE3	1:B:582:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TYR:CE2	1:B:87:GLY:HA2	2.44	0.52
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.45	0.52
1:A:425:VAL:O	1:A:429:MET:HG3	2.10	0.52
1:A:561:PHE:CZ	1:A:585:LEU:HD21	2.45	0.52
1:A:18:THR:HG22	1:A:41:MET:HB2	1.90	0.52
1:B:44:SER:OG	1:B:45:VAL:N	2.42	0.52
1:B:78:VAL:HG13	1:B:79:CYS:H	1.75	0.52
1:A:31:TYR:CD2	1:A:35:ILE:HD11	2.45	0.52
1:B:215:THR:HB	1:B:216:THR:HG22	1.91	0.52
1:B:19:CYS:SG	1:B:39:HIS:CE1	3.03	0.51
1:B:585:LEU:HD23	1:B:587:PHE:CE2	2.46	0.51
1:A:343:TYR:CE2	1:A:345:ARG:HB2	2.46	0.51
1:B:182:PHE:O	1:B:198:TYR:N	2.44	0.51
1:B:279:THR:HG23	1:B:435:ASP:H	1.76	0.51
1:A:340:VAL:HG12	1:A:341:GLU:H	1.76	0.51
1:B:167:TRP:CZ2	1:B:176:LEU:HD21	2.41	0.51
1:B:262:PHE:HE1	1:B:290:HIS:CD2	2.29	0.51
1:B:451:THR:CG2	1:B:586:GLU:H	2.23	0.51
1:B:425:VAL:O	1:B:429:MET:HG3	2.11	0.51
1:B:520:ALA:O	1:B:523:ARG:HB2	2.11	0.51
1:A:59:ASP:OD1	1:A:61:THR:HG22	2.11	0.51
1:B:467:LEU:H	1:B:467:LEU:HD12	1.76	0.51
1:B:105:GLU:HG2	1:B:122:LEU:HD11	1.93	0.51
1:B:155:LYS:HB2	1:B:166:VAL:HG21	1.93	0.50
1:B:487:ALA:O	1:B:517:SER:OG	2.29	0.50
1:A:410:THR:OG1	1:A:411:LEU:N	2.44	0.50
1:A:476:TYR:O	1:A:492:GLN:NE2	2.34	0.50
1:B:161:ARG:HB2	1:B:211:TYR:CD2	2.47	0.49
1:A:445:PRO:HD3	1:A:569:GLN:O	2.11	0.49
1:B:491:PRO:O	1:B:494:THR:HG22	2.12	0.49
1:B:447:GLU:O	1:B:451:THR:HG23	2.12	0.49
1:B:198:TYR:HD2	1:B:211:TYR:HE1	1.61	0.49
1:B:371:LEU:HD13	1:B:391:ILE:HG21	1.94	0.49
1:A:34:VAL:HG12	1:A:40:LYS:HA	1.94	0.49
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.47	0.49
1:B:59:ASP:OD1	1:B:61:THR:OG1	2.27	0.48
1:A:254:PRO:HB3	1:A:298:TYR:CE2	2.49	0.48
1:B:121:THR:HG22	1:B:421:ASN:HD22	1.79	0.48
1:A:18:THR:CG2	1:A:39:HIS:HB3	2.44	0.48
1:B:160:GLU:HA	1:B:161:ARG:HA	1.52	0.48
1:B:258:VAL:HG23	1:B:262:PHE:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:LYS:HG2	1:B:582:PHE:CE1	2.48	0.48
1:A:59:ASP:OD1	1:A:59:ASP:C	2.53	0.47
1:B:376:VAL:HG12	1:B:400:GLY:HA3	1.95	0.47
1:A:304:VAL:HG22	1:A:355:TYR:HD1	1.79	0.47
1:A:532:THR:N	1:A:535:SER:HB3	2.29	0.47
1:B:185:TYR:HA	1:B:193:VAL:O	2.14	0.47
1:B:451:THR:O	1:B:455:LEU:HB2	2.13	0.47
1:B:55:CYS:SG	1:B:75:HIS:CE1	3.07	0.47
1:A:250:THR:O	1:A:395:HIS:NE2	2.32	0.47
1:B:138:LEU:O	1:B:142:GLU:HG3	2.15	0.47
1:B:37:THR:CG2	1:B:39:HIS:H	2.28	0.47
1:A:444:CYS:HB2	1:A:449:VAL:HG23	1.97	0.47
1:B:35:ILE:HD13	1:A:497:LYS:HG2	1.96	0.47
1:B:122:LEU:O	1:B:126:THR:OG1	2.33	0.47
1:B:262:PHE:CE1	1:B:290:HIS:NE2	2.82	0.47
1:A:444:CYS:HB3	1:A:448:ILE:CG1	2.44	0.47
1:B:304:VAL:HG22	1:B:355:TYR:CD1	2.50	0.47
1:A:544:VAL:HG23	1:A:572:ILE:HG13	1.96	0.46
1:B:16:CYS:SG	1:B:19:CYS:SG	3.13	0.46
1:B:245:ARG:NH1	1:B:275:SER:OG	2.48	0.46
1:B:496:VAL:O	1:B:500:ILE:HG22	2.15	0.46
1:A:47:PRO:O	1:A:49:VAL:HG22	2.15	0.46
1:A:5:CYS:C	1:A:7:VAL:H	2.18	0.46
1:B:256:ILE:HA	1:B:257:THR:HA	1.62	0.46
1:B:280:VAL:HG22	1:B:436:ILE:HB	1.97	0.46
1:B:248:LYS:HA	1:B:274:TYR:HE1	1.80	0.46
1:A:383:ASP:O	1:A:387:ILE:HG13	2.16	0.46
1:B:258:VAL:CG2	1:B:262:PHE:HB2	2.45	0.46
1:B:406:PRO:HB3	1:B:422:PHE:CE2	2.51	0.46
1:A:78:VAL:HG23	1:A:79:CYS:H	1.81	0.46
1:B:72:CYS:HB3	1:B:75:HIS:H	1.81	0.46
1:B:60:VAL:HG12	1:B:84:CYS:HB2	1.96	0.46
1:A:516:ASN:HA	1:A:519:ASN:HD22	1.81	0.46
1:B:266:VAL:HG13	1:B:298:TYR:CE1	2.51	0.46
1:A:327:ILE:H	1:A:327:ILE:HD12	1.80	0.46
1:A:489:ASN:OD1	1:A:492:GLN:HG3	2.15	0.46
1:A:585:LEU:HD22	1:A:587:PHE:CE2	2.50	0.46
1:B:535:SER:O	1:B:535:SER:OG	2.33	0.46
1:A:471:CYS:O	1:A:587:PHE:HB3	2.16	0.45
1:A:142:GLU:O	1:A:144:ALA:N	2.49	0.45
1:A:47:PRO:O	1:A:49:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLU:O	1:B:352:ASN:N	2.49	0.45
1:A:32:ASP:N	1:A:32:ASP:OD1	2.47	0.45
1:A:443:ARG:NE	1:A:540:GLU:OE1	2.49	0.45
1:B:215:THR:HB	1:B:216:THR:HA	1.97	0.45
1:B:471:CYS:HA	1:B:572:ILE:O	2.17	0.45
1:A:279:THR:HG22	1:A:435:ASP:OD2	2.17	0.45
1:B:563:VAL:O	1:B:567:ARG:NE	2.49	0.45
1:A:55:CYS:SG	1:A:75:HIS:HE1	2.39	0.45
1:B:12:THR:HB	1:B:26:CYS:HA	1.98	0.45
1:B:304:VAL:HG12	1:B:370:ILE:HB	1.98	0.45
1:B:498:ASN:HA	1:B:501:THR:HG22	1.98	0.45
1:B:546:PHE:CE2	1:B:548:GLN:HB3	2.51	0.44
1:B:376:VAL:HG21	1:B:425:VAL:HG11	1.99	0.44
1:A:16:CYS:SG	1:A:19:CYS:SG	3.14	0.44
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.86	0.44
1:A:448:ILE:O	1:A:452:VAL:HG22	2.18	0.44
1:B:175:PRO:HG2	1:B:180:TYR:CE1	2.52	0.44
1:B:479:ASN:H	1:B:491:PRO:HG2	1.82	0.44
1:B:150:ALA:HB1	1:B:168:GLU:HG3	2.00	0.44
1:B:358:SER:OG	1:B:359:THR:O	2.36	0.44
1:A:307:THR:HA	1:A:358:SER:O	2.18	0.44
1:B:505:ALA:O	1:B:507:SER:N	2.50	0.44
1:A:139:ARG:HG3	1:A:139:ARG:O	2.16	0.43
1:A:506:TRP:N	1:A:506:TRP:CD1	2.86	0.43
1:B:500:ILE:HD11	1:B:507:SER:HA	2.00	0.43
1:A:8:CYS:SG	1:A:26:CYS:SG	3.13	0.43
1:B:42:VAL:CG2	1:B:60:VAL:HG21	2.48	0.43
1:B:323:LYS:HG3	1:B:324:TYR:CD1	2.52	0.43
1:B:519:ASN:ND2	1:B:530:THR:OG1	2.33	0.43
1:B:154:ILE:HA	1:B:154:ILE:HD13	1.91	0.43
1:B:384:LEU:HD11	1:B:423:ASN:HB3	1.99	0.43
1:B:451:THR:HG22	1:B:586:GLU:HG3	1.99	0.43
1:B:71:PHE:CD2	1:B:77:PRO:HD3	2.54	0.43
1:A:255:THR:OG1	1:A:256:ILE:N	2.51	0.43
1:B:200:PHE:HB3	1:B:209:VAL:HG21	2.01	0.43
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.73	0.43
1:B:1:ALA:HA	1:B:15:ARG:NH2	2.34	0.43
1:A:108:ARG:CZ	1:A:122:LEU:HD22	2.49	0.43
1:A:115:THR:O	1:A:412:LEU:HD12	2.19	0.43
1:A:531:GLN:HB3	1:A:535:SER:HG	1.82	0.43
1:A:142:GLU:C	1:A:144:ALA:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:HB3	1:A:320:LYS:HG3	2.01	0.42
1:A:386:ILE:O	1:A:390:ARG:HG3	2.20	0.42
1:A:121:THR:O	1:A:125:THR:OG1	2.36	0.42
1:A:488:ILE:HG12	1:A:517:SER:HB3	2.01	0.42
1:B:32:ASP:HB2	1:B:103:ILE:HG12	2.00	0.42
1:A:453:SER:HB2	1:A:461:LEU:HB3	2.02	0.42
1:B:198:TYR:CD2	1:B:211:TYR:HE1	2.38	0.42
1:A:544:VAL:CG2	1:A:572:ILE:HG13	2.50	0.42
1:A:63:LEU:HA	1:A:71:PHE:O	2.20	0.42
1:A:21:ARG:HD2	1:A:21:ARG:HA	1.82	0.42
1:A:280:VAL:HG22	1:A:436:ILE:HB	2.02	0.42
1:B:94:LYS:HB3	1:B:94:LYS:HE2	1.88	0.42
1:A:37:THR:O	1:A:39:HIS:N	2.53	0.42
1:A:444:CYS:HB3	1:A:448:ILE:HD11	2.02	0.42
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.85	0.42
1:B:548:GLN:NE2	1:B:576:MET:SD	2.93	0.42
1:A:105:GLU:OE1	1:A:126:THR:HG22	2.20	0.41
1:A:78:VAL:HG23	1:A:79:CYS:N	2.35	0.41
1:B:271:LYS:C	1:B:273:GLY:H	2.23	0.41
1:B:453:SER:HA	1:B:457:TYR:HB2	2.02	0.41
1:B:158:VAL:HG23	1:B:162:GLN:HB2	2.02	0.41
1:B:1:ALA:HA	1:B:15:ARG:HH21	1.85	0.41
1:A:143:GLU:OE1	1:A:231:SER:N	2.53	0.41
1:A:240:ILE:HG21	1:A:240:ILE:HD13	1.74	0.41
1:A:18:THR:OG1	1:A:39:HIS:CG	2.73	0.41
1:B:350:GLU:C	1:B:352:ASN:H	2.24	0.41
1:B:423:ASN:HB2	1:B:425:VAL:H	1.84	0.41
1:A:318:CYS:HB3	1:A:346:PHE:CE2	2.55	0.41
1:B:446:LYS:HA	1:B:449:VAL:HG12	2.03	0.41
1:B:272:SER:HA	1:B:278:VAL:HG21	2.01	0.41
1:A:581:LEU:HA	1:A:581:LEU:HD12	1.86	0.41
1:B:548:GLN:OE1	1:B:577:THR:HG22	2.21	0.41
1:A:289:SER:O	1:A:293:ILE:HG12	2.21	0.41
1:A:384:LEU:HD11	1:A:423:ASN:HB3	2.03	0.41
1:A:428:LEU:HA	1:A:428:LEU:HD23	1.90	0.41
1:B:92:LEU:HA	1:B:92:LEU:HD23	1.71	0.41
1:B:544:VAL:CG2	1:B:568:ALA:HB2	2.51	0.40
1:A:26:CYS:HB2	1:A:97:CYS:HB3	2.03	0.40
1:A:31:TYR:CE1	1:A:35:ILE:HG12	2.55	0.40
1:A:340:VAL:HG12	1:A:341:GLU:N	2.36	0.40
1:A:561:PHE:CE2	1:A:565:ILE:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LYS:HA	1:B:449:VAL:CG1	2.51	0.40
1:B:449:VAL:HG11	1:B:463:ALA:HB2	2.03	0.40
1:B:326:ASN:O	1:B:328:ALA:N	2.54	0.40
1:A:409:ARG:NH2	1:A:422:PHE:O	2.55	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:B:79:CYS:CB	1:A:79:CYS:SG[8_445]	1.40	0.80

## 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	511/600 (85%)	458 (90%)	48 (9%)	5 (1%)	18	59
1	B	587/600 (98%)	532 (91%)	50 (8%)	5 (1%)	20	62
All	All	1098/1200 (92%)	990 (90%)	98 (9%)	10 (1%)	20	62

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	504	PRO
1	B	215	THR
1	B	123	ALA
1	B	351	THR
1	B	506	TRP
1	A	45	VAL
1	A	126	THR
1	A	406	PRO
1	A	38	PRO

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Mol	Chain	Res	Type
1	A	73	VAL

### 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	443/521 (85%)	426 (96%)	17 (4%)	38	75
1	B	512/521 (98%)	497 (97%)	15 (3%)	48	82
All	All	955/1042 (92%)	923 (97%)	32 (3%)	42	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	THR
1	B	72	CYS
1	B	79	CYS
1	B	97	CYS
1	B	126	THR
1	B	148	SER
1	B	203	ILE
1	B	227	LEU
1	B	303	ARG
1	B	359	THR
1	B	366	THR
1	B	377	SER
1	B	476	TYR
1	B	524	SER
1	B	592	PHE
1	A	2	VAL
1	A	6	VAL
1	A	18	THR
1	A	35	ILE
1	A	50	CYS
1	A	55	CYS
1	A	102	SER

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Mol	Chain	Res	Type
1	A	125	THR
1	A	126	THR
1	A	241	VAL
1	A	275	SER
1	A	278	VAL
1	A	342	CYS
1	A	358	SER
1	A	376	VAL
1	A	377	SER
1	A	592	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	421	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](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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	SO4	A	604	-	4,4,4	0.11	0	6,6,6	0.30	0
3	SO4	A	605	-	4,4,4	0.10	0	6,6,6	0.18	0
3	SO4	A	606	-	4,4,4	0.11	0	6,6,6	0.19	0
3	SO4	A	607	-	4,4,4	0.20	0	6,6,6	0.22	0
3	SO4	B	604	-	4,4,4	0.10	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	A	607	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	SO4	1	0
3	B	604	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<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	515/600 (85%)	-0.21	5 (0%) 82 58	33, 54, 87, 140	0
1	B	591/600 (98%)	-0.04	12 (2%) 65 36	39, 74, 113, 133	0
All	All	1106/1200 (92%)	-0.12	17 (1%) 74 47	33, 62, 109, 140	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	ALA	5.1
1	B	485	SER	3.9
1	A	341	GLU	3.3
1	B	338	ALA	3.3
1	A	340	VAL	3.1
1	A	339	ARG	2.9
1	A	39	HIS	2.5
1	B	224	ILE	2.5
1	A	38	PRO	2.5
1	B	331	SER	2.5
1	B	345	ARG	2.4
1	B	336	ALA	2.3
1	B	170	GLY	2.3
1	B	335	PRO	2.2
1	B	593	THR	2.2
1	B	483	ASP	2.1
1	B	475	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	SO4	A	605	5/5	0.90	0.47	6.17	85,94,108,118	0
3	SO4	A	604	5/5	0.83	0.43	5.95	73,79,87,113	0
3	SO4	A	607	5/5	0.94	0.20	0.63	70,71,73,79	0
3	SO4	B	604	5/5	0.76	0.17	0.42	89,94,101,120	0
3	SO4	A	606	5/5	0.87	0.16	-0.43	74,79,87,107	0
2	ZN	A	603	1/1	0.85	0.15	-1.14	167,167,167,167	0
2	ZN	A	601	1/1	0.95	0.13	-1.34	52,52,52,52	0
2	ZN	A	602	1/1	0.98	0.06	-1.56	50,50,50,50	0
2	ZN	B	603	1/1	0.98	0.08	-1.97	52,52,52,52	0
2	ZN	B	601	1/1	0.99	0.11	-2.61	45,45,45,45	0
2	ZN	B	602	1/1	0.99	0.09	-4.18	42,42,42,42	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.