



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:25 PM GMT

PDB ID : 4ES5  
Title : Crystal structure of the cap-binding domain of polymerase basic protein 2 from influenza virus A/Bar-headed Gs/Qinghai/15c/2005 (h5n1) with bound m7GTP  
Authors : Meng, G.; Liu, Y.; Zheng, X.  
Deposited on : 2012-04-22  
Resolution : 1.80 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

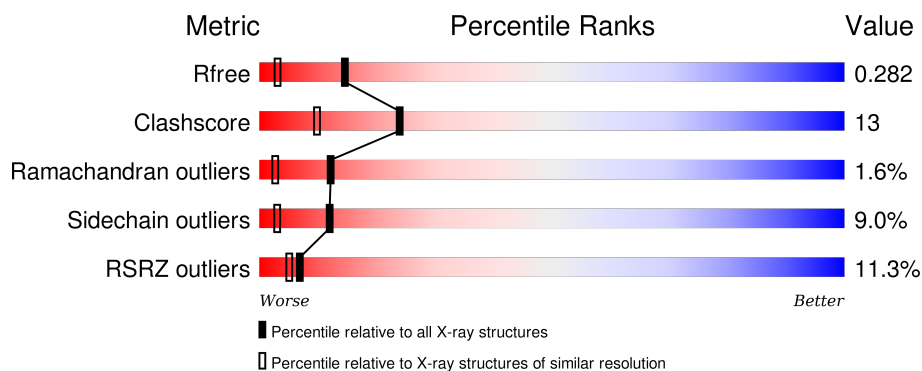
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	170	<div> <div>78%</div> <div>13%</div> <div>5%</div> <div>• •</div> </div>
1	B	170	<div> <div>4%</div> <div>80%</div> <div>12%</div> <div>5%</div> <div>•</div> </div>
1	C	170	<div> <div>12%</div> <div>73%</div> <div>20%</div> <div>• • •</div> </div>
1	D	170	<div> <div>27%</div> <div>58%</div> <div>27%</div> <div>9%</div> <div>• 6%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	502	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5889 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.

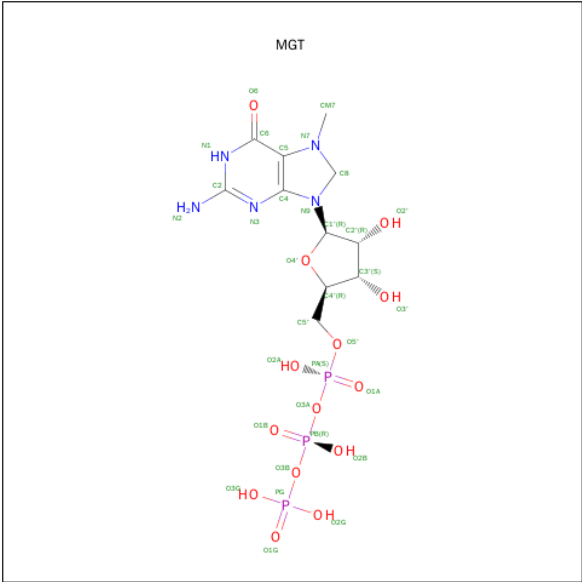
- Molecule 1 is a protein called Polymerase basic subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	1	0
			1313	821	243	240	9			
1	B	165	Total	C	N	O	S	0	0	0
			1299	814	236	239	10			
1	C	163	Total	C	N	O	S	0	0	0
			1285	805	234	236	10			
1	D	160	Total	C	N	O	S	0	0	0
			1262	791	230	232	9			

There are 16 discrepancies between the modelled and reference sequences:

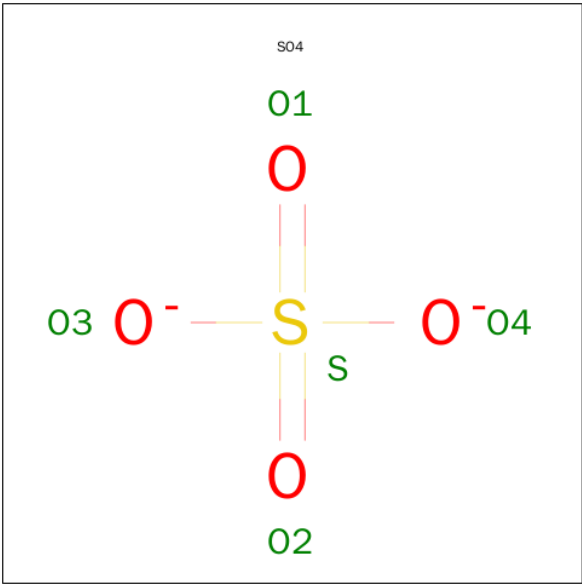
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	GLY	-	EXPRESSION TAG	UNP Q4FAV8
A	315	SER	-	EXPRESSION TAG	UNP Q4FAV8
A	316	HIS	-	EXPRESSION TAG	UNP Q4FAV8
A	317	MET	-	EXPRESSION TAG	UNP Q4FAV8
B	314	GLY	-	EXPRESSION TAG	UNP Q4FAV8
B	315	SER	-	EXPRESSION TAG	UNP Q4FAV8
B	316	HIS	-	EXPRESSION TAG	UNP Q4FAV8
B	317	MET	-	EXPRESSION TAG	UNP Q4FAV8
C	314	GLY	-	EXPRESSION TAG	UNP Q4FAV8
C	315	SER	-	EXPRESSION TAG	UNP Q4FAV8
C	316	HIS	-	EXPRESSION TAG	UNP Q4FAV8
C	317	MET	-	EXPRESSION TAG	UNP Q4FAV8
D	314	GLY	-	EXPRESSION TAG	UNP Q4FAV8
D	315	SER	-	EXPRESSION TAG	UNP Q4FAV8
D	316	HIS	-	EXPRESSION TAG	UNP Q4FAV8
D	317	MET	-	EXPRESSION TAG	UNP Q4FAV8

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (three-letter code: MGT) (formula: C<sub>11</sub>H<sub>20</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			33	11	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			33	11	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			33	11	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			33	11	5	14	3		

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



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

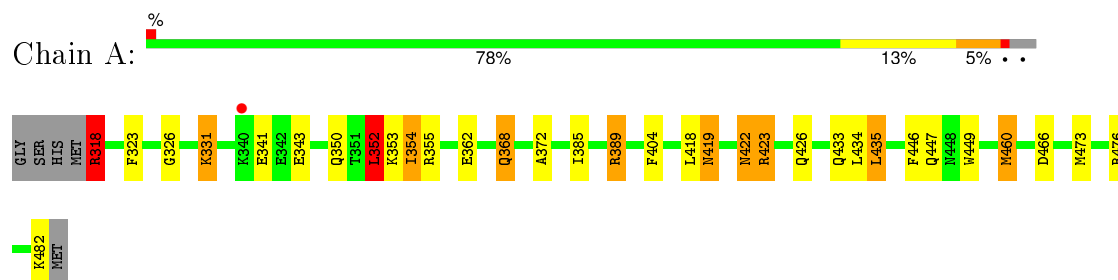
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	271	Total O 271 271	0	0
4	B	182	Total O 182 182	0	0
4	C	80	Total O 80 80	0	0
4	D	45	Total O 45 45	0	0

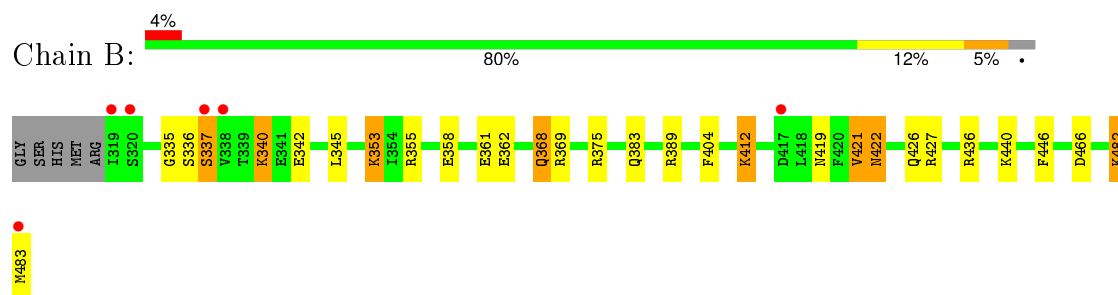
### 3 Residue-property plots

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.

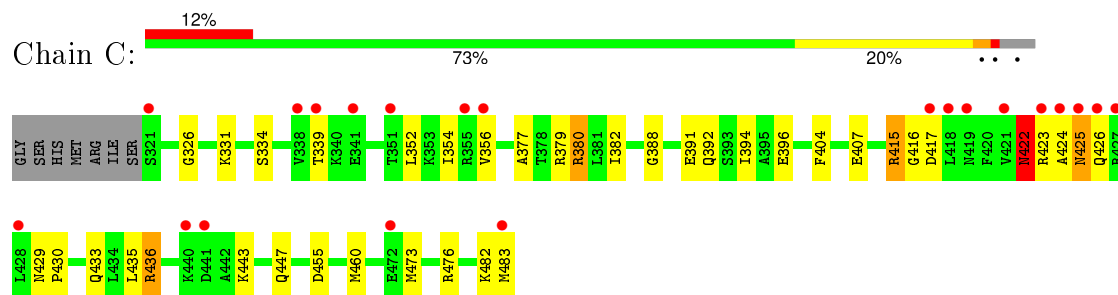
#### • Molecule 1: Polymerase basic subunit 2



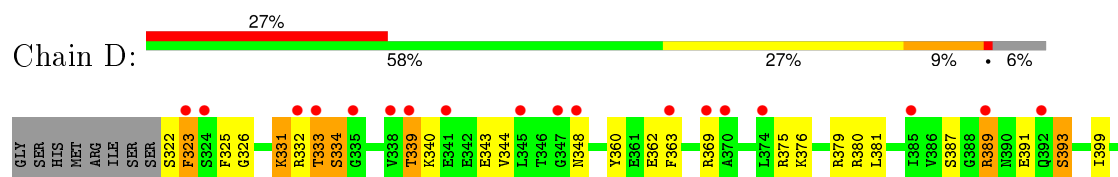
#### • Molecule 1: Polymerase basic subunit 2

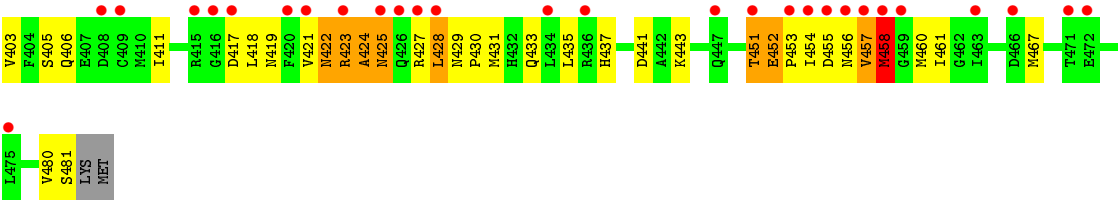


#### • Molecule 1: Polymerase basic subunit 2



#### • Molecule 1: Polymerase basic subunit 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.48Å 39.10Å 141.08Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	14.91 – 1.80 14.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (14.91-1.80) 99.7 (14.91-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.197 , 0.285 0.195 , 0.282	Depositor DCC
$R_{free}$ test set	3166 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.1	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 62222 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: SO4, MGT

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	1.42	6/1331 (0.5%)	1.17	8/1786 (0.4%)
1	B	1.25	0/1317	1.06	3/1768 (0.2%)
1	C	0.86	0/1303	0.87	1/1749 (0.1%)
1	D	0.72	0/1280	0.80	0/1720
All	All	1.10	6/5231 (0.1%)	0.99	12/7023 (0.2%)

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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	449	TRP	CE3-CZ3	5.73	1.48	1.38
1	A	372	ALA	CA-CB	5.69	1.64	1.52
1	A	362	GLU	CD-OE1	-5.52	1.19	1.25
1	A	446	PHE	CE2-CZ	5.46	1.47	1.37
1	A	434	LEU	C-O	5.13	1.33	1.23
1	A	323	PHE	CG-CD1	5.01	1.46	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	MET	CB-CG-SD	-7.24	90.69	112.40
1	A	352	LEU	CA-CB-CG	7.13	131.70	115.30
1	A	476	ARG	NE-CZ-NH1	-6.60	117.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	VAL	CG1-CB-CG2	6.59	121.44	110.90
1	A	404	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	A	466	ASP	CB-CG-OD1	6.15	123.84	118.30
1	B	466	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	416	GLY	N-CA-C	-5.76	98.70	113.10
1	A	460	MET	CG-SD-CE	-5.46	91.46	100.20
1	B	446	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	435	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	354	ILE	CG1-CB-CG2	-5.07	100.24	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	ARG	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	1313	0	1344	31	0
1	B	1299	0	1328	29	0
1	C	1285	0	1312	33	0
1	D	1262	0	1285	51	0
2	A	33	0	16	0	0
2	B	33	0	16	2	0
2	C	33	0	16	2	0
2	D	33	0	16	4	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	271	0	0	8	1
4	B	182	0	0	7	1
4	C	80	0	0	6	0
4	D	45	0	0	6	0
All	All	5889	0	5333	139	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 13.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD13	1:A:354:ILE:HD11	1.31	1.12
1:C:415:ARG:HG3	1:C:415:ARG:HH11	0.98	1.09
1:B:353:LYS:HD2	1:B:353:LYS:H	1.00	1.07
1:D:369:ARG:HB3	1:D:393:SER:HB3	1.35	1.03
1:B:353:LYS:H	1:B:353:LYS:CD	1.75	0.95
1:B:353:LYS:N	1:B:353:LYS:HD2	1.86	0.90
1:B:412:LYS:HD2	1:B:412:LYS:N	1.86	0.90
1:C:460:MET:HG3	4:C:652:HOH:O	1.71	0.89
1:C:415:ARG:HG3	1:C:415:ARG:NH1	1.77	0.88
1:D:326:GLY:CA	1:D:435:LEU:HD21	2.08	0.84
1:A:419:ASN:H	1:A:419:ASN:HD22	1.27	0.81
1:B:419:ASN:HD22	1:B:427:ARG:HH12	1.26	0.80
1:A:423[A]:ARG:H	1:A:423[A]:ARG:CD	1.94	0.80
1:A:447:GLN:NE2	4:A:772:HOH:O	2.14	0.80
1:A:318:ARG:HG3	4:A:656:HOH:O	1.81	0.79
1:B:419:ASN:HD22	1:B:427:ARG:NH1	1.81	0.78
1:D:379:ARG:NH2	1:D:411:ILE:HD12	1.99	0.77
1:A:423[A]:ARG:H	1:A:423[A]:ARG:HD2	1.50	0.77
1:B:436:ARG:HG3	4:B:662:HOH:O	1.86	0.75
1:B:353:LYS:HD3	4:B:682:HOH:O	1.85	0.74
1:C:436:ARG:HD2	4:C:650:HOH:O	1.88	0.73
1:A:419:ASN:N	1:A:419:ASN:HD22	1.85	0.71
1:A:318:ARG:CG	4:A:656:HOH:O	2.38	0.70
1:B:412:LYS:NZ	4:B:733:HOH:O	2.26	0.69
1:C:460:MET:CG	4:C:652:HOH:O	2.35	0.69
1:C:404:PHE:CD1	2:C:501:MGT:HM73	2.27	0.69
1:B:419:ASN:ND2	1:B:427:ARG:HH12	1.91	0.69
1:D:326:GLY:HA2	1:D:435:LEU:HD21	1.75	0.69
1:A:350:GLN:HB2	4:A:800:HOH:O	1.93	0.69
1:A:326:GLY:HA2	1:A:435:LEU:HD21	1.75	0.67
1:D:326:GLY:HA3	1:D:435:LEU:HD21	1.75	0.67
1:D:480:VAL:HG13	1:D:481:SER:H	1.61	0.66
1:C:404:PHE:CE1	2:C:501:MGT:HM73	2.31	0.65
1:A:353:LYS:C	1:A:354:ILE:HD12	2.18	0.64
1:C:415:ARG:CG	1:C:415:ARG:HH11	1.90	0.64
1:D:406:GLN:CA	4:D:639:HOH:O	2.46	0.64
1:B:375:ARG:NH1	1:B:383:GLN:OE1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:C	1:A:422:ASN:HD22	2.01	0.63
1:A:423[A]:ARG:N	1:A:423[A]:ARG:CD	2.62	0.63
1:D:480:VAL:CG1	1:D:481:SER:N	2.61	0.62
1:A:368:GLN:HG2	4:A:817:HOH:O	2.00	0.62
1:D:428:LEU:HA	4:D:638:HOH:O	1.99	0.62
1:A:385:ILE:HG12	1:A:460:MET:HE1	1.81	0.62
1:C:482:LYS:O	1:C:483:MET:HG2	2.01	0.61
1:A:423[A]:ARG:N	1:A:423[A]:ARG:HD2	2.15	0.61
1:C:380:ARG:HD2	1:D:380:ARG:HG3	1.83	0.61
1:D:406:GLN:HA	4:D:639:HOH:O	2.00	0.60
1:C:380:ARG:HG3	1:C:380:ARG:HH11	1.66	0.60
1:D:418:LEU:HD21	1:D:437:HIS:HB2	1.82	0.60
1:C:352:LEU:HD22	1:C:430:PRO:HB3	1.83	0.60
1:C:380:ARG:NE	1:D:380:ARG:HG3	2.17	0.59
1:D:429:ASN:HB2	1:D:430:PRO:HD2	1.83	0.59
1:D:344:VAL:HG21	1:D:411:ILE:HD13	1.84	0.59
1:D:429:ASN:ND2	2:D:501:MGT:O2A	2.33	0.58
1:C:380:ARG:CD	1:D:380:ARG:HG3	2.33	0.58
1:B:340:LYS:HD2	1:B:358:GLU:HG3	1.86	0.57
1:D:427:ARG:HD2	1:D:427:ARG:N	2.19	0.57
1:B:353:LYS:N	1:B:353:LYS:CD	2.55	0.57
1:C:380:ARG:CG	1:C:380:ARG:HH11	2.18	0.57
1:D:451:THR:OG1	1:D:452:GLU:N	2.37	0.56
1:B:342:GLU:OE2	4:B:666:HOH:O	2.18	0.56
1:C:392:GLN:HG3	1:C:396:GLU:OE2	2.05	0.56
1:D:480:VAL:HG13	1:D:481:SER:N	2.20	0.56
1:D:431:MET:CE	2:D:501:MGT:HM72	2.36	0.56
1:C:354:ILE:HG13	1:C:356:VAL:HG23	1.87	0.55
1:D:427:ARG:H	1:D:427:ARG:HD2	1.72	0.55
1:D:339:THR:HG22	4:D:625:HOH:O	2.07	0.55
1:D:422:ASN:HD21	1:D:425:ASN:HB3	1.71	0.55
1:A:343:GLU:CD	1:A:353:LYS:HG3	2.28	0.54
1:A:419:ASN:ND2	1:A:419:ASN:N	2.56	0.54
1:A:354:ILE:HD12	1:A:354:ILE:N	2.23	0.53
1:D:379:ARG:HH21	1:D:411:ILE:HD12	1.70	0.53
1:C:423:ARG:CG	1:C:424:ALA:N	2.72	0.53
1:B:337:SER:HB3	1:B:361:GLU:CD	2.30	0.53
1:C:476:ARG:HD2	4:C:621:HOH:O	2.07	0.53
1:C:422:ASN:HD21	1:C:426:GLN:H	1.56	0.52
1:A:419:ASN:ND2	4:A:717:HOH:O	2.41	0.52
1:D:424:ALA:O	1:D:425:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLN:HG2	4:B:667:HOH:O	2.11	0.51
1:D:323:PHE:N	1:D:323:PHE:CD2	2.79	0.51
1:C:415:ARG:CG	1:C:415:ARG:NH1	2.60	0.51
1:D:457:VAL:O	1:D:457:VAL:HG12	2.10	0.51
1:B:368:GLN:OE1	1:B:369:ARG:HD3	2.10	0.51
1:B:404:PHE:CD1	2:B:501:MGT:HM73	2.46	0.50
1:B:422:ASN:HD22	1:B:422:ASN:C	2.15	0.50
1:D:362:GLU:HG2	1:D:375:ARG:HG2	1.94	0.49
1:C:423:ARG:HG2	1:C:424:ALA:H	1.77	0.49
1:B:412:LYS:CE	4:B:733:HOH:O	2.59	0.49
1:D:418:LEU:HD22	1:D:433:GLN:HB3	1.95	0.49
1:D:391:GLU:OE2	1:D:467:MET:HG3	2.12	0.48
1:B:362:GLU:HG2	1:B:375:ARG:HG2	1.95	0.48
1:D:406:GLN:CB	4:D:639:HOH:O	2.62	0.48
1:D:423:ARG:HB2	4:D:604:HOH:O	2.13	0.48
1:A:422:ASN:ND2	1:A:426:GLN:H	2.11	0.48
1:D:431:MET:HE1	2:D:501:MGT:HM72	1.96	0.48
1:B:436:ARG:NH1	4:B:694:HOH:O	2.47	0.47
1:C:460:MET:CB	4:C:652:HOH:O	2.60	0.47
1:D:456:ASN:O	1:D:458:MET:N	2.48	0.47
1:D:421:VAL:HA	1:D:427:ARG:HA	1.97	0.47
1:D:332:ARG:HA	1:D:363:PHE:CD1	2.50	0.47
1:D:419:ASN:OD1	1:D:427:ARG:HG2	2.14	0.46
1:D:431:MET:HE2	2:D:501:MGT:HM72	1.98	0.46
1:C:377:ALA:HB2	1:C:382:ILE:HD11	1.98	0.46
1:A:422:ASN:C	1:A:422:ASN:ND2	2.70	0.45
1:B:335:GLY:O	1:B:336:SER:OG	2.27	0.45
1:A:354:ILE:HG22	1:A:355:ARG:N	2.31	0.45
1:B:404:PHE:CE1	2:B:501:MGT:HM73	2.51	0.45
1:C:422:ASN:HD21	1:C:425:ASN:HA	1.82	0.44
1:A:482:LYS:NZ	4:A:677:HOH:O	2.47	0.44
1:B:355:ARG:NH1	1:D:339:THR:HG21	2.31	0.44
1:C:388:GLY:HA3	1:C:394:ILE:HG13	2.00	0.44
1:C:430:PRO:O	1:C:433:GLN:HB2	2.18	0.43
1:D:399:ILE:O	1:D:403:VAL:HG23	2.19	0.43
1:B:337:SER:HB3	1:B:361:GLU:OE2	2.19	0.43
1:D:443:LYS:HB2	1:D:443:LYS:HE3	1.86	0.43
1:D:441:ASP:OD1	1:D:443:LYS:HG2	2.18	0.43
1:C:331:LYS:HE3	4:C:640:HOH:O	2.17	0.43
1:B:345:LEU:O	1:B:412:LYS:HE3	2.18	0.43
1:C:455:ASP:OD1	1:D:340:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:CD1	1:A:354:ILE:HD11	2.23	0.42
1:D:333:THR:O	1:D:334:SER:CB	2.68	0.42
1:A:318:ARG:HG2	4:A:656:HOH:O	2.15	0.41
1:A:331:LYS:HE2	1:A:331:LYS:HB2	1.37	0.41
1:D:331:LYS:HG3	1:D:333:THR:HG22	2.03	0.41
1:C:326:GLY:CA	1:C:435:LEU:HD21	2.51	0.41
1:A:418:LEU:HB3	1:A:433:GLN:HB3	2.01	0.41
1:D:389:ARG:H	1:D:389:ARG:HD3	1.86	0.41
1:D:325:PHE:CZ	1:D:435:LEU:HB2	2.56	0.41
1:D:360:TYR:HA	1:D:376:LYS:O	2.21	0.41
1:B:482:LYS:HD3	1:B:482:LYS:HA	1.22	0.41
1:A:389:ARG:HE	1:A:389:ARG:HB2	1.62	0.41
1:D:379:ARG:HA	1:D:405:SER:O	2.21	0.40
1:B:422:ASN:ND2	1:B:426:GLN:H	2.20	0.40
1:C:422:ASN:ND2	1:C:425:ASN:HA	2.37	0.40
1:C:379:ARG:HB3	1:C:379:ARG:HE	1.75	0.40
1:C:380:ARG:HA	1:C:407:GLU:HG2	2.02	0.40
1:D:381:LEU:HD23	1:D:381:LEU:C	2.42	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)
4:A:817:HOH:O	4:B:750:HOH:O[1_455]	2.15	0.05

## 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	164/170 (96%)	163 (99%)	1 (1%)	0	100	100
1	B	163/170 (96%)	159 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	161/170 (95%)	150 (93%)	9 (6%)	2 (1%)	16	4
1	D	158/170 (93%)	142 (90%)	8 (5%)	8 (5%)	2	0
All	All	646/680 (95%)	614 (95%)	22 (3%)	10 (2%)	12	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	425	ASN
1	D	425	ASN
1	D	457	VAL
1	D	334	SER
1	D	422	ASN
1	C	422	ASN
1	D	453	PRO
1	D	423	ARG
1	D	458	MET
1	D	424	ALA

### 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	145/148 (98%)	135 (93%)	10 (7%)	19	6
1	B	144/148 (97%)	133 (92%)	11 (8%)	16	5
1	C	142/148 (96%)	130 (92%)	12 (8%)	13	3
1	D	139/148 (94%)	120 (86%)	19 (14%)	4	1
All	All	570/592 (96%)	518 (91%)	52 (9%)	12	3

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	ARG
1	A	331	LYS

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Mol	Chain	Res	Type
1	A	341	GLU
1	A	352	LEU
1	A	368	GLN
1	A	389	ARG
1	A	419	ASN
1	A	422	ASN
1	A	423[A]	ARG
1	A	423[B]	ARG
1	B	337	SER
1	B	340	LYS
1	B	353	LYS
1	B	368	GLN
1	B	389	ARG
1	B	412	LYS
1	B	421	VAL
1	B	422	ASN
1	B	440	LYS
1	B	482	LYS
1	B	483	MET
1	C	334	SER
1	C	339	THR
1	C	380	ARG
1	C	391	GLU
1	C	415	ARG
1	C	417	ASP
1	C	422	ASN
1	C	429	ASN
1	C	436	ARG
1	C	443	LYS
1	C	447	GLN
1	C	473	MET
1	D	322	SER
1	D	323	PHE
1	D	331	LYS
1	D	333	THR
1	D	339	THR
1	D	343	GLU
1	D	348	ASN
1	D	387	SER
1	D	389	ARG
1	D	393	SER
1	D	417	ASP

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Mol	Chain	Res	Type
1	D	428	LEU
1	D	451	THR
1	D	452	GLU
1	D	454	ILE
1	D	455	ASP
1	D	458	MET
1	D	460	MET
1	D	461	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	ASN
1	A	422	ASN
1	B	419	ASN
1	B	422	ASN
1	C	422	ASN
1	C	426	GLN
1	D	383	GLN
1	D	425	ASN
1	D	426	GLN

### 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](#)

8 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	MGT	A	501	-	28,35,35	1.21	3 (10%)	39,56,56	1.95	8 (20%)
3	SO4	A	502	-	4,4,4	0.29	0	6,6,6	0.50	0
2	MGT	B	501	-	28,35,35	1.14	3 (10%)	39,56,56	2.02	8 (20%)
3	SO4	B	502	-	4,4,4	1.11	0	6,6,6	0.39	0
2	MGT	C	501	-	28,35,35	0.74	1 (3%)	39,56,56	1.82	8 (20%)
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.43	0
2	MGT	D	501	-	28,35,35	0.92	1 (3%)	39,56,56	2.11	11 (28%)
3	SO4	D	502	-	4,4,4	0.20	0	6,6,6	0.22	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	MGT	A	501	-	-	0/22/50/50	0/3/3/3
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	MGT	B	501	-	-	0/22/50/50	0/3/3/3
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	MGT	C	501	-	-	0/22/50/50	0/3/3/3
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	MGT	D	501	-	-	0/22/50/50	0/3/3/3
3	SO4	D	502	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MGT	C8-N9	2.03	1.48	1.45
2	A	501	MGT	O3'-C3'	2.14	1.48	1.43
2	B	501	MGT	C5-C4	2.20	1.45	1.39
2	D	501	MGT	C5-C4	2.35	1.45	1.39
2	C	501	MGT	C6-N1	2.49	1.37	1.33
2	A	501	MGT	C6-N1	2.61	1.37	1.33
2	B	501	MGT	CM7-N7	2.61	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MGT	C5-C4	2.84	1.47	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	MGT	C5-C4-N3	-6.15	120.83	126.82
2	A	501	MGT	C5-C6-N1	-5.21	115.44	123.46
2	B	501	MGT	C5-C6-N1	-5.08	115.65	123.46
2	A	501	MGT	C5-C4-N3	-4.84	122.11	126.82
2	C	501	MGT	C5-C6-N1	-4.54	116.47	123.46
2	C	501	MGT	C5-C4-N3	-3.82	123.09	126.82
2	D	501	MGT	C5-C6-N1	-3.78	117.65	123.46
2	D	501	MGT	PB-O3B-PG	-3.66	120.41	132.67
2	B	501	MGT	C5-C4-N3	-3.56	123.35	126.82
2	A	501	MGT	O3A-PA-O5'	-3.35	94.05	102.94
2	C	501	MGT	PB-O3B-PG	-3.23	121.83	132.67
2	D	501	MGT	CM7-N7-C5	-3.06	113.86	124.09
2	C	501	MGT	CM7-N7-C8	-2.68	112.92	120.52
2	A	501	MGT	C3'-C2'-C1'	-2.61	96.17	101.40
2	B	501	MGT	N1-C2-N3	-2.58	121.31	125.53
2	C	501	MGT	PA-O3A-PB	-2.32	126.20	132.73
2	B	501	MGT	CM7-N7-C5	-2.23	116.63	124.09
2	B	501	MGT	PB-O3B-PG	-2.09	125.66	132.67
2	D	501	MGT	O3'-C3'-C4'	-2.05	104.89	111.05
2	D	501	MGT	N1-C2-N3	-2.00	122.25	125.53
2	D	501	MGT	C2'-C3'-C4'	2.04	106.80	102.61
2	A	501	MGT	O3G-PG-O2G	2.07	115.27	107.38
2	D	501	MGT	O2A-PA-O1A	2.27	124.81	112.53
2	A	501	MGT	O2B-PB-O3B	2.41	116.04	105.09
2	A	501	MGT	N3-C4-N9	2.56	130.59	126.75
2	C	501	MGT	N3-C4-N9	2.69	130.80	126.75
2	D	501	MGT	N2-C2-N3	2.70	121.68	117.20
2	B	501	MGT	O3G-PG-O1G	2.70	119.29	110.58
2	C	501	MGT	N2-C2-N1	3.08	122.29	117.20
2	B	501	MGT	N3-C4-N9	3.20	131.55	126.75
2	D	501	MGT	N3-C4-N9	4.21	133.07	126.75
2	C	501	MGT	C6-N1-C2	4.90	122.74	115.94
2	D	501	MGT	C6-N1-C2	5.25	123.22	115.94
2	A	501	MGT	C6-N1-C2	5.82	124.02	115.94
2	B	501	MGT	C6-N1-C2	7.09	125.78	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	MGT	2	0
2	C	501	MGT	2	0
2	D	501	MGT	4	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	165/170 (97%)	-0.23	1 (0%) 90 88	7, 14, 29, 38	2 (1%)
1	B	165/170 (97%)	-0.05	6 (3%) 46 40	9, 19, 38, 45	2 (1%)
1	C	163/170 (95%)	0.61	21 (12%) 5 4	16, 35, 57, 66	1 (0%)
1	D	160/170 (94%)	1.48	46 (28%) 1 0	32, 51, 71, 74	1 (0%)
All	All	653/680 (96%)	0.44	74 (11%) 7 5	7, 28, 63, 74	6 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	457	VAL	8.4
1	B	319	ILE	6.1
1	D	338	VAL	5.7
1	D	428	LEU	5.5
1	D	458	MET	5.1
1	D	420	PHE	5.0
1	D	421	VAL	4.7
1	C	321	SER	4.7
1	B	320	SER	4.1
1	D	471	THR	4.1
1	D	389	ARG	4.0
1	D	425	ASN	3.5
1	D	463	ILE	3.5
1	D	332	ARG	3.4
1	D	456	ASN	3.4
1	D	335	GLY	3.3
1	C	355	ARG	3.2
1	D	459	GLY	3.2
1	C	440	LYS	3.1
1	D	370	ALA	3.1
1	D	427	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	454	ILE	3.1
1	C	424	ALA	3.0
1	C	356	VAL	3.0
1	A	340	LYS	3.0
1	B	483	MET	3.0
1	B	337	SER	2.9
1	D	426	GLN	2.9
1	D	345	LEU	2.9
1	C	483	MET	2.9
1	D	423	ARG	2.9
1	C	425	ASN	2.7
1	D	347	GLY	2.7
1	D	339	THR	2.7
1	C	419	ASN	2.7
1	C	426	GLN	2.7
1	D	417	ASP	2.7
1	C	351	THR	2.7
1	C	427	ARG	2.7
1	D	341	GLU	2.7
1	C	423	ARG	2.6
1	D	434	LEU	2.6
1	D	416	GLY	2.6
1	C	339	THR	2.6
1	D	392	GLN	2.6
1	D	455	ASP	2.6
1	C	421	VAL	2.5
1	D	408	ASP	2.5
1	D	374	LEU	2.5
1	D	447	GLN	2.5
1	D	385	ILE	2.5
1	C	341	GLU	2.4
1	C	472	GLU	2.4
1	D	369	ARG	2.4
1	D	323	PHE	2.4
1	D	333	THR	2.4
1	D	451	THR	2.4
1	D	324	SER	2.4
1	C	338	VAL	2.4
1	D	453	PRO	2.4
1	D	348	ASN	2.3
1	D	472	GLU	2.3
1	D	363	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	409	CYS	2.3
1	B	338	VAL	2.3
1	C	417	ASP	2.2
1	C	428	LEU	2.2
1	D	436	ARG	2.2
1	D	466	ASP	2.2
1	B	417	ASP	2.1
1	D	475	LEU	2.1
1	C	418	LEU	2.1
1	D	415	ARG	2.0
1	C	441	ASP	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	SO4	B	502	5/5	0.83	0.20	4.46	32,37,44,46	0
2	MGT	C	501	33/33	0.76	0.16	0.35	36,48,78,78	0
3	SO4	A	502	5/5	0.95	0.11	0.31	27,28,35,36	0
2	MGT	B	501	33/33	0.88	0.12	-0.00	21,26,53,54	0
3	SO4	C	502	5/5	0.85	0.16	-0.01	74,75,76,77	0
2	MGT	D	501	33/33	0.72	0.18	-0.21	43,50,65,66	0
3	SO4	D	502	5/5	0.73	0.18	-0.23	85,86,86,86	0
2	MGT	A	501	33/33	0.94	0.09	-0.54	10,19,29,30	0



## 6.5 Other polymers

There are no such residues in this entry.