



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2016 – 04:13 PM EDT

PDB ID : 5E7P  
Title : Crystal Structure of MSMEG\_0858 (Uniprot A0QQS4), a AAA ATPase.  
Authors : Unciulac-Carp, M.; Smith, P.; Shuman, S.  
Deposited on : 2015-10-12  
Resolution : 2.51 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

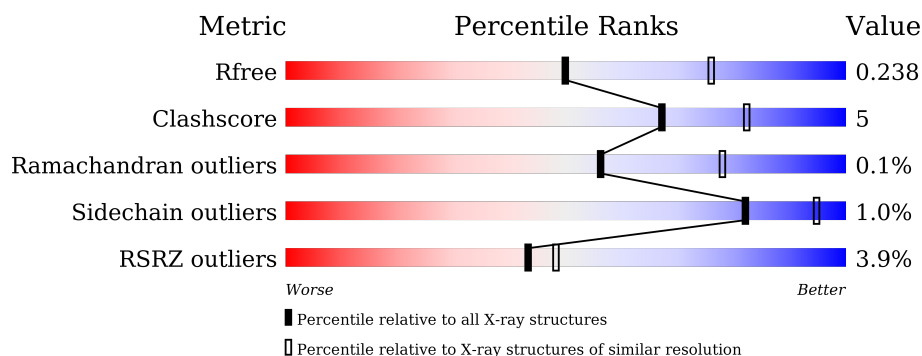
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	745	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	B	745	<div> <div>3%</div> <div>84%</div> <div>10%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PG4	A	903	-	-	X	X
4	GOL	A	904	-	-	-	X
4	GOL	A	905	-	-	-	X
4	GOL	B	905	-	-	X	X
5	PGE	B	903	-	-	-	X
5	PGE	B	904	-	-	X	X

## 2 Entry composition [i](#)

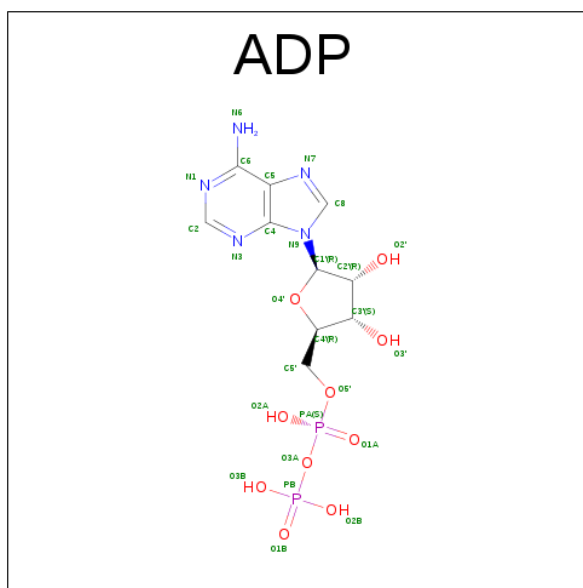
There are 6 unique types of molecules in this entry. The entry contains 10908 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division control protein Cdc48.

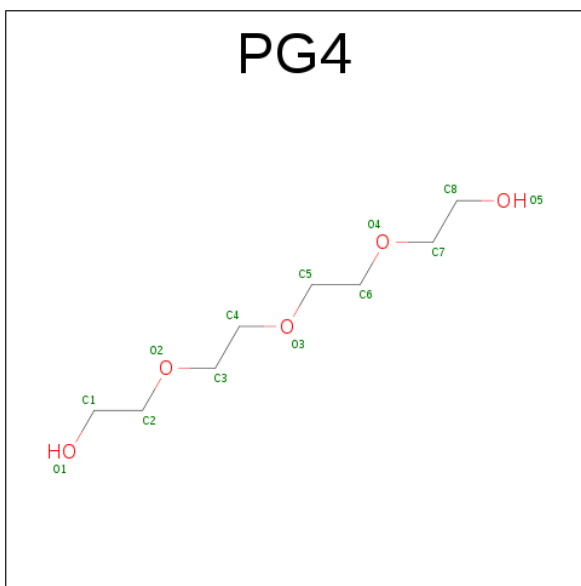
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	1	0
			5267	3284	943	1028	12			
1	B	704	Total	C	N	O	S	0	0	0
			5150	3209	917	1011	13			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



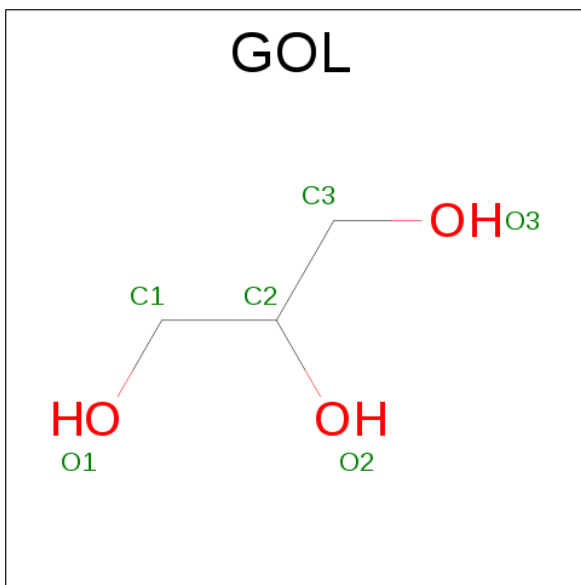
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



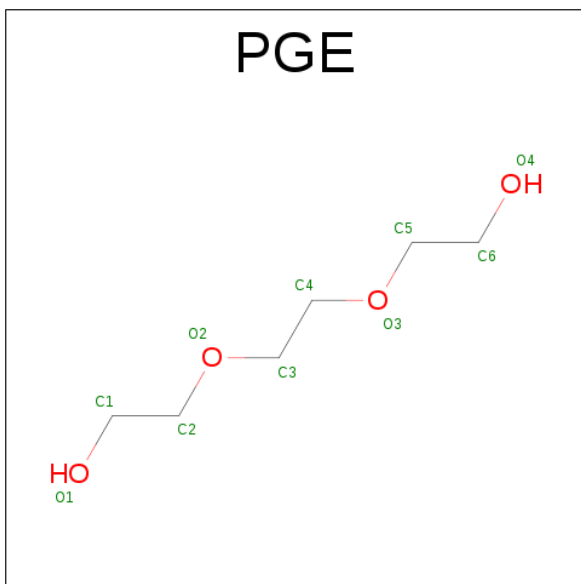
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

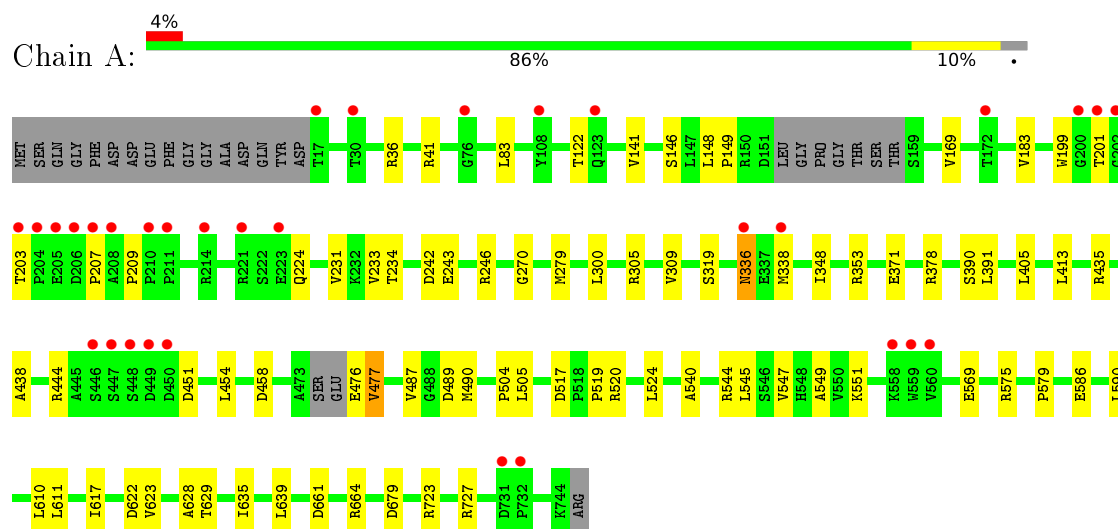
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	180	Total	O	0	0
			180	180		
6	B	152	Total	O	0	0
			152	152		

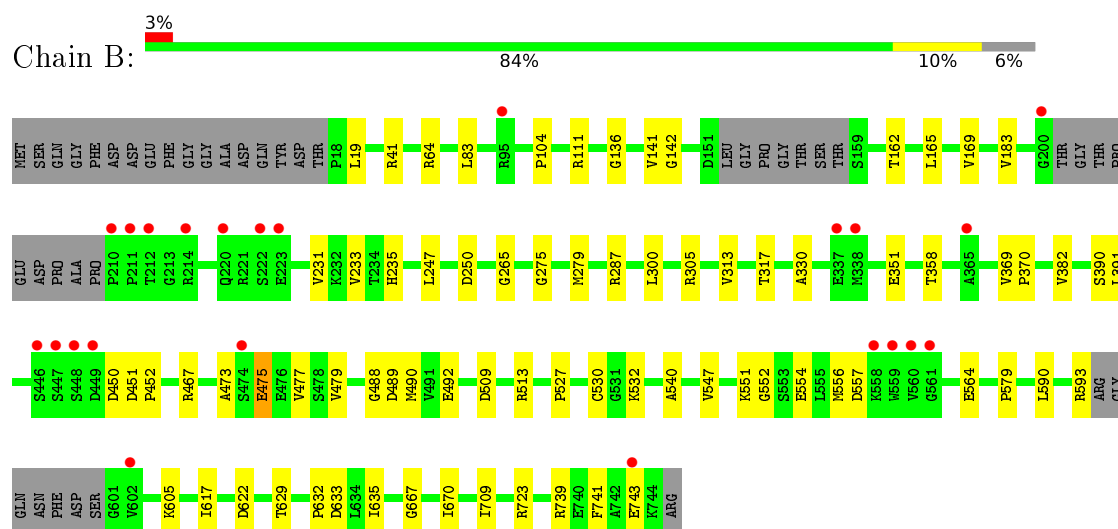
### 3 Residue-property plots [i](#)

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

- Molecule 1: Cell division control protein Cdc48



- Molecule 1: Cell division control protein Cdc48



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.80Å 111.82Å 151.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 2.51 29.52 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.52-2.51) 99.8 (29.52-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_833)	Depositor
R, $R_{free}$	0.206 , 0.251 0.195 , 0.238	Depositor DCC
$R_{free}$ test set	2601 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.9797e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, PGE, ADP

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	0.21	0/5352	0.42	1/7317 (0.0%)
1	B	0.21	0/5228	0.41	0/7146
All	All	0.21	0/10580	0.42	1/14463 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	PRO	N-CA-CB	5.90	110.38	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5267	0	5354	51	0
1	B	5150	0	5224	49	0
2	A	54	0	24	1	0
2	B	54	0	24	2	0
3	A	13	0	18	8	0
4	A	12	0	16	3	0
4	B	6	0	8	4	0
5	B	20	0	28	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	180	0	0	6	0
6	B	152	0	0	4	0
All	All	10908	0	10696	102	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 (102) 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:41:ARG:HB2	1:A:83:LEU:HB2	1.65	0.78
1:B:391:LEU:H	5:B:904:PGE:H22	1.51	0.76
1:B:489:ASP:CG	1:B:490:MET:H	1.90	0.75
1:B:41:ARG:HB2	1:B:83:LEU:HB2	1.70	0.73
1:A:231:VAL:HG22	4:A:904:GOL:H12	1.71	0.72
1:B:629:THR:HG21	1:B:635:ILE:HD11	1.80	0.64
1:B:532:LYS:NZ	6:B:1002:HOH:O	2.26	0.61
1:B:547:VAL:H	5:B:904:PGE:H3	1.65	0.61
1:B:275:GLY:HA3	4:B:905:GOL:H31	1.84	0.60
1:A:444:ARG:NH2	1:A:458:ASP:OD2	2.35	0.59
1:B:739:ARG:O	6:B:1001:HOH:O	2.17	0.59
1:A:540:ALA:HB1	1:A:547:VAL:HG21	1.85	0.59
1:B:250:ASP:OD2	1:B:287:ARG:NH2	2.33	0.58
1:A:353:ARG:NH1	6:A:1008:HOH:O	2.36	0.58
1:B:235:HIS:HD2	4:B:905:GOL:H32	1.69	0.57
1:A:169:VAL:HG12	1:A:435:ARG:HG2	1.87	0.57
1:A:270:GLY:HA2	3:A:903:PG4:H52	1.86	0.56
1:B:743:GLU:OE2	6:B:1001:HOH:O	2.18	0.56
1:A:489:ASP:CG	1:A:490:MET:H	2.09	0.56
1:A:544:ARG:NH2	6:A:1010:HOH:O	2.39	0.55
1:A:549:ALA:HB1	4:A:905:GOL:H11	1.88	0.55
1:B:235:HIS:CD2	4:B:905:GOL:H32	2.42	0.55
2:B:901:ADP:N7	4:B:905:GOL:O2	2.31	0.55
1:A:390:SER:HA	3:A:903:PG4:H31	1.89	0.54
1:A:629:THR:HG21	1:A:635:ILE:HD11	1.89	0.54
1:A:487:VAL:HG13	1:A:490:MET:HE3	1.89	0.54
1:B:547:VAL:N	5:B:904:PGE:H3	2.23	0.54
1:B:488:GLY:O	2:B:902:ADP:N6	2.30	0.54
1:B:552:GLY:HA2	1:B:590:LEU:HG	1.90	0.54
1:A:224:GLN:NE2	6:A:1011:HOH:O	2.39	0.53
1:A:540:ALA:O	3:A:903:PG4:H12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LYS:NZ	1:A:586:GLU:OE2	2.41	0.53
1:A:505:LEU:HD13	1:A:545:LEU:HD13	1.91	0.53
1:B:564:GLU:HG3	1:B:605:LYS:HG2	1.91	0.52
2:A:901:ADP:HN61	4:A:904:GOL:H31	1.74	0.52
1:A:391:LEU:H	3:A:903:PG4:C2	2.21	0.52
1:B:593:ARG:NH1	1:B:633:ASP:O	2.42	0.52
1:A:517:ASP:OD1	6:A:1001:HOH:O	2.19	0.52
1:B:390:SER:HA	5:B:904:PGE:H32	1.92	0.52
1:B:450:ASP:OD1	1:B:451:ASP:N	2.43	0.51
1:A:723:ARG:O	1:A:727:ARG:NH1	2.40	0.51
1:A:664:ARG:NH1	1:A:679:ASP:OD1	2.39	0.51
1:A:547:VAL:HB	3:A:903:PG4:H41	1.93	0.51
1:A:547:VAL:H	3:A:903:PG4:H41	1.76	0.50
1:B:64:ARG:HH12	1:B:142:GLY:HA3	1.77	0.50
1:B:136:GLY:O	1:B:467:ARG:NH2	2.38	0.50
1:B:473:ALA:HB1	1:B:475:GLU:HG3	1.94	0.50
1:B:551:LYS:HB2	1:B:554:GLU:HG2	1.93	0.49
1:B:111:ARG:HA	5:B:903:PGE:H42	1.94	0.49
1:B:231:VAL:HG11	1:B:279:MET:HG3	1.94	0.49
1:A:504:PRO:HB2	1:A:519:PRO:HG3	1.94	0.49
1:A:489:ASP:CG	1:A:490:MET:N	2.66	0.49
1:B:723:ARG:NH2	6:B:1009:HOH:O	2.37	0.49
1:B:479:VAL:HG21	5:B:904:PGE:H42	1.94	0.48
1:A:391:LEU:H	3:A:903:PG4:H22	1.78	0.48
1:A:231:VAL:HG11	1:A:279:MET:HG3	1.95	0.48
1:B:556:MET:HA	1:B:557:ASP:HA	1.50	0.47
1:A:489:ASP:HB2	1:A:661:ASP:HB2	1.96	0.47
1:B:390:SER:HB2	5:B:904:PGE:H2	1.95	0.47
1:B:527:PRO:HG2	1:B:530:CYS:SG	2.55	0.47
1:A:201:THR:HG22	1:A:209:PRO:HG2	1.96	0.47
1:A:476:GLU:HG2	1:A:477:VAL:H	1.80	0.47
1:B:489:ASP:CG	1:B:490:MET:N	2.62	0.47
1:A:438:ALA:HA	1:A:454:LEU:HD11	1.96	0.47
1:B:165:LEU:O	1:B:169:VAL:HG23	2.15	0.46
1:B:667:GLY:HA2	1:B:670:ILE:HD12	1.97	0.46
1:B:313:VAL:HG21	1:B:351:GLU:HB3	1.96	0.46
1:B:330:ALA:HB1	5:B:903:PGE:H52	1.97	0.46
1:A:233:VAL:HG23	1:A:234:THR:HG23	1.97	0.45
1:A:579:PRO:HA	1:A:622:ASP:O	2.17	0.45
1:B:111:ARG:O	5:B:903:PGE:H5	2.17	0.44
1:B:300:LEU:O	1:B:305:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:O	1:A:305:ARG:NH1	2.51	0.44
1:B:265:GLY:HA3	1:B:382:VAL:O	2.18	0.44
1:A:141:VAL:HG23	1:A:183:VAL:HG22	1.99	0.44
1:A:122:THR:HA	1:A:199:TRP:CE2	2.53	0.43
1:A:336:ASN:O	1:A:338:MET:N	2.44	0.43
1:B:391:LEU:N	5:B:904:PGE:H22	2.28	0.43
1:B:540:ALA:HB1	1:B:547:VAL:HG21	2.01	0.43
1:A:617:ILE:HD12	1:A:623:VAL:HG11	2.00	0.42
1:A:378:ARG:HD2	1:A:569:GLU:OE2	2.19	0.42
1:A:611:LEU:HD21	1:A:639:LEU:HD22	2.01	0.42
1:A:148:LEU:HA	1:A:149:PRO:HD3	1.90	0.42
1:A:309:VAL:HG11	1:A:348:ILE:HG23	2.00	0.42
1:B:19:LEU:HD21	1:B:104:PRO:HB2	2.01	0.42
1:A:371:GLU:OE2	6:A:1002:HOH:O	2.21	0.42
1:B:162:THR:HA	1:B:452:PRO:HG3	2.02	0.42
1:A:524:LEU:O	1:A:628:ALA:HA	2.21	0.41
1:A:36:ARG:HG2	1:A:146:SER:OG	2.19	0.41
1:A:590:LEU:HD22	1:A:610:LEU:HD22	2.01	0.41
1:B:247:LEU:HA	1:B:247:LEU:HD12	1.94	0.41
1:B:509:ASP:O	1:B:513:ARG:HG3	2.20	0.41
1:A:405:LEU:HD13	1:A:413:LEU:HD13	2.01	0.41
1:B:317:THR:HG23	1:B:358:THR:HG21	2.01	0.41
1:A:242:ASP:O	1:A:246:ARG:HG3	2.21	0.41
1:A:575:ARG:NH1	6:A:1029:HOH:O	2.53	0.41
1:B:632:PRO:HB2	1:B:741:PHE:CZ	2.56	0.41
1:A:391:LEU:H	3:A:903:PG4:H21	1.85	0.41
1:A:487:VAL:CG1	1:A:490:MET:HE3	2.50	0.41
1:B:369:VAL:HA	1:B:370:PRO:HD3	1.85	0.40
1:B:579:PRO:HA	1:B:622:ASP:O	2.20	0.40
1:B:141:VAL:HG23	1:B:183:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	714/745 (96%)	695 (97%)	18 (2%)	1 (0%)	56	78
1	B	696/745 (93%)	682 (98%)	13 (2%)	1 (0%)	56	78
All	All	1410/1490 (95%)	1377 (98%)	31 (2%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	VAL
1	B	477	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	566/594 (95%)	560 (99%)	6 (1%)	80	94
1	B	554/594 (93%)	549 (99%)	5 (1%)	84	95
All	All	1120/1188 (94%)	1109 (99%)	11 (1%)	82	95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	A	243	GLU
1	A	319	SER
1	A	336	ASN
1	A	451	ASP
1	A	520	ARG
1	B	233	VAL
1	B	475	GLU
1	B	492	GLU
1	B	617	ILE
1	B	709	ILE

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

Mol	Chain	Res	Type
1	A	215	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADP	A	901	-	24,29,29	0.98	1 (4%)	23,45,45	1.82	1 (4%)
2	ADP	A	902	-	24,29,29	1.02	1 (4%)	23,45,45	1.64	2 (8%)
3	PG4	A	903	-	12,12,12	0.73	0	11,11,11	1.56	1 (9%)
4	GOL	A	904	-	5,5,5	0.39	0	5,5,5	0.19	0
4	GOL	A	905	-	5,5,5	0.35	0	5,5,5	0.28	0
2	ADP	B	901	-	24,29,29	1.00	1 (4%)	23,45,45	1.67	1 (4%)
2	ADP	B	902	-	24,29,29	0.99	1 (4%)	23,45,45	1.73	2 (8%)
5	PGE	B	903	-	9,9,9	0.68	0	8,8,8	1.50	1 (12%)
5	PGE	B	904	-	9,9,9	0.68	0	8,8,8	1.66	2 (25%)
4	GOL	B	905	-	5,5,5	0.37	0	5,5,5	0.16	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	ADP	A	901	-	-	0/12/32/32	0/3/3/3
2	ADP	A	902	-	-	0/12/32/32	0/3/3/3
3	PG4	A	903	-	-	0/10/10/10	0/0/0/0
4	GOL	A	904	-	-	0/4/4/4	0/0/0/0
4	GOL	A	905	-	-	0/4/4/4	0/0/0/0
2	ADP	B	901	-	-	0/12/32/32	0/3/3/3
2	ADP	B	902	-	-	0/12/32/32	0/3/3/3
5	PGE	B	903	-	-	0/7/7/7	0/0/0/0
5	PGE	B	904	-	-	0/7/7/7	0/0/0/0
4	GOL	B	905	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADP	C5-C4	3.00	1.47	1.40
2	B	902	ADP	C5-C4	3.05	1.47	1.40
2	B	901	ADP	C5-C4	3.11	1.47	1.40
2	A	902	ADP	C5-C4	3.17	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ADP	N3-C2-N1	-7.14	123.26	128.87
2	B	901	ADP	N3-C2-N1	-6.45	123.81	128.87
2	B	902	ADP	N3-C2-N1	-6.33	123.90	128.87
2	A	902	ADP	N3-C2-N1	-6.08	124.09	128.87
2	B	902	ADP	C2'-C1'-N9	-2.54	106.68	113.47
2	A	902	ADP	C2'-C1'-N9	-2.05	107.98	113.47
5	B	904	PGE	O3-C4-C3	2.03	119.40	110.40
5	B	903	PGE	O3-C4-C3	2.11	119.75	110.40
5	B	904	PGE	O2-C2-C1	2.38	120.22	110.25
3	A	903	PG4	O2-C2-C1	2.77	121.82	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ADP	1	0
3	A	903	PG4	8	0
4	A	904	GOL	2	0
4	A	905	GOL	1	0
2	B	901	ADP	1	0
2	B	902	ADP	1	0
5	B	903	PGE	3	0
5	B	904	PGE	7	0
4	B	905	GOL	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	719/745 (96%)	-0.03	32 (4%) 37 42	22, 44, 88, 147	0
1	B	704/745 (94%)	-0.01	23 (3%) 50 55	19, 46, 89, 134	0
All	All	1423/1490 (95%)	-0.02	55 (3%) 43 48	19, 45, 89, 147	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	MET	6.2
1	B	210	PRO	5.9
1	B	560	VAL	5.5
1	A	338	MET	5.1
1	A	201	THR	5.0
1	B	474	SER	4.6
1	B	559	TRP	4.5
1	A	202	GLY	4.3
1	A	203	THR	4.2
1	A	207	PRO	4.1
1	A	447	SER	4.1
1	A	450	ASP	4.1
1	A	204	PRO	3.9
1	B	223	GLU	3.9
1	A	208	ALA	3.8
1	B	200	GLY	3.6
1	B	211	PRO	3.5
1	B	448	SER	3.5
1	A	336	ASN	3.5
1	A	448	SER	3.4
1	A	200	GLY	3.2
1	B	337	GLU	3.0
1	A	560	VAL	3.0
1	A	731	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	214	ARG	2.9
1	A	558	LYS	2.9
1	B	222	SER	2.9
1	A	449	ASP	2.8
1	A	211	PRO	2.7
1	A	210	PRO	2.7
1	A	206	ASP	2.7
1	A	205	GLU	2.7
1	B	212	THR	2.6
1	A	123	GLN	2.4
1	B	561	GLY	2.4
1	A	17	THR	2.4
1	B	220	GLN	2.4
1	A	108	TYR	2.3
1	A	30	THR	2.3
1	B	602	VAL	2.3
1	B	447	SER	2.3
1	B	449	ASP	2.2
1	A	732	PRO	2.2
1	A	446	SER	2.2
1	A	214	ARG	2.2
1	A	76	GLY	2.1
1	B	558	LYS	2.1
1	A	559	TRP	2.1
1	A	223	GLU	2.1
1	B	365	ALA	2.0
1	B	446	SER	2.0
1	B	743	GLU	2.0
1	B	95	ARG	2.0
1	A	172	THR	2.0
1	A	221	ARG	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	PG4	A	903	13/13	0.68	0.48	14.25	84,89,91,91	0
4	GOL	A	905	6/6	0.88	0.40	13.51	96,96,96,97	0
5	PGE	B	904	10/10	0.69	0.45	11.07	70,72,74,75	0
4	GOL	A	904	6/6	0.79	0.45	9.78	66,68,69,71	0
5	PGE	B	903	10/10	0.73	0.39	9.49	79,80,80,80	0
4	GOL	B	905	6/6	0.90	0.34	9.06	48,50,52,55	0
2	ADP	A	901	27/27	0.96	0.18	1.29	24,46,57,59	0
2	ADP	B	901	27/27	0.96	0.18	1.10	20,44,56,57	0
2	ADP	A	902	27/27	0.92	0.15	0.01	50,63,91,92	0
2	ADP	B	902	27/27	0.93	0.13	-0.16	56,62,72,147	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.