



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:36 PM BST

PDB ID : 2P8Y  
EMDB ID: : EMD-1344  
Title : Fitted structure of ADPR-eEF2 in the 80S:ADPR-eEF2:GDP:sordarin cryo-EM reconstruction  
Authors : Taylor, D.J.; Nilsson, J.; Merrill, A.R.; Andersen, G.R.; Nissen, P.; Frank, J.  
Deposited on : 2007-03-23  
Resolution : 11.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

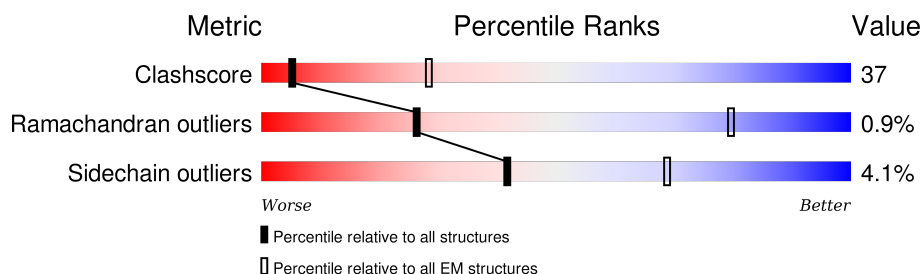
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.70 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	T	842	

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
1	DDE	T	699	-	-	X	-
2	APR	T	1699	X	-	-	-
3	SO1	T	1700	X	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

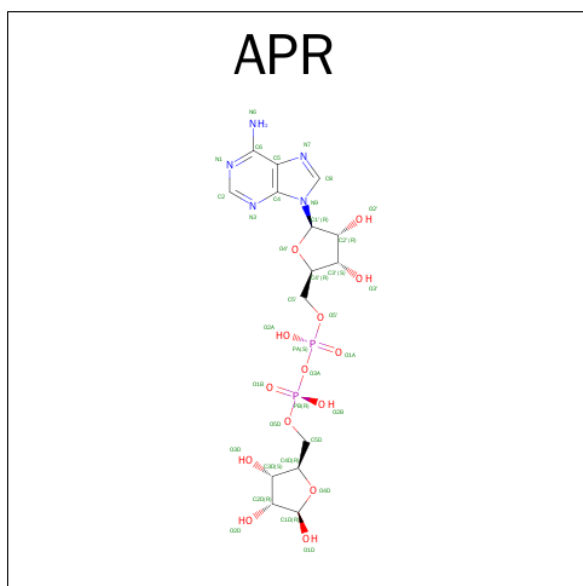
- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	T	814	6342	4035	1082	1195	30	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324

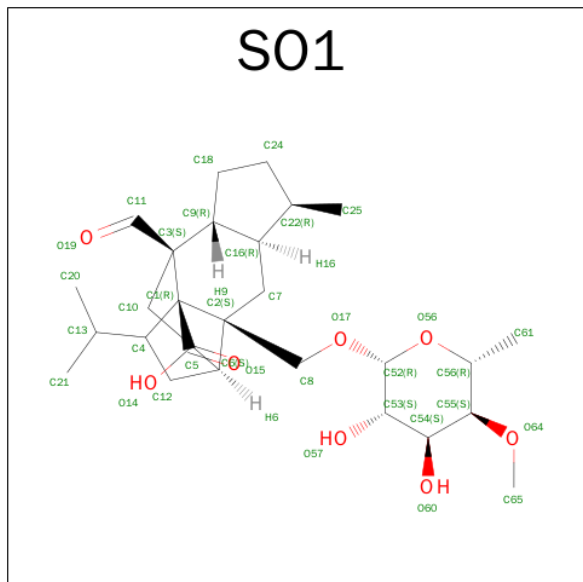
- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula:  $C_{15}H_{23}N_5O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	T	1	35	15	5	13	2	0

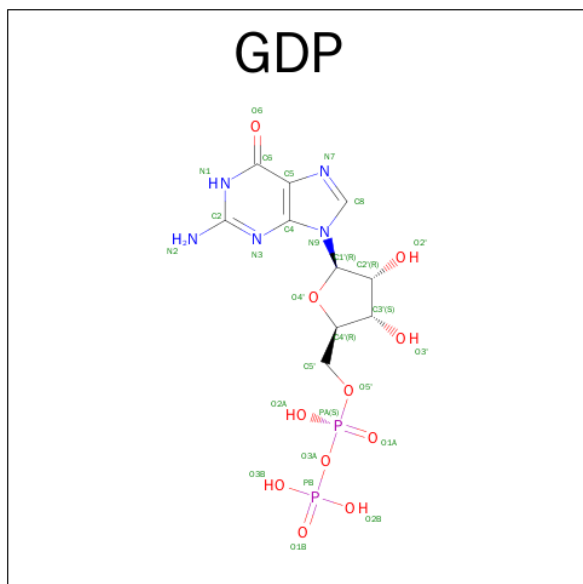
- Molecule 3 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.B.ETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-M

ETHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula:  $C_{27}H_{42}O_8$ ).



Mol	Chain	Residues	Atoms			AltConf
3	T	1	Total	C	O	0
			35	27	8	

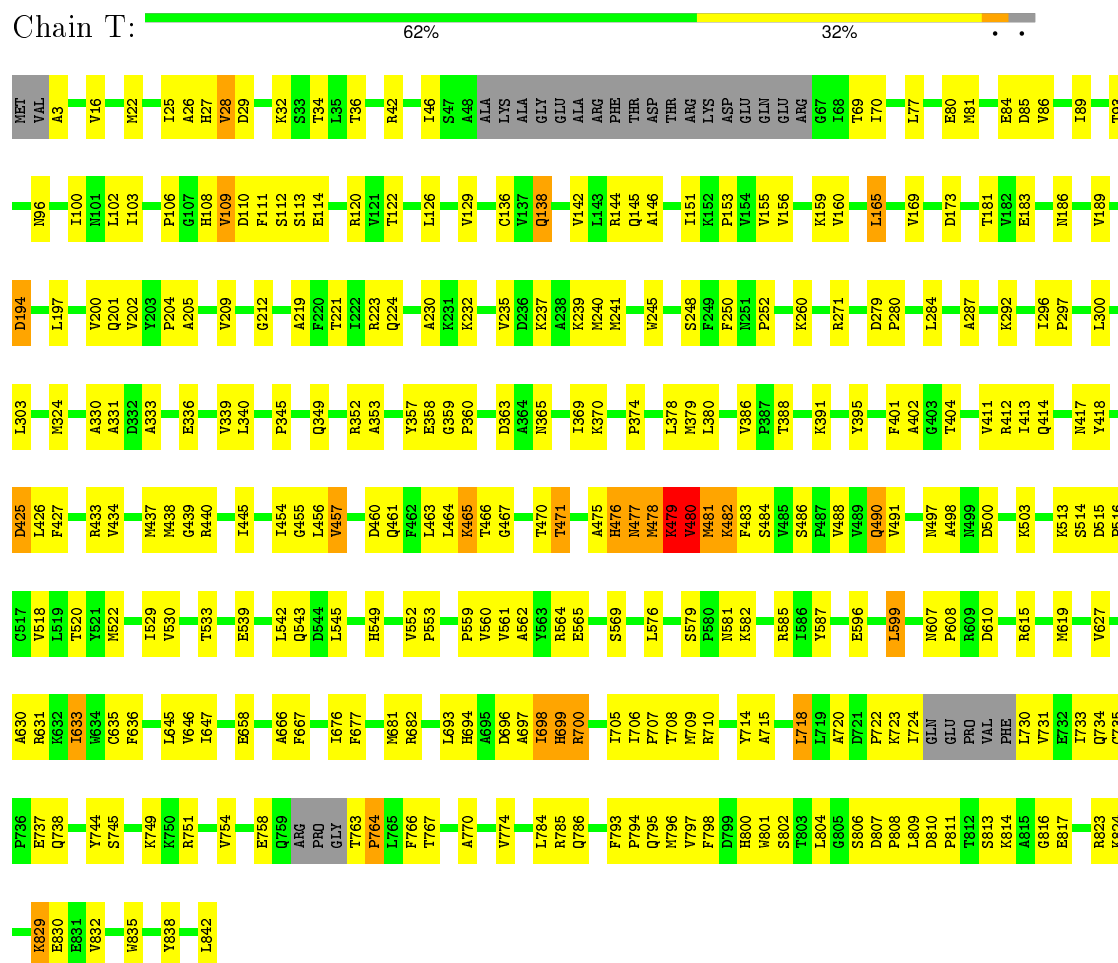
- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



### 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. 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. 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: Elongation factor 2



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of 3D-maps by Wiener filtration	Depositor
Microscope	FEI Tecnai F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2500	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	39000	Depositor
Image detector	Kodak SO163 film	Depositor

## 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: GDP, SO1, DDE, APR

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	T	1.03	11/6431 (0.2%)	0.80	17/8688 (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	T	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	481	MET	N-CA	35.95	2.18	1.46
1	T	480	VAL	N-CA	32.97	2.12	1.46
1	T	480	VAL	CA-C	30.56	2.32	1.52
1	T	479	LYS	C-N	28.36	1.99	1.34
1	T	479	LYS	N-CA	22.20	1.90	1.46
1	T	479	LYS	CA-C	21.18	2.08	1.52
1	T	481	MET	CA-C	14.97	1.91	1.52
1	T	478	MET	C-N	14.95	1.68	1.34
1	T	482	LYS	N-CA	14.21	1.74	1.46
1	T	478	MET	CA-C	9.71	1.78	1.52
1	T	478	MET	N-CA	6.00	1.58	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	480	VAL	N-CA-C	19.14	162.66	111.00
1	T	481	MET	CB-CA-C	-14.71	80.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	479	LYS	CA-C-N	13.31	146.49	117.20
1	T	479	LYS	N-CA-C	12.82	145.61	111.00
1	T	481	MET	N-CA-C	11.71	142.62	111.00
1	T	480	VAL	N-CA-CB	-11.47	86.27	111.50
1	T	479	LYS	C-N-CA	10.03	146.76	121.70
1	T	479	LYS	O-C-N	-9.17	108.02	122.70
1	T	481	MET	N-CA-CB	9.10	126.98	110.60
1	T	480	VAL	CA-C-O	-8.95	101.31	120.10
1	T	478	MET	C-N-CA	8.68	143.40	121.70
1	T	482	LYS	N-CA-CB	7.96	124.93	110.60
1	T	479	LYS	N-CA-CB	-7.66	96.80	110.60
1	T	478	MET	CA-C-N	7.17	132.97	117.20
1	T	482	LYS	CB-CA-C	-7.04	96.32	110.40
1	T	479	LYS	CA-C-O	-6.96	105.48	120.10
1	T	478	MET	O-C-N	-5.75	113.50	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	698	ILE	Mainchain
1	T	699	DDE	Mainchain,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	T	6342	0	6400	471	0
2	T	35	0	19	7	0
3	T	35	0	40	67	0
4	T	28	0	12	3	0
All	All	6440	0	6471	471	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 37.

All (471) 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:T:798:PHE:CB	3:T:1700:SO1:H6	1.24	1.61
1:T:145:GLN:HA	1:T:481:MET:CB	1.12	1.60
1:T:798:PHE:CD1	3:T:1700:SO1:H102	1.06	1.57
1:T:144:ARG:CD	1:T:482:LYS:N	1.69	1.53
1:T:798:PHE:CG	3:T:1700:SO1:H102	1.44	1.53
1:T:798:PHE:HB2	3:T:1700:SO1:C6	1.35	1.53
1:T:800:HIS:HB2	1:T:801:TRP:CA	1.35	1.52
1:T:111:PHE:CD1	1:T:483:PHE:HZ	1.24	1.51
1:T:798:PHE:CZ	3:T:1700:SO1:H182	1.47	1.50
1:T:111:PHE:CD1	1:T:483:PHE:CZ	2.00	1.49
1:T:481:MET:C	1:T:481:MET:HG3	1.24	1.48
1:T:145:GLN:CG	1:T:481:MET:HB3	1.39	1.47
1:T:478:MET:CA	1:T:478:MET:C	1.78	1.47
1:T:145:GLN:CA	1:T:481:MET:HB2	0.99	1.47
1:T:482:LYS:N	1:T:482:LYS:CA	1.74	1.47
1:T:478:MET:C	1:T:479:LYS:N	1.68	1.44
1:T:800:HIS:CB	1:T:801:TRP:N	1.80	1.44
1:T:800:HIS:HB2	1:T:801:TRP:N	1.11	1.42
1:T:111:PHE:CE1	1:T:483:PHE:HZ	1.38	1.42
1:T:798:PHE:CD2	3:T:1700:SO1:H16	0.87	1.40
1:T:221:THR:HG21	1:T:336:GLU:CD	1.40	1.40
1:T:481:MET:C	1:T:481:MET:CA	1.91	1.37
1:T:144:ARG:HD3	1:T:482:LYS:N	1.13	1.36
1:T:113:SER:OG	1:T:516:PRO:CG	1.74	1.35
1:T:798:PHE:CE2	3:T:1700:SO1:H182	1.61	1.35
1:T:479:LYS:CA	1:T:479:LYS:N	1.90	1.32
1:T:561:VAL:CG2	1:T:774:VAL:CG1	2.07	1.32
1:T:111:PHE:HD1	1:T:483:PHE:CZ	1.40	1.29
1:T:481:MET:C	1:T:481:MET:CG	2.01	1.29
1:T:561:VAL:HG21	1:T:774:VAL:CB	1.62	1.29
1:T:465:LYS:HE3	1:T:513:LYS:O	1.30	1.27
1:T:221:THR:HG21	1:T:336:GLU:OE1	1.35	1.26
1:T:70:ILE:HD11	1:T:439:GLY:O	1.08	1.24
1:T:120:ARG:HH22	1:T:480:VAL:CA	1.48	1.24
1:T:561:VAL:CG2	1:T:774:VAL:HG11	1.68	1.22
1:T:479:LYS:CA	1:T:479:LYS:C	2.08	1.22
1:T:70:ILE:CD1	1:T:439:GLY:O	1.88	1.22
1:T:798:PHE:CE2	3:T:1700:SO1:H16	1.74	1.21
1:T:114:GLU:OE1	1:T:516:PRO:HD3	1.06	1.21
1:T:798:PHE:CE2	3:T:1700:SO1:C18	2.23	1.20
1:T:145:GLN:CG	1:T:481:MET:CB	2.19	1.20
1:T:798:PHE:CE1	3:T:1700:SO1:H102	1.76	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:144:ARG:NH1	1:T:482:LYS:N	1.88	1.18
1:T:113:SER:OG	1:T:516:PRO:HG3	1.30	1.17
1:T:561:VAL:CG2	1:T:774:VAL:CB	2.22	1.17
1:T:797:VAL:HG23	3:T:1700:SO1:O57	1.41	1.16
1:T:561:VAL:CG2	1:T:774:VAL:HB	1.75	1.16
1:T:114:GLU:OE1	1:T:516:PRO:CD	1.93	1.16
1:T:221:THR:HG21	1:T:336:GLU:OE2	1.42	1.15
1:T:479:LYS:C	1:T:480:VAL:N	1.99	1.15
1:T:800:HIS:HB2	1:T:801:TRP:HA	1.27	1.14
1:T:70:ILE:H	1:T:440:ARG:HB3	1.10	1.13
1:T:480:VAL:N	1:T:480:VAL:CA	2.12	1.13
1:T:120:ARG:NH2	1:T:480:VAL:HA	1.65	1.12
1:T:221:THR:CG2	1:T:336:GLU:OE1	1.96	1.12
1:T:798:PHE:CG	3:T:1700:SO1:C10	2.13	1.12
1:T:480:VAL:N	1:T:480:VAL:CG2	2.12	1.12
1:T:798:PHE:CG	3:T:1700:SO1:H16	1.84	1.11
1:T:797:VAL:HG22	3:T:1700:SO1:O57	1.43	1.10
1:T:798:PHE:CE2	3:T:1700:SO1:C16	2.32	1.10
1:T:111:PHE:CE1	1:T:483:PHE:CZ	2.25	1.10
1:T:120:ARG:NH2	1:T:480:VAL:CA	2.13	1.10
1:T:480:VAL:C	1:T:481:MET:N	2.05	1.10
1:T:464:LEU:HD13	1:T:513:LYS:NZ	1.66	1.09
1:T:561:VAL:HG22	1:T:774:VAL:HG11	1.12	1.09
1:T:481:MET:HE3	1:T:482:LYS:N	1.65	1.07
1:T:69:THR:HB	1:T:440:ARG:NH1	1.70	1.07
1:T:481:MET:CA	1:T:481:MET:N	2.18	1.07
1:T:561:VAL:HG22	1:T:774:VAL:CG1	1.78	1.05
1:T:798:PHE:CB	3:T:1700:SO1:C6	2.08	1.04
1:T:798:PHE:CG	3:T:1700:SO1:C6	2.38	1.04
1:T:560:VAL:O	3:T:1700:SO1:C20	2.06	1.04
1:T:113:SER:H	1:T:516:PRO:HG2	1.23	1.03
1:T:109:VAL:HG21	1:T:138:GLN:HG2	1.37	1.02
1:T:219:ALA:HB1	1:T:333:ALA:HB2	1.42	1.02
1:T:145:GLN:CB	1:T:481:MET:CB	2.39	1.01
1:T:481:MET:C	1:T:481:MET:CB	2.29	1.01
1:T:111:PHE:CZ	1:T:482:LYS:N	2.30	1.00
1:T:111:PHE:HZ	1:T:482:LYS:N	1.59	1.00
1:T:800:HIS:CB	1:T:801:TRP:CA	2.27	0.99
1:T:126:LEU:HD11	1:T:156:VAL:HG23	1.43	0.99
1:T:480:VAL:HG22	1:T:480:VAL:N	1.75	0.99
1:T:480:VAL:C	1:T:480:VAL:CA	2.32	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:145:GLN:CB	1:T:481:MET:HB2	1.93	0.98
1:T:798:PHE:CZ	3:T:1700:SO1:C18	2.43	0.97
1:T:145:GLN:HG2	1:T:481:MET:HB3	0.97	0.97
1:T:465:LYS:CE	1:T:513:LYS:O	2.12	0.97
1:T:481:MET:CE	1:T:482:LYS:N	2.28	0.96
1:T:464:LEU:HD13	1:T:513:LYS:HZ3	1.22	0.96
1:T:800:HIS:CB	1:T:801:TRP:HA	1.94	0.96
1:T:797:VAL:HG23	3:T:1700:SO1:C53	1.96	0.96
1:T:113:SER:HG	1:T:516:PRO:HG3	1.31	0.96
1:T:221:THR:CG2	1:T:336:GLU:CD	2.32	0.95
1:T:724:ILE:HD11	1:T:804:LEU:HD12	1.50	0.94
1:T:145:GLN:CA	1:T:481:MET:CB	1.89	0.94
1:T:561:VAL:HG21	1:T:774:VAL:HB	0.94	0.93
1:T:144:ARG:CZ	1:T:482:LYS:N	2.32	0.93
1:T:481:MET:HA	1:T:481:MET:N	1.84	0.93
1:T:145:GLN:HG3	1:T:481:MET:HB3	1.49	0.92
1:T:70:ILE:HD11	1:T:439:GLY:C	1.81	0.92
1:T:144:ARG:HD2	1:T:482:LYS:N	1.84	0.92
1:T:798:PHE:CE2	3:T:1700:SO1:C24	2.53	0.91
1:T:113:SER:OG	1:T:516:PRO:HG2	1.71	0.91
1:T:798:PHE:CG	3:T:1700:SO1:H6	2.02	0.90
1:T:145:GLN:HG2	1:T:481:MET:CB	1.93	0.90
1:T:70:ILE:O	1:T:440:ARG:CG	2.19	0.89
1:T:27:HIS:CD2	1:T:138:GLN:HB2	2.07	0.89
1:T:800:HIS:HB3	1:T:801:TRP:N	1.87	0.89
1:T:70:ILE:O	1:T:440:ARG:HD2	1.73	0.88
1:T:463:LEU:HD21	1:T:467:GLY:HA3	1.55	0.88
1:T:126:LEU:HD11	1:T:156:VAL:CG2	2.03	0.88
1:T:798:PHE:CD1	3:T:1700:SO1:H101	2.07	0.87
1:T:144:ARG:NE	1:T:482:LYS:N	2.21	0.87
1:T:70:ILE:HG23	1:T:440:ARG:O	1.73	0.87
1:T:797:VAL:HG23	3:T:1700:SO1:C54	2.06	0.86
1:T:797:VAL:HA	3:T:1700:SO1:H53	1.58	0.84
1:T:111:PHE:HE1	1:T:483:PHE:CZ	1.94	0.84
1:T:221:THR:CG2	1:T:336:GLU:OE2	2.24	0.84
1:T:70:ILE:N	1:T:440:ARG:HB3	1.93	0.83
1:T:145:GLN:HG3	1:T:481:MET:CB	2.05	0.83
1:T:562:ALA:CB	3:T:1700:SO1:C11	2.56	0.83
1:T:113:SER:N	1:T:516:PRO:HG2	1.93	0.82
1:T:560:VAL:O	3:T:1700:SO1:H203	1.79	0.82
1:T:145:GLN:CB	1:T:481:MET:HB3	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:145:GLN:HG3	1:T:481:MET:HG2	1.59	0.82
1:T:70:ILE:O	1:T:440:ARG:CD	2.28	0.82
1:T:798:PHE:CE2	3:T:1700:SO1:C22	2.63	0.81
1:T:562:ALA:CB	3:T:1700:SO1:H11	2.10	0.81
1:T:109:VAL:CG2	1:T:138:GLN:HG2	2.11	0.81
1:T:111:PHE:CE2	1:T:481:MET:HG2	2.16	0.81
1:T:111:PHE:HE2	1:T:481:MET:HG2	1.45	0.81
1:T:488:VAL:CG1	1:T:796:MET:HE2	2.11	0.80
1:T:798:PHE:HD2	3:T:1700:SO1:H16	0.97	0.80
1:T:70:ILE:O	1:T:440:ARG:HG2	1.79	0.80
1:T:486:SER:OG	1:T:795:GLN:HG3	1.82	0.79
1:T:120:ARG:HH21	1:T:480:VAL:HA	1.45	0.79
1:T:145:GLN:HA	1:T:481:MET:CA	2.13	0.79
1:T:562:ALA:HB3	3:T:1700:SO1:C11	2.13	0.78
1:T:562:ALA:HB2	3:T:1700:SO1:H11	1.64	0.78
1:T:798:PHE:CD2	3:T:1700:SO1:C7	2.67	0.78
1:T:488:VAL:HG12	1:T:796:MET:HE2	1.65	0.78
1:T:120:ARG:NH2	1:T:480:VAL:N	2.33	0.77
1:T:698:ILE:HG23	1:T:699:DDE:CG	2.13	0.77
1:T:751:ARG:HD2	1:T:814:LYS:HZ2	1.50	0.77
1:T:813:SER:O	1:T:817:GLU:HG3	1.84	0.76
1:T:69:THR:CB	1:T:440:ARG:NH1	2.47	0.76
1:T:560:VAL:O	3:T:1700:SO1:H201	1.86	0.76
1:T:114:GLU:CD	1:T:516:PRO:HD3	2.04	0.76
1:T:145:GLN:HG3	1:T:481:MET:CG	2.16	0.76
1:T:561:VAL:HG21	1:T:774:VAL:CG1	1.97	0.76
1:T:798:PHE:CD2	3:T:1700:SO1:C22	2.69	0.76
1:T:22:MET:SD	1:T:102:LEU:HD12	2.26	0.75
1:T:120:ARG:HH22	1:T:480:VAL:N	1.85	0.75
1:T:576:LEU:HD21	1:T:842:LEU:HG	1.69	0.74
1:T:34:THR:HG23	4:T:843:GDP:O2A	1.86	0.74
1:T:205:ALA:HB2	1:T:245:TRP:CD1	2.22	0.74
1:T:698:ILE:HG23	1:T:699:DDE:CD2	2.18	0.74
1:T:751:ARG:CD	1:T:814:LYS:NZ	2.50	0.73
1:T:219:ALA:HB1	1:T:333:ALA:CB	2.16	0.73
1:T:698:ILE:HG23	1:T:699:DDE:CE1	2.19	0.73
1:T:378:LEU:H	1:T:471:THR:HG22	1.54	0.73
1:T:219:ALA:HB2	1:T:330:ALA:HA	1.70	0.72
1:T:111:PHE:HE2	1:T:481:MET:CG	2.01	0.72
1:T:797:VAL:HG23	3:T:1700:SO1:H54	1.70	0.72
1:T:221:THR:HG22	1:T:336:GLU:OE1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:464:LEU:O	1:T:465:LYS:HB2	1.90	0.72
1:T:145:GLN:CA	1:T:481:MET:CG	2.67	0.72
1:T:480:VAL:HG23	1:T:480:VAL:N	2.02	0.72
1:T:219:ALA:CB	1:T:333:ALA:HB2	2.19	0.71
1:T:353:ALA:CB	1:T:370:LYS:HG2	2.19	0.71
1:T:561:VAL:HG22	1:T:774:VAL:CB	2.07	0.71
1:T:694:HIS:O	1:T:700:ARG:HD3	1.89	0.71
1:T:70:ILE:CG2	1:T:440:ARG:O	2.39	0.71
1:T:798:PHE:HE2	3:T:1700:SO1:C24	2.01	0.70
1:T:698:ILE:CG2	1:T:699:DDE:CD2	2.70	0.70
1:T:699:DDE:HAA1	2:T:1699:APR:H5'2	1.74	0.70
1:T:798:PHE:CD2	3:T:1700:SO1:H102	2.22	0.70
1:T:488:VAL:HB	1:T:796:MET:HE1	1.73	0.70
1:T:223:ARG:HH11	1:T:223:ARG:HG2	1.57	0.70
1:T:32:LYS:O	1:T:36:THR:HG23	1.92	0.69
1:T:479:LYS:N	1:T:479:LYS:CB	2.56	0.69
1:T:374:PRO:O	1:T:404:THR:HG23	1.92	0.69
1:T:111:PHE:HD1	1:T:483:PHE:CE1	2.07	0.69
1:T:488:VAL:HB	1:T:796:MET:CE	2.23	0.68
1:T:189:VAL:CG1	1:T:200:VAL:HG13	2.22	0.68
1:T:480:VAL:CB	1:T:480:VAL:N	2.56	0.67
1:T:561:VAL:HG23	1:T:774:VAL:CG1	2.19	0.67
1:T:798:PHE:CE1	3:T:1700:SO1:C10	2.57	0.67
1:T:630:ALA:O	1:T:633:ILE:HG23	1.94	0.67
1:T:559:PRO:HB2	3:T:1700:SO1:C20	2.24	0.67
1:T:103:ILE:HD12	1:T:122:THR:HG22	1.77	0.67
1:T:478:MET:HA	1:T:478:MET:C	2.08	0.67
1:T:699:DDE:HAA1	2:T:1699:APR:C5'	2.26	0.66
1:T:751:ARG:HD2	1:T:814:LYS:NZ	2.10	0.66
1:T:731:VAL:HG12	1:T:770:ALA:O	1.95	0.66
1:T:737:GLU:HB2	1:T:766:PHE:CE2	2.30	0.66
1:T:490:GLN:H	1:T:559:PRO:HD3	1.62	0.65
1:T:763:THR:N	1:T:764:PRO:HD3	2.12	0.65
1:T:798:PHE:CB	3:T:1700:SO1:C2	2.75	0.65
1:T:798:PHE:HZ	1:T:801:TRP:CH2	2.14	0.64
1:T:829:LYS:CE	1:T:830:GLU:H	2.11	0.64
1:T:800:HIS:CG	1:T:801:TRP:N	2.62	0.64
1:T:829:LYS:HE3	1:T:829:LYS:HA	1.78	0.64
1:T:800:HIS:HD2	1:T:802:SER:N	1.95	0.63
1:T:284:LEU:HD13	1:T:324:MET:HE1	1.80	0.63
1:T:237:LYS:O	1:T:241:MET:HG2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:113:SER:OG	1:T:516:PRO:CB	2.45	0.63
1:T:627:VAL:O	1:T:631:ARG:HG3	1.98	0.63
1:T:798:PHE:CE2	3:T:1700:SO1:C9	2.81	0.63
1:T:633:ILE:HD12	1:T:635:CYS:N	2.14	0.63
1:T:734:GLN:HG3	1:T:767:THR:HG22	1.80	0.63
1:T:86:VAL:HG13	1:T:93:THR:HG21	1.81	0.63
1:T:698:ILE:HG23	1:T:699:DDE:ND1	2.14	0.62
1:T:433:ARG:HB3	1:T:457:VAL:CG1	2.30	0.62
1:T:718:LEU:HB3	1:T:835:TRP:HB3	1.82	0.62
1:T:204:PRO:HB2	1:T:245:TRP:CZ2	2.35	0.61
1:T:797:VAL:HA	3:T:1700:SO1:C53	2.30	0.61
1:T:559:PRO:HB2	3:T:1700:SO1:H201	1.82	0.61
1:T:520:THR:HG22	1:T:530:VAL:HG22	1.81	0.61
1:T:576:LEU:HD11	1:T:585:ARG:HD3	1.82	0.61
1:T:284:LEU:CD1	1:T:324:MET:HE1	2.31	0.61
1:T:561:VAL:HG23	1:T:774:VAL:HG11	1.77	0.61
1:T:798:PHE:HB3	3:T:1700:SO1:H72	1.83	0.61
1:T:694:HIS:CD2	1:T:696:ASP:H	2.19	0.61
1:T:698:ILE:CG2	1:T:699:DDE:NE2	2.64	0.61
1:T:800:HIS:CD2	1:T:802:SER:N	2.69	0.60
1:T:324:MET:HA	1:T:324:MET:HE2	1.82	0.60
1:T:800:HIS:CG	1:T:801:TRP:CA	2.84	0.60
1:T:284:LEU:HD13	1:T:324:MET:CE	2.32	0.60
1:T:564:ARG:HG3	1:T:682:ARG:HB2	1.83	0.60
1:T:126:LEU:CD1	1:T:156:VAL:HG23	2.25	0.59
1:T:379:MET:HB2	1:T:402:ALA:HB3	1.83	0.59
1:T:202:VAL:HG12	1:T:209:VAL:CG2	2.33	0.59
1:T:561:VAL:CG2	1:T:774:VAL:HG12	2.23	0.59
1:T:111:PHE:CD1	1:T:483:PHE:CE1	2.82	0.59
1:T:365:ASN:O	1:T:369:ILE:HG12	2.03	0.58
1:T:479:LYS:C	1:T:480:VAL:HG22	2.24	0.58
1:T:497:ASN:HB3	1:T:500:ASP:OD2	2.04	0.58
1:T:751:ARG:HD3	1:T:814:LYS:NZ	2.20	0.57
1:T:464:LEU:HD13	1:T:513:LYS:CE	2.33	0.57
1:T:797:VAL:CG2	3:T:1700:SO1:C53	2.65	0.57
1:T:464:LEU:CD1	1:T:513:LYS:HZ3	2.08	0.57
1:T:545:LEU:HA	1:T:549:HIS:HB2	1.85	0.57
1:T:386:VAL:HG11	1:T:437:MET:CE	2.34	0.57
1:T:581:ASN:O	1:T:582:LYS:HB2	2.05	0.57
1:T:296:ILE:O	1:T:300:LEU:HD13	2.05	0.57
1:T:797:VAL:HG22	3:T:1700:SO1:H57	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3:ALA:HA	1:T:46:ILE:O	2.05	0.56
1:T:500:ASP:HB3	1:T:552:VAL:HG11	1.87	0.56
1:T:500:ASP:CB	1:T:552:VAL:HG11	2.35	0.56
1:T:798:PHE:HE2	3:T:1700:SO1:H242	1.71	0.56
1:T:106:PRO:HB3	1:T:108:HIS:NE2	2.21	0.56
1:T:751:ARG:CD	1:T:814:LYS:HZ3	2.17	0.56
1:T:89:ILE:HG12	1:T:340:LEU:HD23	1.88	0.56
1:T:615:ARG:HG2	1:T:619:MET:HE3	1.87	0.55
1:T:490:GLN:HG3	1:T:559:PRO:HG3	1.88	0.55
1:T:108:HIS:CE1	1:T:114:GLU:HB2	2.41	0.55
1:T:26:ALA:HB3	1:T:32:LYS:HB2	1.88	0.55
1:T:829:LYS:HE3	1:T:830:GLU:H	1.71	0.55
1:T:129:VAL:HG11	1:T:181:THR:CG2	2.36	0.55
1:T:800:HIS:C	1:T:801:TRP:HA	2.27	0.55
1:T:698:ILE:HG23	1:T:699:DDE:NE2	2.21	0.55
1:T:223:ARG:HA	1:T:241:MET:HE2	1.88	0.55
1:T:615:ARG:HG2	1:T:619:MET:CE	2.36	0.55
1:T:194:ASP:HB2	1:T:197:LEU:HD13	1.89	0.55
1:T:413:ILE:HB	1:T:427:PHE:HB2	1.88	0.54
1:T:490:GLN:HB2	1:T:559:PRO:HB3	1.89	0.54
1:T:700:ARG:O	1:T:705:ILE:HD12	2.08	0.54
1:T:369:ILE:HD12	1:T:401:PHE:HB3	1.90	0.54
1:T:296:ILE:HB	1:T:297:PRO:HD3	1.89	0.54
1:T:279:ASP:HB3	1:T:280:PRO:HD3	1.89	0.54
1:T:108:HIS:HE1	1:T:114:GLU:HB2	1.72	0.54
1:T:378:LEU:H	1:T:471:THR:CG2	2.21	0.54
1:T:560:VAL:O	3:T:1700:SO1:C13	2.55	0.53
1:T:798:PHE:CD2	3:T:1700:SO1:C9	2.85	0.53
1:T:520:THR:HA	1:T:529:ILE:O	2.08	0.53
1:T:360:PRO:O	1:T:363:ASP:HB3	2.08	0.53
1:T:798:PHE:CG	3:T:1700:SO1:C16	2.66	0.53
1:T:829:LYS:HE2	1:T:830:GLU:H	1.74	0.53
1:T:111:PHE:CE1	1:T:483:PHE:CE2	2.95	0.53
1:T:806:SER:HB2	1:T:813:SER:HB2	1.90	0.53
1:T:500:ASP:CG	1:T:552:VAL:HG11	2.29	0.53
1:T:109:VAL:HG11	1:T:142:VAL:CG2	2.38	0.52
1:T:798:PHE:H	3:T:1700:SO1:H53	1.74	0.52
1:T:515:ASP:HB3	1:T:518:VAL:CG1	2.39	0.52
1:T:28:VAL:HG22	1:T:138:GLN:OE1	2.08	0.52
1:T:646:VAL:C	1:T:647:ILE:HD12	2.29	0.52
1:T:129:VAL:HG11	1:T:181:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:561:VAL:HA	3:T:1700:SO1:H203	1.91	0.52
1:T:464:LEU:CD1	1:T:513:LYS:NZ	2.57	0.52
1:T:693:LEU:HB3	1:T:700:ARG:HD2	1.92	0.52
1:T:745:SER:O	1:T:749:LYS:HG3	2.10	0.52
1:T:471:THR:HG23	1:T:471:THR:O	2.09	0.51
1:T:250:PHE:O	1:T:252:PRO:HD3	2.10	0.51
1:T:113:SER:CB	1:T:516:PRO:HG2	2.39	0.51
1:T:426:LEU:HD12	1:T:427:PHE:H	1.76	0.51
1:T:785:ARG:HH11	1:T:785:ARG:HG3	1.75	0.51
1:T:694:HIS:CD2	1:T:699:DDE:HD2	2.46	0.51
1:T:569:SER:O	1:T:720:ALA:HB1	2.10	0.51
1:T:559:PRO:C	3:T:1700:SO1:H201	2.31	0.51
1:T:800:HIS:CG	1:T:801:TRP:HA	2.46	0.51
1:T:479:LYS:N	1:T:479:LYS:HB2	2.26	0.51
1:T:751:ARG:HD3	1:T:814:LYS:HZ3	1.76	0.51
1:T:223:ARG:HG2	1:T:223:ARG:NH1	2.21	0.51
1:T:189:VAL:HG13	1:T:200:VAL:HG13	1.92	0.51
1:T:718:LEU:HD12	1:T:722:PRO:HG2	1.92	0.51
1:T:470:THR:HG21	1:T:475:ALA:HB1	1.93	0.51
1:T:576:LEU:HD21	1:T:585:ARG:HH11	1.76	0.50
1:T:360:PRO:HB2	1:T:363:ASP:HB2	1.94	0.50
1:T:562:ALA:HB3	3:T:1700:SO1:H181	1.93	0.50
1:T:414:GLN:HB2	1:T:477:ASN:HD21	1.77	0.50
1:T:706:ILE:HB	1:T:707:PRO:HD3	1.94	0.50
1:T:798:PHE:H	3:T:1700:SO1:C53	2.25	0.50
1:T:576:LEU:HD21	1:T:585:ARG:NH1	2.27	0.50
1:T:386:VAL:HG11	1:T:437:MET:HE1	1.94	0.50
1:T:576:LEU:HD13	1:T:587:TYR:CE1	2.46	0.50
1:T:607:ASN:HB2	1:T:610:ASP:OD2	2.11	0.50
1:T:539:GLU:O	1:T:543:GLN:HG3	2.12	0.49
1:T:345:PRO:O	1:T:349:GLN:HG3	2.11	0.49
1:T:488:VAL:CB	1:T:796:MET:HE2	2.43	0.49
1:T:411:VAL:HG12	1:T:412:ARG:N	2.27	0.49
1:T:699:DDE:HAD2	1:T:699:DDE:HAA3	1.77	0.49
1:T:552:VAL:HG13	1:T:553:PRO:HD2	1.95	0.49
1:T:111:PHE:CE2	1:T:481:MET:CG	2.86	0.49
1:T:202:VAL:CG1	1:T:209:VAL:CG2	2.91	0.49
1:T:464:LEU:HD13	1:T:513:LYS:HZ1	1.67	0.48
1:T:503:LYS:HD2	1:T:552:VAL:HG21	1.94	0.48
1:T:153:PRO:HD2	1:T:200:VAL:HG22	1.95	0.48
1:T:109:VAL:CG1	1:T:142:VAL:CG2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:200:VAL:HG22	1:T:200:VAL:O	2.13	0.48
1:T:798:PHE:HB3	3:T:1700:SO1:C7	2.43	0.48
1:T:433:ARG:HB3	1:T:457:VAL:HG11	1.95	0.48
1:T:797:VAL:CA	3:T:1700:SO1:H53	2.39	0.48
1:T:69:THR:CB	1:T:440:ARG:HH12	2.25	0.48
1:T:646:VAL:HG23	1:T:667:PHE:CD2	2.49	0.48
1:T:271:ARG:HH11	1:T:271:ARG:HG3	1.79	0.48
1:T:186:ASN:HB3	1:T:201:GLN:OE1	2.14	0.48
1:T:699:DDE:HAC1	2:T:1699:APR:H5'1	1.96	0.48
1:T:360:PRO:HD2	1:T:363:ASP:HB2	1.96	0.48
1:T:699:DDE:HAB1	2:T:1699:APR:O3A	2.14	0.47
1:T:110:ASP:OD2	1:T:112:SER:HB3	2.14	0.47
1:T:823:ARG:HE	1:T:832:VAL:HG22	1.79	0.47
1:T:461:GLN:CD	1:T:461:GLN:H	2.16	0.47
1:T:237:LYS:HA	1:T:240:MET:HB2	1.95	0.47
1:T:114:GLU:CD	1:T:514:SER:O	2.53	0.47
1:T:807:ASP:OD1	1:T:809:LEU:N	2.44	0.47
1:T:784:LEU:HD23	1:T:794:PRO:HD3	1.97	0.47
1:T:698:ILE:CG2	1:T:699:DDE:CE1	2.92	0.47
1:T:80:GLU:HA	1:T:96:ASN:O	2.15	0.47
1:T:106:PRO:HB3	1:T:108:HIS:CD2	2.50	0.46
1:T:70:ILE:O	1:T:440:ARG:CB	2.64	0.46
1:T:823:ARG:NH1	1:T:829:LYS:O	2.47	0.46
1:T:84:GLU:HG3	1:T:85:ASP:N	2.30	0.46
1:T:515:ASP:O	1:T:518:VAL:HG12	2.15	0.46
1:T:565:GLU:O	1:T:681:MET:HA	2.14	0.46
1:T:454:ILE:HG13	1:T:455:GLY:N	2.30	0.46
1:T:559:PRO:HB2	3:T:1700:SO1:C21	2.45	0.46
1:T:480:VAL:HA	1:T:480:VAL:C	2.33	0.46
1:T:809:LEU:O	1:T:811:PRO:HD3	2.16	0.46
1:T:800:HIS:CD2	1:T:801:TRP:C	2.89	0.46
1:T:411:VAL:HG12	1:T:412:ARG:H	1.80	0.46
1:T:111:PHE:CE1	1:T:482:LYS:C	2.89	0.46
1:T:114:GLU:OE1	1:T:516:PRO:CG	2.62	0.46
1:T:126:LEU:HD11	1:T:156:VAL:HG21	1.93	0.46
1:T:113:SER:CB	1:T:516:PRO:CG	2.87	0.46
1:T:785:ARG:HG3	1:T:786:GLN:N	2.30	0.46
1:T:798:PHE:CG	3:T:1700:SO1:C7	2.99	0.45
1:T:113:SER:CA	1:T:516:PRO:HG2	2.46	0.45
1:T:42:ARG:HG2	1:T:331:ALA:CB	2.47	0.45
1:T:483:PHE:N	1:T:793:PHE:HE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:378:LEU:N	1:T:471:THR:HG22	2.28	0.45
1:T:434:VAL:HG12	1:T:445:ILE:HG22	1.98	0.45
1:T:221:THR:OG1	1:T:224:GLN:HG3	2.15	0.45
1:T:733:ILE:O	1:T:767:THR:HA	2.17	0.45
1:T:202:VAL:CG1	1:T:209:VAL:HG22	2.47	0.45
1:T:800:HIS:C	1:T:801:TRP:CE3	2.90	0.45
1:T:202:VAL:HG12	1:T:209:VAL:HG23	1.98	0.45
1:T:699:DDE:HAU3	1:T:699:DDE:HAB2	1.71	0.45
1:T:81:MET:HG3	1:T:339:VAL:HG11	1.99	0.45
1:T:109:VAL:HG12	1:T:142:VAL:HG22	1.99	0.45
1:T:699:DDE:CAB	2:T:1699:APR:H5R1	2.47	0.45
1:T:560:VAL:O	3:T:1700:SO1:H13	2.16	0.44
1:T:479:LYS:C	1:T:479:LYS:HA	2.25	0.44
1:T:515:ASP:HB3	1:T:518:VAL:HG12	2.00	0.44
1:T:25:ILE:HG23	1:T:142:VAL:HB	2.00	0.44
1:T:561:VAL:HG22	1:T:774:VAL:CG2	2.47	0.44
1:T:29:ASP:HA	4:T:843:GDP:H5'	2.00	0.44
1:T:718:LEU:HA	1:T:722:PRO:HG3	2.00	0.44
1:T:479:LYS:C	1:T:479:LYS:CB	2.81	0.44
1:T:159:LYS:HG3	4:T:843:GDP:C2	2.53	0.44
1:T:607:ASN:HA	1:T:608:PRO:HD3	1.83	0.44
1:T:763:THR:N	1:T:764:PRO:CD	2.79	0.44
1:T:715:ALA:HB2	1:T:838:TYR:HB2	2.00	0.44
1:T:490:GLN:OE1	3:T:1700:SO1:H213	2.18	0.44
1:T:564:ARG:HG3	1:T:682:ARG:CB	2.47	0.44
1:T:560:VAL:C	3:T:1700:SO1:C20	2.82	0.44
1:T:633:ILE:O	1:T:633:ILE:HG13	2.18	0.44
1:T:16:VAL:HB	1:T:345:PRO:HD2	2.00	0.44
1:T:28:VAL:O	1:T:29:ASP:HB2	2.17	0.43
1:T:737:GLU:HB2	1:T:766:PHE:HE2	1.79	0.43
1:T:699:DDE:HAB1	2:T:1699:APR:H5'2	1.99	0.43
1:T:69:THR:CG2	1:T:440:ARG:NH1	2.81	0.43
1:T:380:LEU:HD13	1:T:456:LEU:HD11	2.00	0.43
1:T:414:GLN:CB	1:T:477:ASN:HD21	2.31	0.43
1:T:235:VAL:HG12	1:T:239:LYS:HB3	2.01	0.43
1:T:491:VAL:HG21	1:T:542:LEU:HD11	2.01	0.43
1:T:77:LEU:HB2	1:T:100:ILE:HB	2.00	0.43
1:T:108:HIS:CE1	1:T:112:SER:HG	2.36	0.43
1:T:114:GLU:OE1	1:T:515:ASP:HA	2.19	0.43
1:T:798:PHE:CB	3:T:1700:SO1:C7	2.97	0.43
1:T:800:HIS:CD2	1:T:801:TRP:CA	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:153:PRO:HD2	1:T:200:VAL:CG2	2.49	0.43
1:T:798:PHE:CD1	3:T:1700:SO1:C6	2.78	0.43
1:T:357:TYR:OH	1:T:476:HIS:HB2	2.19	0.43
1:T:478:MET:O	1:T:478:MET:CA	2.54	0.42
1:T:465:LYS:HB3	1:T:466:THR:H	1.67	0.42
1:T:697:ALA:C	1:T:699:DDE:N	2.63	0.42
1:T:763:THR:O	1:T:763:THR:HG22	2.19	0.42
1:T:114:GLU:OE1	1:T:514:SER:O	2.37	0.42
1:T:69:THR:CG2	1:T:440:ARG:NH2	2.82	0.42
1:T:386:VAL:HG11	1:T:437:MET:HE3	2.00	0.42
1:T:197:LEU:HD12	1:T:197:LEU:N	2.34	0.42
1:T:810:ASP:O	1:T:816:GLY:HA3	2.19	0.42
1:T:426:LEU:HD12	1:T:427:PHE:N	2.34	0.42
1:T:798:PHE:HD2	3:T:1700:SO1:C16	1.73	0.42
1:T:378:LEU:HD11	1:T:380:LEU:HB2	2.02	0.42
1:T:560:VAL:C	3:T:1700:SO1:H203	2.37	0.42
1:T:69:THR:HG21	1:T:440:ARG:HH22	1.84	0.42
1:T:205:ALA:HB2	1:T:245:TRP:NE1	2.35	0.42
1:T:552:VAL:CG1	1:T:553:PRO:HD2	2.50	0.42
1:T:388:THR:HG21	1:T:395:TYR:CD1	2.55	0.42
1:T:230:ALA:C	1:T:232:LYS:H	2.23	0.41
1:T:353:ALA:HB3	1:T:370:LYS:HG2	1.99	0.41
1:T:763:THR:O	1:T:764:PRO:O	2.38	0.41
1:T:284:LEU:HD11	1:T:303:LEU:CD1	2.50	0.41
1:T:417:ASN:HB2	1:T:425:ASP:OD2	2.20	0.41
1:T:744:TYR:CE1	1:T:754:VAL:HG21	2.55	0.41
1:T:710:ARG:NH1	1:T:714:TYR:OH	2.54	0.41
1:T:658:GLU:OE1	1:T:700:ARG:NH2	2.54	0.41
1:T:698:ILE:HG21	2:T:1699:APR:O4D	2.21	0.41
1:T:369:ILE:HD13	1:T:402:ALA:HB2	2.01	0.41
1:T:454:ILE:HG13	1:T:455:GLY:H	1.84	0.41
1:T:666:ALA:CB	1:T:709:MET:HB3	2.51	0.41
1:T:636:PHE:CE1	1:T:645:LEU:HD21	2.55	0.41
1:T:731:VAL:HG13	1:T:731:VAL:O	2.21	0.41
1:T:490:GLN:N	1:T:559:PRO:HD3	2.32	0.41
1:T:106:PRO:CB	1:T:108:HIS:NE2	2.84	0.41
1:T:576:LEU:CD2	1:T:842:LEU:HG	2.45	0.41
1:T:287:ALA:HA	1:T:292:LYS:HD2	2.02	0.41
1:T:110:ASP:O	1:T:111:PHE:HB2	2.21	0.41
1:T:169:VAL:HG12	1:T:173:ASP:HB2	2.03	0.41
1:T:418:TYR:C	1:T:418:TYR:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:800:HIS:CA	1:T:801:TRP:HA	2.49	0.41
1:T:599:LEU:HD12	1:T:599:LEU:HA	1.88	0.41
1:T:69:THR:HB	1:T:440:ARG:CZ	2.45	0.40
1:T:824:LYS:HD3	1:T:830:GLU:OE1	2.22	0.40
1:T:358:GLU:OE2	1:T:479:LYS:HG3	2.21	0.40
1:T:484:SER:HB3	1:T:533:THR:HG23	2.03	0.40
1:T:579:SER:HB3	1:T:708:THR:OG1	2.20	0.40
1:T:260:LYS:HB3	1:T:260:LYS:HE2	1.80	0.40
1:T:751:ARG:HD3	1:T:814:LYS:CE	2.50	0.40
1:T:565:GLU:CD	1:T:676:ILE:HB	2.41	0.40
1:T:27:HIS:CD2	1:T:136:CYS:HB2	2.57	0.40
1:T:155:VAL:CG1	1:T:156:VAL:N	2.84	0.40
1:T:722:PRO:O	1:T:723:LYS:HD2	2.20	0.40
1:T:807:ASP:HA	1:T:808:PRO:HD3	1.96	0.40
1:T:633:ILE:C	1:T:633:ILE:HD12	2.42	0.40
1:T:718:LEU:HA	1:T:722:PRO:CG	2.51	0.40
1:T:146:ALA:HA	1:T:151:ILE:HD12	2.04	0.40
1:T:160:VAL:HG23	1:T:212:GLY:O	2.22	0.40
1:T:165:LEU:HD12	1:T:165:LEU:HA	1.90	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 PDB entries followed by that with respect to all EM entries.

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	T	791/842 (94%)	746 (94%)	38 (5%)	7 (1%)	21 67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	700	ARG
1	T	764	PRO

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Mol	Chain	Res	Type
1	T	391	LYS
1	T	465	LYS
1	T	425	ASP
1	T	498	ALA
1	T	359	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	T	691/714 (97%)	663 (96%)	28 (4%)	37 71

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	28	VAL
1	T	109	VAL
1	T	138	GLN
1	T	165	LEU
1	T	183	GLU
1	T	194	ASP
1	T	248	SER
1	T	352	ARG
1	T	438	MET
1	T	457	VAL
1	T	460	ASP
1	T	471	THR
1	T	476	HIS
1	T	477	ASN
1	T	479	LYS
1	T	480	VAL
1	T	490	GLN
1	T	522	MET
1	T	596	GLU
1	T	599	LEU
1	T	633	ILE

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Mol	Chain	Res	Type
1	T	677	PHE
1	T	718	LEU
1	T	730	LEU
1	T	735	CYS
1	T	738	GLN
1	T	758	GLU
1	T	829	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	21	ASN
1	T	27	HIS
1	T	101	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	DDE	T	699	1,2	13,20,21	2.00	3 (23%)	12,28,30	2.67	2 (16%)

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
1	DDE	T	699	1,2	-	0/19/21/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	699	DDE	CG-ND1	-2.40	1.33	1.37
1	T	699	DDE	CAC-NCB	3.00	1.60	1.50
1	T	699	DDE	OAG-CBI	4.96	1.33	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	699	DDE	OAG-CBI-NAD	4.93	131.22	123.06
1	T	699	DDE	CAU-CAT-CE1	7.07	150.72	112.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	T	699	DDE	18	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	APR	T	1699	1	33,38,39	1.42	5 (15%)	36,58,60	1.73	9 (25%)
3	SO1	T	1700	1	36,39,39	2.36	12 (33%)	36,64,64	2.43	7 (19%)
4	GDP	T	843	-	24,30,30	1.35	3 (12%)	26,47,47	2.27	4 (15%)

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	APR	T	1699	1	1/1/9/10	0/18/51/54	0/4/4/4
3	SO1	T	1700	1	1/1/15/16	0/15/104/104	0/2/5/5
4	GDP	T	843	-	-	0/12/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1700	SO1	C12-C4	-4.84	1.42	1.54
2	T	1699	APR	O4D-C4D	2.07	1.48	1.44
4	T	843	GDP	O3'-C3'	2.17	1.48	1.43
2	T	1699	APR	C4-N3	2.20	1.38	1.35
3	T	1700	SO1	C8-C2	2.23	1.57	1.53
3	T	1700	SO1	C10-C3	2.23	1.59	1.55
4	T	843	GDP	C2-N1	2.24	1.39	1.35
3	T	1700	SO1	C52-C53	2.28	1.59	1.52
3	T	1700	SO1	C10-C6	2.35	1.58	1.53
3	T	1700	SO1	C3-C11	2.57	1.56	1.51
3	T	1700	SO1	O56-C52	2.63	1.48	1.41
2	T	1699	APR	O2'-C2'	2.75	1.49	1.43
2	T	1699	APR	C3'-C4'	2.76	1.60	1.53
3	T	1700	SO1	C55-C56	3.12	1.58	1.52
2	T	1699	APR	C2-N1	4.03	1.41	1.33
3	T	1700	SO1	C1-C4	4.06	1.62	1.55
4	T	843	GDP	C6-N1	4.99	1.42	1.33
3	T	1700	SO1	C1-C5	5.02	1.59	1.50
3	T	1700	SO1	C3-C1	5.77	1.68	1.57
3	T	1700	SO1	C7-C2	6.36	1.64	1.54

All (20) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	843	GDP	C5-C6-N1	-7.68	113.48	123.52
3	T	1700	SO1	C7-C2-C8	-6.09	99.15	110.16
2	T	1699	APR	O2D-C2D-C3D	-4.94	101.92	111.26
3	T	1700	SO1	C18-C9-C16	-3.56	98.41	103.42
4	T	843	GDP	N3-C2-N1	-3.26	123.12	127.56
2	T	1699	APR	O4D-C4D-C5D	-2.94	103.07	109.53
2	T	1699	APR	O4D-C1D-C2D	-2.68	100.67	106.05
2	T	1699	APR	C1'-N9-C4	-2.23	124.32	126.81
4	T	843	GDP	O3'-C3'-C4'	-2.14	104.61	111.01
3	T	1700	SO1	C24-C18-C9	-2.04	101.02	105.11
2	T	1699	APR	O2A-PA-O3A	2.20	114.68	105.27
2	T	1699	APR	N3-C2-N1	2.36	130.72	128.87
2	T	1699	APR	O4'-C1'-N9	2.75	113.30	108.11
3	T	1700	SO1	O17-C52-C53	2.98	111.67	108.00
2	T	1699	APR	C1D-O4D-C4D	2.99	115.75	108.11
2	T	1699	APR	C1D-C2D-C3D	3.59	107.33	101.65
3	T	1700	SO1	C10-C6-C2	3.94	112.00	103.68
4	T	843	GDP	C6-N1-C2	6.25	123.20	115.88
3	T	1700	SO1	C12-C4-C13	7.02	129.03	112.51
3	T	1700	SO1	C1-C4-C13	8.57	128.15	118.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	T	1700	SO1	C4
2	T	1699	APR	C1D

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	1699	APR	7	0
3	T	1700	SO1	67	0
4	T	843	GDP	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.