



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:11 am GMT

PDB ID : 2P8X  
EMDB ID: : EMD-1343  
Title : Fitted structure of ADPR-eEF2 in the 80S:ADPR-eEF2:GDPNP 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 : 9.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

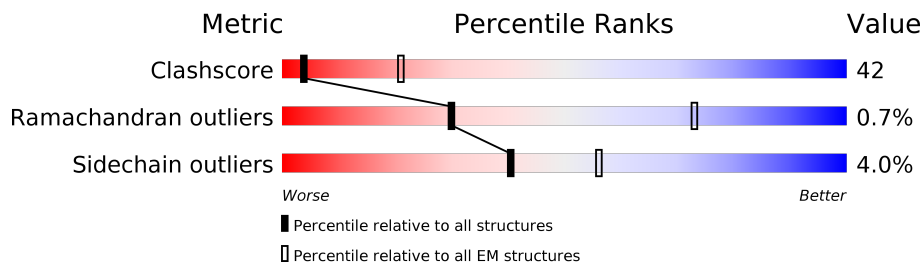
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.70 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	
2	S	35	

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	-
3	APR	T	1699	X	-	-	-
4	GNP	T	843	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6677 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

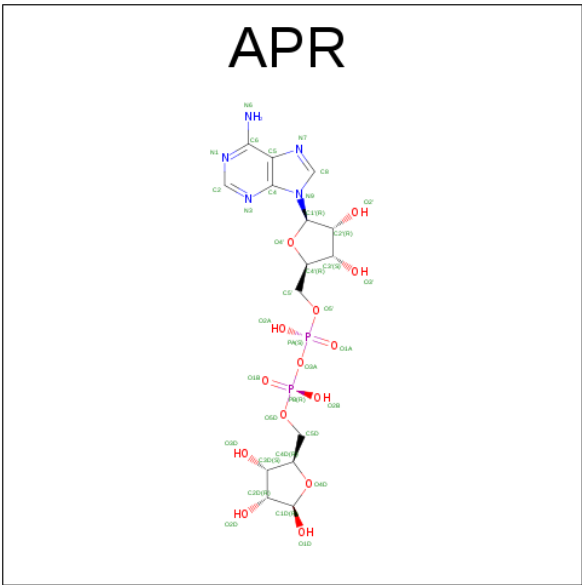
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Elongation factor Tu-B.

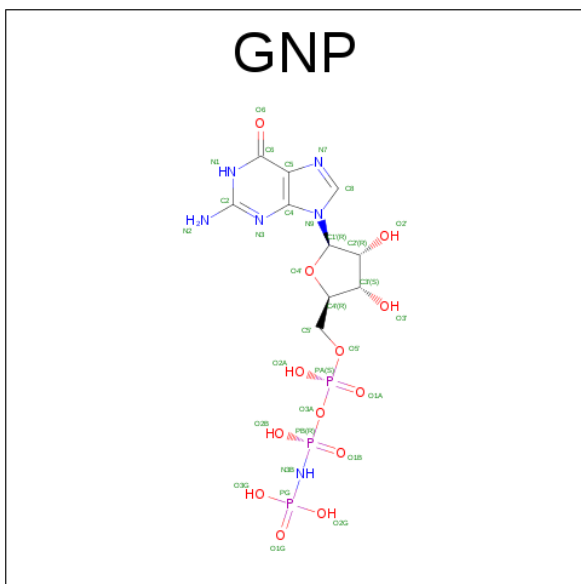
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	35	268	162	48	58	0	0

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).



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

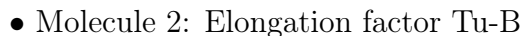
- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
4	T	1	Total	C	N	O	P	0
			32	10	6	13	3	



- Molecule 1: Elongation factor 2



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	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)	3500	Depositor
Magnification	37642	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: APR, GNP, DDE

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	1.16	13/6434 (0.2%)	0.93	26/8698 (0.3%)
2	S	0.53	0/271	0.61	0/368
All	All	1.14	13/6705 (0.2%)	0.92	26/9066 (0.3%)

All (13) 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	344	SER	C-N	34.54	1.99	1.34
1	T	480	VAL	N-CA	32.97	2.12	1.46
1	T	480	VAL	CA-C	30.59	2.32	1.52
1	T	479	LYS	C-N	28.39	1.99	1.34
1	T	216	HIS	C-N	23.64	1.75	1.33
1	T	479	LYS	N-CA	22.16	1.90	1.46
1	T	479	LYS	CA-C	21.18	2.08	1.52
1	T	481	MET	CA-C	15.03	1.92	1.52
1	T	478	MET	C-N	14.96	1.68	1.34
1	T	482	LYS	N-CA	14.25	1.74	1.46
1	T	478	MET	CA-C	9.68	1.78	1.52
1	T	478	MET	N-CA	6.03	1.58	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	216	HIS	O-C-N	-22.87	84.32	123.20
1	T	480	VAL	N-CA-C	19.14	162.68	111.00
1	T	216	HIS	CA-C-N	18.82	153.84	116.20
1	T	344	SER	O-C-N	-17.27	88.29	121.10
1	T	216	HIS	C-N-CA	16.64	157.25	122.30
1	T	481	MET	CB-CA-C	-14.73	80.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	479	LYS	CA-C-N	13.30	146.47	117.20
1	T	479	LYS	N-CA-C	12.83	145.65	111.00
1	T	344	SER	C-N-CD	-12.38	93.36	120.60
1	T	344	SER	CA-C-N	12.03	150.77	117.10
1	T	481	MET	N-CA-C	11.72	142.64	111.00
1	T	480	VAL	N-CA-CB	-11.48	86.25	111.50
1	T	479	LYS	C-N-CA	10.01	146.74	121.70
1	T	479	LYS	O-C-N	-9.15	108.07	122.70
1	T	481	MET	N-CA-CB	9.12	127.01	110.60
1	T	480	VAL	CA-C-O	-8.98	101.25	120.10
1	T	478	MET	C-N-CA	8.70	143.44	121.70
1	T	800	HIS	O-C-N	8.32	136.01	122.70
1	T	482	LYS	N-CA-CB	7.95	124.91	110.60
1	T	479	LYS	N-CA-CB	-7.68	96.78	110.60
1	T	344	SER	C-N-CA	7.37	152.95	122.00
1	T	478	MET	CA-C-N	7.18	133.00	117.20
1	T	482	LYS	CB-CA-C	-7.01	96.39	110.40
1	T	479	LYS	CA-C-O	-6.97	105.46	120.10
1	T	800	HIS	CA-C-N	-6.59	102.71	117.20
1	T	478	MET	O-C-N	-5.77	113.47	122.70

There are no chirality outliers.

There are no planarity outliers.

## 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	6397	550	0
2	S	268	0	247	149	0
3	T	35	0	19	7	0
4	T	32	0	13	42	0
All	All	6677	0	6676	552	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 42.

All (552) 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:478:MET:CA	1:T:478:MET:C	1.78	1.51
1:T:482:LYS:N	1:T:482:LYS:CA	1.74	1.50
1:T:145:GLN:HG3	1:T:481:MET:CB	1.40	1.50
1:T:46:ILE:CD1	2:S:43:GLU:HA	1.38	1.49
1:T:481:MET:HG3	1:T:481:MET:C	1.24	1.46
1:T:478:MET:C	1:T:479:LYS:N	1.68	1.45
1:T:104:ASP:HB3	2:S:67:HIS:CG	1.50	1.45
1:T:3:ALA:HB3	2:S:40:PRO:CB	1.17	1.44
1:T:46:ILE:CG1	2:S:43:GLU:N	1.77	1.44
1:T:104:ASP:HB3	2:S:67:HIS:CD2	1.53	1.44
1:T:145:GLN:CG	1:T:481:MET:HB3	1.48	1.42
1:T:46:ILE:CG1	2:S:43:GLU:CA	1.98	1.42
1:T:46:ILE:HG12	2:S:43:GLU:CA	1.48	1.40
1:T:438:MET:CB	2:S:69:GLU:OE1	1.68	1.40
1:T:216:HIS:C	1:T:217:GLY:N	1.75	1.39
1:T:104:ASP:HB2	2:S:67:HIS:CA	1.49	1.39
1:T:3:ALA:CB	2:S:40:PRO:HB2	1.05	1.38
1:T:481:MET:C	1:T:481:MET:CA	1.92	1.37
1:T:3:ALA:C	2:S:40:PRO:HG2	1.44	1.36
1:T:3:ALA:O	2:S:40:PRO:CG	1.70	1.35
1:T:145:GLN:CG	1:T:481:MET:CB	2.01	1.35
1:T:46:ILE:O	2:S:41:ASN:CA	1.75	1.34
1:T:479:LYS:CA	1:T:479:LYS:N	1.90	1.34
1:T:46:ILE:CG1	2:S:42:VAL:C	1.88	1.34
1:T:46:ILE:HG13	2:S:42:VAL:O	1.23	1.33
1:T:46:ILE:HG13	2:S:43:GLU:N	1.33	1.33
1:T:696:ASP:OD2	3:T:1699:APR:HR'4	1.14	1.32
1:T:698:ILE:C	1:T:699:DDE:HA	1.48	1.31
1:T:46:ILE:CG1	2:S:43:GLU:HA	1.58	1.31
1:T:215:LEU:H	4:T:843:GNP:C5	1.44	1.31
1:T:46:ILE:HG13	2:S:42:VAL:C	0.92	1.30
1:T:111:PHE:CZ	1:T:482:LYS:CA	2.15	1.29
1:T:215:LEU:HB2	4:T:843:GNP:C4	1.55	1.29
1:T:120:ARG:HH22	1:T:480:VAL:N	1.31	1.28
1:T:481:MET:C	1:T:481:MET:CG	2.01	1.27
1:T:144:ARG:NH1	1:T:482:LYS:HA	1.50	1.25
1:T:144:ARG:HH11	1:T:482:LYS:CA	1.49	1.25
1:T:111:PHE:HE1	1:T:482:LYS:C	1.41	1.24
1:T:111:PHE:CE1	1:T:482:LYS:C	2.11	1.24
1:T:215:LEU:CB	4:T:843:GNP:C5	2.14	1.23
1:T:479:LYS:CA	1:T:479:LYS:C	2.08	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:72:SER:OG	2:S:67:HIS:O	1.54	1.22
1:T:215:LEU:HB2	4:T:843:GNP:N9	1.54	1.21
1:T:45:ILE:CG2	2:S:41:ASN:O	1.88	1.19
1:T:104:ASP:CB	2:S:67:HIS:CG	2.27	1.18
1:T:45:ILE:HG22	2:S:41:ASN:O	1.08	1.16
1:T:479:LYS:C	1:T:480:VAL:N	1.99	1.16
1:T:215:LEU:HD13	4:T:843:GNP:O2'	1.00	1.16
1:T:88:GLU:OE2	1:T:223:ARG:NH2	1.77	1.16
1:T:344:SER:C	1:T:345:PRO:N	1.99	1.16
1:T:215:LEU:HB3	4:T:843:GNP:C4	1.69	1.16
1:T:46:ILE:CG1	2:S:42:VAL:O	1.90	1.16
1:T:76:SER:OG	2:S:69:GLU:HG3	1.46	1.16
1:T:161:ASP:CG	4:T:843:GNP:HN21	1.49	1.15
1:T:45:ILE:CG2	2:S:41:ASN:C	2.15	1.14
1:T:480:VAL:N	1:T:480:VAL:CG2	2.12	1.13
1:T:110:ASP:O	1:T:485:VAL:HG13	1.49	1.12
1:T:438:MET:SD	2:S:69:GLU:OE2	2.08	1.12
1:T:114:GLU:OE1	1:T:516:PRO:CB	1.98	1.11
1:T:480:VAL:N	1:T:480:VAL:CA	2.12	1.11
1:T:144:ARG:HH11	1:T:482:LYS:CB	1.63	1.11
1:T:110:ASP:HB2	1:T:484:SER:O	1.46	1.11
1:T:34:THR:HG23	4:T:843:GNP:O2A	1.51	1.11
1:T:215:LEU:HB3	4:T:843:GNP:C5	1.79	1.09
1:T:46:ILE:CD1	2:S:43:GLU:CA	2.27	1.09
1:T:76:SER:OG	2:S:69:GLU:CG	1.99	1.09
1:T:215:LEU:N	4:T:843:GNP:C5	2.14	1.09
1:T:480:VAL:C	1:T:481:MET:N	2.05	1.09
1:T:3:ALA:O	2:S:40:PRO:HG2	0.93	1.08
1:T:46:ILE:HD11	2:S:43:GLU:HA	1.13	1.08
1:T:144:ARG:NH1	1:T:482:LYS:CA	2.10	1.08
1:T:481:MET:CA	1:T:481:MET:N	2.18	1.07
1:T:145:GLN:CG	1:T:481:MET:HB2	1.79	1.07
1:T:104:ASP:OD1	2:S:66:ALA:N	1.87	1.07
1:T:145:GLN:CA	1:T:481:MET:HB2	1.84	1.07
1:T:76:SER:CB	2:S:69:GLU:HG2	1.84	1.07
1:T:104:ASP:CB	2:S:67:HIS:CD2	2.38	1.06
1:T:438:MET:HB3	2:S:69:GLU:OE1	0.91	1.06
1:T:37:ASP:OD1	2:S:50:ILE:HD12	1.55	1.06
1:T:45:ILE:HG22	2:S:41:ASN:C	1.74	1.06
1:T:161:ASP:CG	4:T:843:GNP:N2	2.07	1.06
1:T:481:MET:CE	1:T:482:LYS:CA	2.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:698:ILE:C	1:T:699:DDE:CA	2.25	1.04
1:T:558:PRO:C	1:T:559:PRO:N	2.11	1.04
1:T:3:ALA:CB	2:S:40:PRO:CB	1.78	1.04
1:T:37:ASP:OD2	2:S:47:TYR:HA	1.56	1.03
1:T:46:ILE:C	2:S:41:ASN:HA	1.72	1.03
1:T:464:LEU:HD13	1:T:513:LYS:HG2	1.40	1.03
1:T:481:MET:HE2	1:T:482:LYS:CA	1.76	1.03
1:T:215:LEU:H	4:T:843:GNP:C6	1.70	1.02
1:T:45:ILE:HG23	2:S:41:ASN:CB	1.89	1.02
1:T:76:SER:CB	2:S:69:GLU:CG	2.38	1.02
1:T:141:THR:HG21	1:T:483:PHE:CE2	1.95	1.01
1:T:109:VAL:HG21	1:T:138:GLN:HG2	1.37	1.01
1:T:104:ASP:HB2	2:S:67:HIS:HA	1.00	1.00
1:T:696:ASP:OD2	3:T:1699:APR:C4D	2.09	1.00
1:T:698:ILE:O	1:T:699:DDE:HA	1.60	1.00
1:T:46:ILE:HD11	2:S:43:GLU:CA	1.88	1.00
1:T:104:ASP:CB	2:S:67:HIS:CA	2.40	0.99
1:T:481:MET:CB	1:T:481:MET:C	2.29	0.99
1:T:145:GLN:HG2	1:T:481:MET:HB3	1.41	0.99
1:T:215:LEU:HB2	4:T:843:GNP:C8	1.92	0.99
1:T:145:GLN:HG3	1:T:481:MET:HB2	1.36	0.98
1:T:126:LEU:HD11	1:T:156:VAL:HG23	1.43	0.98
1:T:120:ARG:NH2	1:T:480:VAL:N	2.10	0.98
1:T:480:VAL:C	1:T:480:VAL:CA	2.32	0.98
1:T:114:GLU:OE1	1:T:516:PRO:HB2	1.15	0.98
1:T:480:VAL:HG22	1:T:480:VAL:N	1.75	0.97
1:T:45:ILE:CG2	2:S:41:ASN:CB	2.42	0.97
1:T:46:ILE:O	2:S:41:ASN:HA	0.81	0.97
1:T:70:ILE:HG12	1:T:440:ARG:O	1.63	0.96
1:T:104:ASP:CB	2:S:67:HIS:HA	1.95	0.96
1:T:46:ILE:CD1	2:S:42:VAL:O	2.14	0.96
1:T:145:GLN:HG2	1:T:481:MET:CB	1.93	0.96
1:T:145:GLN:HG3	1:T:481:MET:HB3	1.01	0.95
1:T:699:DDE:O	1:T:704:GLN:HG3	1.67	0.94
1:T:46:ILE:HG12	2:S:43:GLU:N	1.53	0.94
1:T:37:ASP:OD1	2:S:50:ILE:CD1	2.16	0.93
1:T:145:GLN:HA	1:T:481:MET:HB2	1.51	0.93
1:T:481:MET:HA	1:T:481:MET:N	1.83	0.92
1:T:45:ILE:CG2	2:S:41:ASN:HB3	1.98	0.92
1:T:144:ARG:NH1	1:T:482:LYS:CB	2.31	0.92
1:T:724:ILE:HD11	1:T:804:LEU:HD12	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:141:THR:CG2	1:T:483:PHE:CE2	2.53	0.91
1:T:698:ILE:C	1:T:699:DDE:CB	2.40	0.91
1:T:4:PHE:O	2:S:41:ASN:OD1	1.65	0.90
1:T:558:PRO:C	1:T:559:PRO:CA	2.39	0.90
1:T:110:ASP:O	1:T:485:VAL:CG1	2.19	0.90
1:T:40:VAL:CG1	2:S:44:VAL:HA	2.02	0.90
1:T:215:LEU:HD13	4:T:843:GNP:C2'	2.02	0.89
1:T:216:HIS:O	1:T:217:GLY:N	2.04	0.89
1:T:111:PHE:CE1	1:T:482:LYS:CA	2.53	0.88
1:T:40:VAL:HG12	2:S:44:VAL:HA	1.55	0.88
1:T:110:ASP:CB	1:T:484:SER:O	2.21	0.88
1:T:27:HIS:CD2	1:T:138:GLN:HB2	2.07	0.88
1:T:88:GLU:CD	1:T:223:ARG:HH21	1.77	0.88
1:T:126:LEU:HD11	1:T:156:VAL:CG2	2.03	0.87
1:T:37:ASP:OD2	2:S:47:TYR:CA	2.22	0.87
1:T:438:MET:SD	2:S:69:GLU:CD	2.53	0.87
1:T:463:LEU:HD21	1:T:467:GLY:HA3	1.55	0.87
1:T:43:ALA:O	2:S:42:VAL:HG21	1.73	0.87
1:T:45:ILE:HG23	2:S:41:ASN:HB2	1.56	0.87
1:T:46:ILE:HG12	2:S:43:GLU:CB	2.05	0.85
1:T:215:LEU:HD13	4:T:843:GNP:HO2'	1.38	0.85
1:T:161:ASP:OD2	4:T:843:GNP:C2	2.25	0.85
1:T:215:LEU:HB2	4:T:843:GNP:C5	1.93	0.84
1:T:558:PRO:CA	1:T:559:PRO:N	2.41	0.84
1:T:144:ARG:HH11	1:T:482:LYS:HB2	1.40	0.84
1:T:40:VAL:HG11	2:S:45:LYS:H	1.40	0.83
1:T:72:SER:HA	1:T:439:GLY:O	1.78	0.83
1:T:699:DDE:CA	1:T:700:ARG:N	2.40	0.83
1:T:111:PHE:HZ	1:T:482:LYS:CA	1.59	0.83
1:T:3:ALA:C	2:S:40:PRO:CG	2.27	0.83
1:T:70:ILE:HG12	1:T:440:ARG:C	1.99	0.82
1:T:3:ALA:CA	2:S:40:PRO:CG	2.49	0.82
1:T:76:SER:HB2	2:S:69:GLU:HG2	1.60	0.82
1:T:70:ILE:N	1:T:440:ARG:O	2.11	0.82
1:T:145:GLN:CB	1:T:481:MET:HB2	2.09	0.81
1:T:109:VAL:CG2	1:T:138:GLN:HG2	2.11	0.81
1:T:215:LEU:HB3	4:T:843:GNP:C6	2.09	0.81
1:T:215:LEU:CA	4:T:843:GNP:C5	2.60	0.80
3:T:1699:APR:H5R2	3:T:1699:APR:H8	1.65	0.79
1:T:105:SER:O	2:S:65:THR:CB	2.10	0.78
1:T:72:SER:HA	1:T:439:GLY:C	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:105:SER:O	2:S:65:THR:HB	1.83	0.78
1:T:104:ASP:HB2	2:S:67:HIS:N	1.86	0.77
1:T:696:ASP:HB3	1:T:699:DDE:HAB2	1.66	0.77
1:T:329:PRO:O	1:T:332:ASP:HB2	1.85	0.77
1:T:558:PRO:HA	1:T:559:PRO:N	2.00	0.77
1:T:696:ASP:HB3	1:T:699:DDE:CAB	2.14	0.76
1:T:3:ALA:HB3	2:S:40:PRO:HB3	1.60	0.76
1:T:22:MET:SD	1:T:102:LEU:HD12	2.26	0.76
1:T:73:THR:HG22	2:S:67:HIS:ND1	2.01	0.76
1:T:104:ASP:CG	2:S:66:ALA:N	2.37	0.76
1:T:329:PRO:C	1:T:330:ALA:N	2.39	0.76
1:T:145:GLN:OE1	1:T:483:PHE:HZ	1.69	0.75
1:T:813:SER:O	1:T:817:GLU:HG3	1.84	0.75
1:T:215:LEU:N	4:T:843:GNP:C6	2.44	0.75
1:T:215:LEU:HB3	4:T:843:GNP:N3	2.02	0.75
1:T:464:LEU:HD11	1:T:513:LYS:HE2	1.68	0.75
1:T:45:ILE:HG23	2:S:41:ASN:C	2.07	0.74
1:T:576:LEU:HD21	1:T:842:LEU:HG	1.69	0.74
1:T:344:SER:C	1:T:345:PRO:CD	2.55	0.74
1:T:480:VAL:N	1:T:480:VAL:HG23	2.02	0.74
1:T:70:ILE:CG1	1:T:440:ARG:O	2.35	0.73
1:T:378:LEU:H	1:T:471:THR:HG22	1.54	0.73
1:T:441:PHE:CE2	2:S:43:GLU:OE1	2.42	0.72
1:T:215:LEU:CD2	4:T:843:GNP:N3	2.51	0.72
1:T:438:MET:CA	2:S:69:GLU:OE1	2.37	0.72
1:T:694:HIS:O	1:T:700:ARG:HD3	1.89	0.72
1:T:353:ALA:CB	1:T:370:LYS:HG2	2.20	0.72
1:T:45:ILE:O	2:S:43:GLU:N	2.13	0.71
1:T:70:ILE:CG1	1:T:440:ARG:C	2.59	0.71
1:T:104:ASP:OD2	2:S:65:THR:C	2.29	0.71
1:T:464:LEU:O	1:T:465:LYS:HB2	1.90	0.71
1:T:76:SER:CB	2:S:69:GLU:HG3	2.13	0.71
1:T:215:LEU:HB3	4:T:843:GNP:C2	2.19	0.71
1:T:482:LYS:N	1:T:482:LYS:HA	2.01	0.71
1:T:40:VAL:HG11	2:S:45:LYS:N	2.06	0.70
1:T:698:ILE:O	1:T:699:DDE:CA	2.34	0.70
1:T:438:MET:CG	2:S:69:GLU:OE1	2.39	0.70
1:T:111:PHE:O	1:T:485:VAL:HG11	1.91	0.70
1:T:699:DDE:C	1:T:704:GLN:HG3	2.22	0.70
1:T:374:PRO:O	1:T:404:THR:HG23	1.92	0.70
1:T:104:ASP:HB3	2:S:67:HIS:ND1	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:73:THR:HA	2:S:67:HIS:CD2	1.86	0.69
1:T:223:ARG:HH11	1:T:223:ARG:HG2	1.57	0.69
1:T:32:LYS:O	1:T:36:THR:HG23	1.92	0.69
1:T:45:ILE:HG23	2:S:41:ASN:CA	2.22	0.69
1:T:104:ASP:HB2	2:S:67:HIS:CB	2.21	0.69
1:T:141:THR:HG21	1:T:483:PHE:CD2	2.28	0.69
1:T:73:THR:CG2	2:S:67:HIS:CE1	2.76	0.69
1:T:109:VAL:CB	1:T:483:PHE:CE2	2.63	0.69
1:T:479:LYS:N	1:T:479:LYS:CB	2.56	0.68
1:T:438:MET:SD	2:S:69:GLU:OE1	2.51	0.68
1:T:480:VAL:N	1:T:480:VAL:CB	2.56	0.68
1:T:189:VAL:CG1	1:T:200:VAL:HG13	2.22	0.68
1:T:558:PRO:C	1:T:559:PRO:HA	2.12	0.68
1:T:116:THR:HG21	1:T:480:VAL:CA	2.24	0.68
1:T:630:ALA:O	1:T:633:ILE:HG23	1.94	0.67
1:T:45:ILE:CB	2:S:41:ASN:O	2.38	0.67
1:T:111:PHE:CE2	1:T:481:MET:C	2.68	0.67
1:T:73:THR:HG23	2:S:67:HIS:CE1	2.30	0.67
1:T:3:ALA:CA	2:S:40:PRO:HG2	2.17	0.67
1:T:699:DDE:O	1:T:704:GLN:CG	2.43	0.67
1:T:144:ARG:NH1	1:T:482:LYS:HB2	2.04	0.67
1:T:110:ASP:O	1:T:483:PHE:O	2.12	0.67
1:T:44:GLY:O	2:S:36:ALA:HA	1.94	0.67
1:T:31:GLY:HA2	4:T:843:GNP:PA	2.35	0.67
1:T:103:ILE:HD12	1:T:122:THR:HG22	1.77	0.66
1:T:111:PHE:CZ	1:T:482:LYS:C	2.54	0.66
1:T:737:GLU:HB2	1:T:766:PHE:CE2	2.30	0.66
1:T:45:ILE:HG22	2:S:41:ASN:HB3	1.68	0.66
1:T:104:ASP:HB3	2:S:67:HIS:NE2	2.07	0.66
1:T:478:MET:HA	1:T:478:MET:C	2.07	0.66
1:T:731:VAL:HG12	1:T:770:ALA:O	1.95	0.66
1:T:109:VAL:HB	1:T:483:PHE:CE2	2.30	0.66
1:T:114:GLU:OE1	1:T:517:CYS:N	2.29	0.66
1:T:438:MET:CB	2:S:69:GLU:CD	2.60	0.66
1:T:73:THR:CG2	2:S:67:HIS:ND1	2.59	0.66
1:T:104:ASP:OD2	2:S:67:HIS:CD2	2.48	0.65
1:T:214:GLY:N	4:T:843:GNP:O6	2.29	0.65
1:T:45:ILE:CG2	2:S:41:ASN:CA	2.75	0.65
1:T:763:THR:N	1:T:764:PRO:HD3	2.12	0.65
1:T:110:ASP:HB2	1:T:484:SER:C	2.17	0.65
1:T:141:THR:HG22	1:T:483:PHE:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:237:LYS:O	1:T:241:MET:HG2	1.97	0.65
1:T:284:LEU:HD13	1:T:324:MET:HE1	1.79	0.65
1:T:161:ASP:OD2	4:T:843:GNP:N2	2.30	0.64
1:T:46:ILE:O	2:S:41:ASN:OD1	2.16	0.64
1:T:734:GLN:HG3	1:T:767:THR:HG22	1.80	0.64
1:T:829:LYS:CE	1:T:830:GLU:H	2.11	0.64
1:T:829:LYS:HE3	1:T:829:LYS:HA	1.78	0.64
1:T:30:HIS:N	4:T:843:GNP:O1B	2.31	0.64
1:T:627:VAL:O	1:T:631:ARG:HG3	1.98	0.64
1:T:344:SER:O	1:T:345:PRO:N	2.31	0.63
1:T:104:ASP:HB3	2:S:67:HIS:CE1	2.32	0.63
1:T:110:ASP:HB2	1:T:484:SER:N	2.13	0.63
1:T:141:THR:CG2	1:T:483:PHE:CZ	2.81	0.63
1:T:696:ASP:CG	3:T:1699:APR:HR'4	2.11	0.63
1:T:86:VAL:HG13	1:T:93:THR:HG21	1.81	0.63
1:T:633:ILE:HD12	1:T:635:CYS:N	2.14	0.63
1:T:215:LEU:HD22	4:T:843:GNP:N3	2.14	0.63
1:T:4:PHE:CZ	2:S:39:ASN:CG	2.44	0.63
1:T:74:ALA:O	1:T:439:GLY:N	2.28	0.62
1:T:104:ASP:OD2	2:S:66:ALA:CA	2.45	0.62
3:T:1699:APR:H8	3:T:1699:APR:C5D	2.30	0.62
1:T:215:LEU:HD22	4:T:843:GNP:HI'	1.81	0.62
1:T:433:ARG:HB3	1:T:457:VAL:CG1	2.30	0.62
1:T:40:VAL:CG1	2:S:45:LYS:H	2.12	0.62
1:T:576:LEU:HD11	1:T:585:ARG:HD3	1.82	0.62
1:T:696:ASP:HB3	1:T:699:DDE:HAU3	1.82	0.62
1:T:104:ASP:CB	2:S:67:HIS:CB	2.78	0.62
1:T:520:THR:HG22	1:T:530:VAL:HG22	1.81	0.61
1:T:284:LEU:CD1	1:T:324:MET:HE1	2.30	0.61
1:T:88:GLU:OE1	1:T:223:ARG:NE	2.29	0.61
1:T:718:LEU:HB3	1:T:835:TRP:HB3	1.82	0.61
1:T:46:ILE:HD12	2:S:42:VAL:O	1.99	0.61
1:T:126:LEU:CD1	1:T:156:VAL:HG23	2.25	0.60
1:T:145:GLN:N	1:T:481:MET:HB2	2.16	0.60
1:T:438:MET:CG	2:S:69:GLU:OE2	2.49	0.60
1:T:441:PHE:HE2	2:S:43:GLU:OE1	1.82	0.60
1:T:379:MET:HB2	1:T:402:ALA:HB3	1.84	0.60
1:T:694:HIS:CD2	1:T:696:ASP:H	2.19	0.60
1:T:698:ILE:CD1	1:T:699:DDE:HAT2	2.28	0.60
1:T:284:LEU:HD13	1:T:324:MET:CE	2.32	0.59
1:T:110:ASP:CB	1:T:483:PHE:C	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:324:MET:HE2	1:T:324:MET:HA	1.83	0.59
1:T:110:ASP:HB2	1:T:483:PHE:C	2.22	0.59
1:T:215:LEU:CB	4:T:843:GNP:N3	2.60	0.59
1:T:564:ARG:HG3	1:T:682:ARG:HB2	1.83	0.59
1:T:202:VAL:HG12	1:T:209:VAL:CG2	2.32	0.59
1:T:104:ASP:OD2	2:S:66:ALA:N	2.35	0.58
1:T:73:THR:HG22	2:S:67:HIS:CE1	2.37	0.58
1:T:46:ILE:HD11	2:S:44:VAL:N	2.18	0.58
1:T:464:LEU:CD1	1:T:513:LYS:HE2	2.34	0.58
1:T:365:ASN:O	1:T:369:ILE:HG12	2.03	0.58
1:T:464:LEU:HD13	1:T:513:LYS:CG	2.26	0.58
1:T:479:LYS:C	1:T:480:VAL:HG22	2.24	0.58
1:T:386:VAL:HG11	1:T:437:MET:CE	2.34	0.58
1:T:615:ARG:HG2	1:T:619:MET:HE3	1.86	0.57
1:T:4:PHE:CG	2:S:39:ASN:OD1	2.54	0.57
1:T:698:ILE:C	1:T:699:DDE:CG	2.47	0.57
1:T:34:THR:HG22	2:S:47:TYR:CD1	2.39	0.57
1:T:500:ASP:CB	1:T:552:VAL:HG11	2.35	0.57
1:T:110:ASP:CG	1:T:484:SER:O	2.43	0.57
1:T:497:ASN:HB3	1:T:500:ASP:OD2	2.04	0.57
1:T:386:VAL:HG11	1:T:437:MET:HE3	1.87	0.57
1:T:73:THR:CG2	2:S:67:HIS:CG	2.88	0.56
1:T:102:LEU:O	2:S:68:VAL:O	2.22	0.56
1:T:102:LEU:HD23	2:S:68:VAL:CG2	2.34	0.56
1:T:106:PRO:HB3	1:T:108:HIS:NE2	2.21	0.56
1:T:296:ILE:O	1:T:300:LEU:HD13	2.05	0.56
1:T:545:LEU:HA	1:T:549:HIS:HB2	1.85	0.56
1:T:104:ASP:CB	2:S:67:HIS:N	2.46	0.56
1:T:581:ASN:O	1:T:582:LYS:HB2	2.04	0.56
1:T:89:ILE:HG12	1:T:340:LEU:HD23	1.88	0.56
1:T:129:VAL:HG11	1:T:181:THR:CG2	2.36	0.56
1:T:615:ARG:HG2	1:T:619:MET:CE	2.36	0.56
1:T:108:HIS:CE1	1:T:114:GLU:HB2	2.42	0.55
1:T:500:ASP:HB3	1:T:552:VAL:HG11	1.87	0.55
1:T:279:ASP:HB3	1:T:280:PRO:HD3	1.89	0.55
1:T:44:GLY:N	2:S:36:ALA:N	2.52	0.55
1:T:194:ASP:HB2	1:T:197:LEU:HD13	1.89	0.55
1:T:3:ALA:HA	1:T:46:ILE:O	2.05	0.55
1:T:829:LYS:HE3	1:T:830:GLU:H	1.71	0.55
1:T:413:ILE:HB	1:T:427:PHE:HB2	1.88	0.54
1:T:215:LEU:HB3	4:T:843:GNP:N1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:37:ASP:OD1	2:S:50:ILE:HD11	2.04	0.54
1:T:120:ARG:HH22	1:T:480:VAL:CA	2.21	0.54
1:T:223:ARG:HA	1:T:241:MET:HE2	1.87	0.54
1:T:369:ILE:HD12	1:T:401:PHE:HB3	1.89	0.54
1:T:700:ARG:O	1:T:705:ILE:HD12	2.08	0.54
1:T:221:THR:HG21	1:T:336:GLU:OE1	2.07	0.54
1:T:31:GLY:HA2	4:T:843:GNP:O3A	2.06	0.54
1:T:26:ALA:HB3	1:T:32:LYS:HB2	1.88	0.54
1:T:70:ILE:O	1:T:440:ARG:HB3	2.07	0.54
1:T:215:LEU:HD23	4:T:843:GNP:N3	2.22	0.54
1:T:360:PRO:O	1:T:363:ASP:HB3	2.08	0.54
1:T:109:VAL:CB	1:T:483:PHE:HE2	2.19	0.54
1:T:28:VAL:HG22	1:T:138:GLN:OE1	2.08	0.54
1:T:699:DDE:HA	1:T:700:ARG:N	2.21	0.54
1:T:111:PHE:O	1:T:485:VAL:CG1	2.56	0.53
1:T:108:HIS:HE1	1:T:114:GLU:HB2	1.72	0.53
1:T:109:VAL:HG11	1:T:142:VAL:CG2	2.38	0.53
1:T:481:MET:CE	1:T:482:LYS:CB	2.87	0.53
1:T:696:ASP:HB3	1:T:699:DDE:HAB3	1.89	0.53
1:T:806:SER:HB2	1:T:813:SER:HB2	1.90	0.53
1:T:520:THR:HA	1:T:529:ILE:O	2.08	0.53
1:T:646:VAL:C	1:T:647:ILE:HD12	2.29	0.53
1:T:223:ARG:HG2	1:T:223:ARG:NH1	2.21	0.53
1:T:296:ILE:HB	1:T:297:PRO:HD3	1.89	0.53
1:T:3:ALA:O	2:S:40:PRO:HG3	1.92	0.53
1:T:4:PHE:CD2	2:S:41:ASN:HB2	2.44	0.53
1:T:37:ASP:OD2	2:S:47:TYR:N	2.41	0.53
1:T:378:LEU:H	1:T:471:THR:CG2	2.21	0.53
1:T:70:ILE:HG13	1:T:440:ARG:HA	1.91	0.53
1:T:112:SER:HB2	1:T:517:CYS:SG	2.48	0.53
1:T:34:THR:HG22	2:S:47:TYR:CE1	2.45	0.52
1:T:46:ILE:HD11	2:S:44:VAL:H	1.75	0.52
1:T:76:SER:OG	2:S:69:GLU:CD	2.46	0.52
1:T:74:ALA:O	2:S:69:GLU:HB2	2.09	0.52
1:T:129:VAL:HG11	1:T:181:THR:HG23	1.91	0.52
1:T:693:LEU:HB3	1:T:700:ARG:HD2	1.92	0.52
1:T:441:PHE:CD2	2:S:43:GLU:OE1	2.62	0.52
1:T:500:ASP:CG	1:T:552:VAL:HG11	2.29	0.52
1:T:77:LEU:HG	2:S:35:THR:HG21	1.92	0.52
1:T:46:ILE:O	2:S:41:ASN:CB	2.53	0.52
1:T:515:ASP:HB3	1:T:518:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:785:ARG:HH11	1:T:785:ARG:HG3	1.75	0.52
1:T:215:LEU:CA	4:T:843:GNP:N7	2.70	0.51
1:T:144:ARG:HH12	1:T:482:LYS:HA	1.63	0.51
1:T:145:GLN:HA	1:T:481:MET:CB	2.30	0.51
1:T:215:LEU:HB2	4:T:843:GNP:N7	2.23	0.51
1:T:718:LEU:HD12	1:T:722:PRO:HG2	1.92	0.51
1:T:745:SER:O	1:T:749:LYS:HG3	2.10	0.51
1:T:438:MET:CG	2:S:69:GLU:CD	2.79	0.51
1:T:471:THR:HG23	1:T:471:THR:O	2.09	0.51
1:T:76:SER:HG	2:S:69:GLU:CD	2.14	0.51
1:T:4:PHE:CG	2:S:41:ASN:HB2	2.45	0.51
1:T:829:LYS:HE2	1:T:830:GLU:H	1.74	0.51
1:T:250:PHE:O	1:T:252:PRO:HD3	2.10	0.51
1:T:479:LYS:HB2	1:T:479:LYS:N	2.26	0.51
1:T:104:ASP:CG	2:S:67:HIS:CD2	2.83	0.51
1:T:470:THR:HG21	1:T:475:ALA:HB1	1.93	0.51
1:T:576:LEU:HD13	1:T:587:TYR:CE1	2.46	0.51
1:T:110:ASP:C	1:T:483:PHE:O	2.50	0.51
1:T:215:LEU:CB	4:T:843:GNP:N7	2.72	0.50
1:T:426:LEU:HD12	1:T:427:PHE:H	1.76	0.50
1:T:31:GLY:HA2	4:T:843:GNP:O2A	2.11	0.50
1:T:345:PRO:O	1:T:349:GLN:HG3	2.12	0.50
1:T:576:LEU:HD21	1:T:585:ARG:NH1	2.27	0.50
1:T:76:SER:O	2:S:69:GLU:C	2.49	0.50
1:T:539:GLU:O	1:T:543:GLN:HG3	2.12	0.50
1:T:569:SER:O	1:T:720:ALA:HB1	2.10	0.50
1:T:189:VAL:HG13	1:T:200:VAL:HG13	1.92	0.50
1:T:360:PRO:HB2	1:T:363:ASP:HB2	1.94	0.50
1:T:607:ASN:HB2	1:T:610:ASP:OD2	2.11	0.50
1:T:76:SER:CA	2:S:69:GLU:HG3	2.29	0.50
1:T:807:ASP:OD1	1:T:809:LEU:N	2.44	0.50
1:T:706:ILE:HB	1:T:707:PRO:HD3	1.94	0.50
1:T:46:ILE:HD11	2:S:43:GLU:C	2.31	0.50
1:T:344:SER:C	1:T:345:PRO:HD3	2.31	0.49
1:T:414:GLN:HB2	1:T:477:ASN:HD21	1.77	0.49
1:T:116:THR:HG21	1:T:480:VAL:HA	1.94	0.49
1:T:114:GLU:OE1	1:T:516:PRO:CA	2.59	0.49
1:T:411:VAL:HG12	1:T:412:ARG:N	2.27	0.49
1:T:46:ILE:HG12	2:S:43:GLU:CG	2.41	0.49
1:T:76:SER:OG	2:S:69:GLU:OE2	2.30	0.49
1:T:699:DDE:HAD2	1:T:699:DDE:HAA3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:69:THR:HG22	1:T:441:PHE:CE1	2.47	0.49
1:T:215:LEU:HD23	4:T:843:GNP:C2	2.42	0.49
1:T:699:DDE:HAC3	3:T:1699:APR:O2B	2.13	0.49
1:T:576:LEU:HD21	1:T:585:ARG:HH11	1.76	0.49
1:T:202:VAL:CG1	1:T:209:VAL:CG2	2.91	0.49
1:T:215:LEU:N	4:T:843:GNP:O6	2.44	0.48
1:T:503:LYS:HD2	1:T:552:VAL:HG21	1.94	0.48
1:T:461:GLN:CD	1:T:461:GLN:H	2.16	0.48
1:T:109:VAL:CG1	1:T:142:VAL:CG2	2.92	0.48
1:T:271:ARG:HH11	1:T:271:ARG:HG3	1.79	0.48
1:T:120:ARG:NH2	1:T:479:LYS:C	2.66	0.48
1:T:433:ARG:HB3	1:T:457:VAL:HG11	1.95	0.48
1:T:126:LEU:HD11	1:T:156:VAL:HG21	1.93	0.48
1:T:646:VAL:HG23	1:T:667:PHE:CD2	2.49	0.48
1:T:552:VAL:HG13	1:T:553:PRO:HD2	1.95	0.48
1:T:200:VAL:HG22	1:T:200:VAL:O	2.13	0.48
1:T:70:ILE:HG13	1:T:440:ARG:C	2.34	0.48
1:T:110:ASP:OD2	1:T:112:SER:HB3	2.14	0.47
1:T:823:ARG:NH1	1:T:829:LYS:O	2.47	0.47
1:T:111:PHE:C	1:T:485:VAL:CG1	2.83	0.47
1:T:76:SER:HG	2:S:69:GLU:CG	2.22	0.47
1:T:699:DDE:HAU3	1:T:699:DDE:HAB2	1.76	0.47
1:T:411:VAL:HG12	1:T:412:ARG:H	1.80	0.47
1:T:186:ASN:HB3	1:T:201:GLN:OE1	2.14	0.47
1:T:153:PRO:HD2	1:T:200:VAL:HG22	1.95	0.47
1:T:215:LEU:CD1	4:T:843:GNP:HO2'	2.10	0.47
1:T:3:ALA:O	2:S:40:PRO:CB	2.55	0.47
1:T:698:ILE:HB	1:T:699:DDE:OAG	2.15	0.47
1:T:823:ARG:HE	1:T:832:VAL:HG22	1.80	0.47
1:T:104:ASP:O	2:S:67:HIS:CE1	2.67	0.47
1:T:221:THR:OG1	1:T:224:GLN:HG3	2.15	0.47
1:T:237:LYS:HA	1:T:240:MET:HB2	1.95	0.47
1:T:106:PRO:HB3	1:T:108:HIS:CD2	2.50	0.46
1:T:360:PRO:HD2	1:T:363:ASP:HB2	1.96	0.46
1:T:565:GLU:O	1:T:681:MET:HA	2.14	0.46
1:T:80:GLU:HA	1:T:96:ASN:O	2.16	0.46
1:T:784:LEU:HD23	1:T:794:PRO:HD3	1.97	0.46
1:T:42:ARG:HH12	2:S:38:GLU:HG2	1.81	0.46
1:T:515:ASP:O	1:T:518:VAL:HG12	2.15	0.46
1:T:785:ARG:HG3	1:T:786:GLN:N	2.31	0.46
1:T:73:THR:HG23	2:S:67:HIS:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:84:GLU:HG3	1:T:85:ASP:N	2.30	0.46
1:T:46:ILE:C	2:S:41:ASN:CA	2.50	0.46
1:T:70:ILE:HD13	1:T:442:VAL:HG13	1.98	0.46
1:T:454:ILE:HG13	1:T:455:GLY:N	2.30	0.46
1:T:72:SER:C	2:S:67:HIS:HB2	2.02	0.45
1:T:434:VAL:HG12	1:T:445:ILE:HG22	1.98	0.45
1:T:42:ARG:HG2	1:T:331:ALA:CB	2.47	0.45
1:T:202:VAL:HG12	1:T:209:VAL:HG23	1.98	0.45
1:T:763:THR:N	1:T:764:PRO:CD	2.79	0.45
1:T:202:VAL:CG1	1:T:209:VAL:HG22	2.47	0.45
1:T:733:ILE:O	1:T:767:THR:HA	2.17	0.45
1:T:809:LEU:O	1:T:811:PRO:HD3	2.16	0.45
1:T:78:TYR:HB3	2:S:39:ASN:HB2	1.98	0.45
1:T:46:ILE:HB	2:S:40:PRO:O	2.16	0.44
1:T:145:GLN:HG3	1:T:481:MET:CG	2.33	0.44
1:T:633:ILE:HG13	1:T:633:ILE:O	2.18	0.44
1:T:109:VAL:HG12	1:T:142:VAL:HG22	1.99	0.44
1:T:465:LYS:HE2	1:T:516:PRO:HG3	1.12	0.44
1:T:28:VAL:O	1:T:29:ASP:HB2	2.18	0.44
1:T:378:LEU:N	1:T:471:THR:HG22	2.28	0.44
1:T:515:ASP:HB3	1:T:518:VAL:HG12	1.99	0.44
1:T:77:LEU:HB2	1:T:100:ILE:HB	1.99	0.44
1:T:576:LEU:CD2	1:T:842:LEU:HG	2.45	0.44
1:T:267:LYS:HA	1:T:268:PRO:HD3	1.81	0.44
1:T:29:ASP:OD1	2:S:61:ILE:HG22	2.18	0.44
1:T:81:MET:HG3	1:T:339:VAL:HG11	1.99	0.44
1:T:353:ALA:HB3	1:T:370:LYS:HG2	1.99	0.44
1:T:44:GLY:O	2:S:36:ALA:CA	2.64	0.44
1:T:414:GLN:CB	1:T:477:ASN:HD21	2.31	0.43
1:T:73:THR:HG23	2:S:67:HIS:CD2	2.53	0.43
1:T:25:ILE:HG23	1:T:142:VAL:HB	2.00	0.43
1:T:718:LEU:HA	1:T:722:PRO:HG3	2.00	0.43
1:T:34:THR:CG2	4:T:843:GNP:O2A	2.43	0.43
1:T:380:LEU:HD13	1:T:456:LEU:HD11	2.01	0.43
1:T:810:ASP:O	1:T:816:GLY:HA3	2.19	0.43
1:T:72:SER:H	1:T:440:ARG:HG2	1.82	0.43
1:T:715:ALA:HB2	1:T:838:TYR:HB2	2.00	0.43
1:T:564:ARG:HG3	1:T:682:ARG:CB	2.47	0.43
1:T:438:MET:HA	2:S:69:GLU:CD	2.39	0.43
1:T:491:VAL:HG21	1:T:542:LEU:HD11	2.01	0.43
1:T:197:LEU:HD12	1:T:197:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:110:ASP:OD2	1:T:484:SER:O	2.36	0.42
1:T:763:THR:O	1:T:763:THR:HG22	2.19	0.42
1:T:77:LEU:HB3	2:S:35:THR:HG21	2.00	0.42
1:T:104:ASP:OD2	2:S:67:HIS:HD2	1.98	0.42
1:T:552:VAL:CG1	1:T:553:PRO:HD2	2.50	0.42
1:T:260:LYS:HB3	1:T:260:LYS:HE2	1.80	0.42
1:T:426:LEU:HD12	1:T:427:PHE:N	2.34	0.42
1:T:378:LEU:HD11	1:T:380:LEU:HB2	2.02	0.42
1:T:235:VAL:HG12	1:T:239:LYS:HB3	2.01	0.42
1:T:42:ARG:O	2:S:35:THR:C	2.53	0.42
1:T:230:ALA:C	1:T:232:LYS:H	2.23	0.42
1:T:108:HIS:CE1	1:T:112:SER:HG	2.37	0.42
1:T:357:TYR:OH	1:T:476:HIS:HB2	2.19	0.42
1:T:114:GLU:OE1	1:T:516:PRO:C	2.59	0.42
1:T:153:PRO:HD2	1:T:200:VAL:CG2	2.49	0.42
1:T:737:GLU:HB2	1:T:766:PHE:HE2	1.79	0.42
1:T:369:ILE:HD13	1:T:402:ALA:HB2	2.01	0.42
1:T:144:ARG:HH11	1:T:481:MET:CE	2.33	0.41
1:T:417:ASN:HB2	1:T:425:ASP:OD2	2.20	0.41
1:T:454:ILE:HG13	1:T:455:GLY:H	1.84	0.41
1:T:219:ALA:HB3	1:T:330:ALA:HA	2.02	0.41
1:T:699:DDE:HD2	3:T:1699:APR:O2D	2.20	0.41
1:T:744:TYR:CE1	1:T:754:VAL:HG21	2.55	0.41
1:T:479:LYS:C	1:T:479:LYS:CB	2.81	0.41
1:T:636:PHE:CE1	1:T:645:LEU:HD21	2.55	0.41
1:T:658:GLU:OE1	1:T:700:ARG:NH2	2.54	0.41
1:T:710:ARG:NH1	1:T:714:TYR:OH	2.54	0.41
1:T:722:PRO:O	1:T:723:LYS:HD2	2.20	0.41
1:T:418:TYR:C	1:T:418:TYR:CD1	2.94	0.41
1:T:287:ALA:HA	1:T:292:LYS:HD2	2.02	0.41
1:T:386:VAL:HA	1:T:387:PRO:HD3	1.87	0.41
1:T:388:THR:HG21	1:T:395:TYR:CD1	2.55	0.41
1:T:486:SER:HA	1:T:487:PRO:HD3	1.88	0.41
1:T:78:TYR:CB	2:S:39:ASN:HB2	2.50	0.41
1:T:481:MET:HE3	1:T:482:LYS:HB2	2.03	0.41
1:T:607:ASN:HA	1:T:608:PRO:HD3	1.83	0.41
1:T:829:LYS:HE3	1:T:829:LYS:CA	2.48	0.41
1:T:358:GLU:OE2	1:T:479:LYS:HG3	2.21	0.41
1:T:718:LEU:HA	1:T:722:PRO:CG	2.51	0.41
1:T:155:VAL:CG1	1:T:156:VAL:N	2.84	0.41
1:T:633:ILE:C	1:T:633:ILE:HD12	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:824:LYS:HD3	1:T:830:GLU:OE1	2.21	0.41
1:T:39:LEU:HB3	1:T:77:LEU:HD21	2.03	0.40
1:T:666:ALA:CB	1:T:709:MET:HB3	2.51	0.40
1:T:70:ILE:HG13	1:T:440:ARG:CA	2.50	0.40
1:T:27:HIS:CD2	1:T:136:CYS:HB2	2.57	0.40
1:T:161:ASP:CG	4:T:843:GNP:C2	2.70	0.40
1:T:235:VAL:CG1	1:T:239:LYS:HB3	2.51	0.40
1:T:254:THR:O	1:T:255:LYS:HB2	2.22	0.40
1:T:141:THR:HG22	1:T:483:PHE:CZ	2.52	0.40
1:T:465:LYS:HB3	1:T:466:THR:H	1.67	0.40
1:T:479:LYS:C	1:T:479:LYS:HA	2.25	0.40
1:T:111:PHE:CD2	1:T:481:MET:C	2.95	0.40
1:T:565:GLU:CD	1:T:676:ILE:HB	2.41	0.40
1:T:26:ALA:HB2	1:T:128:VAL:HB	2.04	0.40
1:T:120:ARG:NH2	1:T:480:VAL:CA	2.84	0.40
1:T:579:SER:HB3	1:T:708:THR:OG1	2.20	0.40
1:T:284:LEU:HD11	1:T:303:LEU:CD1	2.51	0.40
1:T:490:GLN:O	1:T:559:PRO:HD3	2.22	0.40
1:T:731:VAL:HG13	1:T:731:VAL:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	796/842 (94%)	750 (94%)	40 (5%)	6 (1%)	22	67
2	S	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
All	All	829/877 (94%)	782 (94%)	41 (5%)	6 (1%)	30	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	764	PRO
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%)	35	65
2	S	28/28 (100%)	27 (96%)	1 (4%)	40	68
All	All	719/742 (97%)	690 (96%)	29 (4%)	40	65

All (29) 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

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Mol	Chain	Res	Type
1	T	596	GLU
1	T	599	LEU
1	T	633	ILE
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
2	S	43	GLU

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	1,3	15,20,21	1.48	2 (13%)	15,28,30	2.06	6 (40%)

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	1,3	-	0/19/21/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	699	DDE	CA-C	2.80	1.53	1.50
1	T	699	DDE	CAT-CE1	3.98	1.54	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	699	DDE	OAG-CBI-CBW	-3.97	115.75	120.64
1	T	699	DDE	CAU-CBW-CBI	-2.65	105.89	111.12
1	T	699	DDE	CAC-NCB-CAB	-2.15	102.23	108.11
1	T	699	DDE	CAC-NCB-CBW	2.78	117.58	110.51
1	T	699	DDE	CAT-CE1-ND1	3.01	130.95	122.54
1	T	699	DDE	OAG-CBI-NAD	3.58	128.55	123.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	T	699	DDE	21	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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
3	APR	T	1699	1	33,38,39	1.68	5 (15%)	32,58,60	2.04	9 (28%)
4	GNP	T	843	1	27,34,34	2.99	10 (37%)	26,54,54	1.76	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	APR	T	1699	1	1/1/9/10	0/18/51/54	0/4/4/4
4	GNP	T	843	1	-	0/16/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	843	GNP	C4-N9	-10.48	1.33	1.47
4	T	843	GNP	C5-C6	-6.52	1.41	1.53
3	T	1699	APR	O5'-C5'	-6.07	1.20	1.44
4	T	843	GNP	C2'-C1'	-3.76	1.41	1.53
4	T	843	GNP	C8-N9	-3.74	1.35	1.46
3	T	1699	APR	PA-O2A	-2.90	1.40	1.55
4	T	843	GNP	PB-N3B	-2.74	1.56	1.63
3	T	1699	APR	PB-O2B	-2.55	1.42	1.55
4	T	843	GNP	PG-N3B	-2.25	1.57	1.63
4	T	843	GNP	O4'-C4'	-2.23	1.40	1.45
4	T	843	GNP	PB-O3A	-2.16	1.56	1.59
4	T	843	GNP	PG-O1G	2.29	1.48	1.46
3	T	1699	APR	O4'-C4'	2.55	1.50	1.45
3	T	1699	APR	C2-N1	3.55	1.40	1.33
4	T	843	GNP	C6-N1	3.73	1.39	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1699	APR	O4'-C4'-C5'	-5.89	89.51	109.40
3	T	1699	APR	O2D-C2D-C3D	-3.77	104.10	111.28
3	T	1699	APR	C1'-N9-C4	-3.09	121.29	126.64
4	T	843	GNP	O6-C6-N1	-2.42	119.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1699	APR	O4D-C1D-C2D	-2.37	101.24	106.00
3	T	1699	APR	C5'-C4'-C3'	-2.03	107.53	115.29
3	T	1699	APR	C4-C5-N7	2.01	111.35	109.41
4	T	843	GNP	C2'-C3'-C4'	2.28	107.07	102.62
4	T	843	GNP	O2G-PG-O1G	2.35	119.38	113.41
3	T	1699	APR	C1D-O4D-C4D	3.25	115.88	108.15
4	T	843	GNP	O3A-PB-N3B	3.33	115.82	106.59
3	T	1699	APR	O5'-C5'-C4'	3.83	122.59	109.00
4	T	843	GNP	O6-C6-C5	3.90	127.15	119.69
3	T	1699	APR	C1D-C2D-C3D	3.95	107.73	101.67
4	T	843	GNP	O1B-PB-N3B	3.98	117.74	111.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	T	1699	APR	C1D

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1699	APR	7	0
4	T	843	GNP	42	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.