wwPDB EM Map/Model Validation Report (i)

May 2, 2016 – 07:11 PM EDT

PDB ID	:	3JD4
EMDB ID:	:	EMD-6633
Title	:	Glutamate dehydrogenase in complex with NADH and GTP, closed conformation
Authors	:	Borgnia, M.J.; Banerjee, S.; Merk, A.; Matthies, D.; Bartesaghi, A.; Rao, P.; Pierson, J.; Earl, L.A.; Falconieri, V.; Subramaniam, S.; Milne, J.L.S.
Deposited on	:	2016-03-28
Resolution	:	3.40 Å(reported)
Based on PDB ID	:	3MW9

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

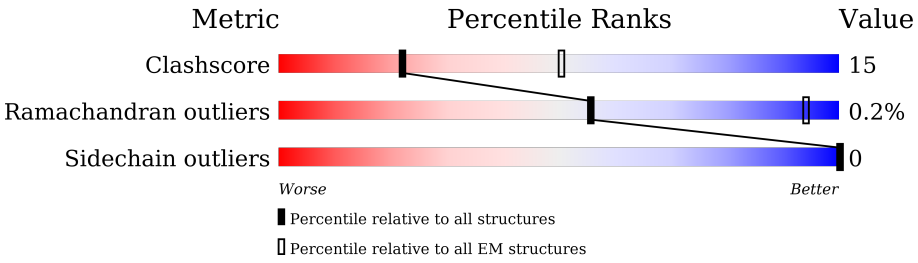
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	501	64% 35% .
1	B	501	64% 35% .
1	C	501	64% 35% .
1	D	501	64% 35% .
1	E	501	64% 35% .
1	F	501	64% 35% .

2 Entry composition

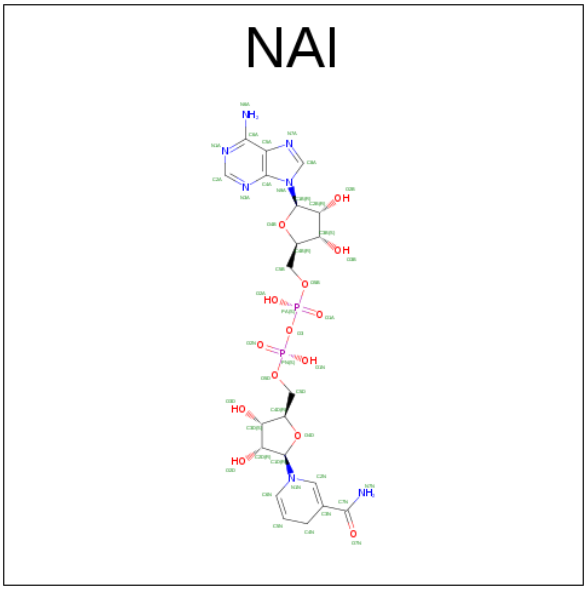
There are 3 unique types of molecules in this entry. The entry contains 24054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

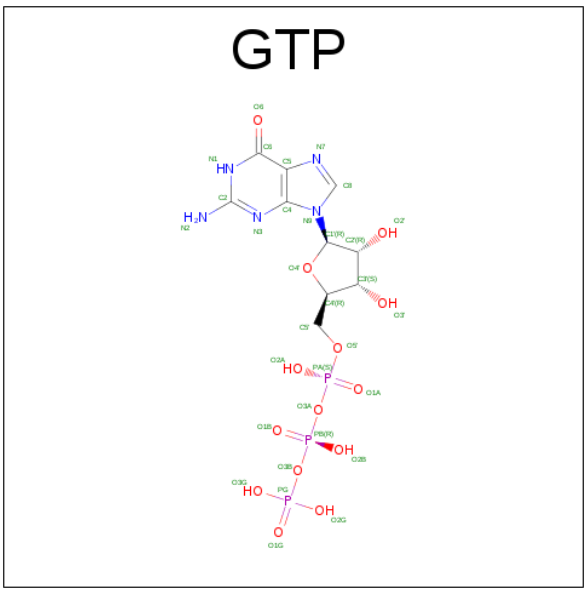
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	497	Total	C	N	O	S	0	0
			3889	2458	680	732	19		
1	B	497	Total	C	N	O	S	0	0
			3889	2458	680	732	19		
1	C	497	Total	C	N	O	S	0	0
			3889	2458	680	732	19		
1	D	497	Total	C	N	O	S	0	0
			3889	2458	680	732	19		
1	E	497	Total	C	N	O	S	0	0
			3889	2458	680	732	19		
1	F	497	Total	C	N	O	S	0	0
			3889	2458	680	732	19		

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	D	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	D	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	E	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	E	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	F	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	F	1	Total	C	N	O	P	0
			88	42	14	28	4	

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



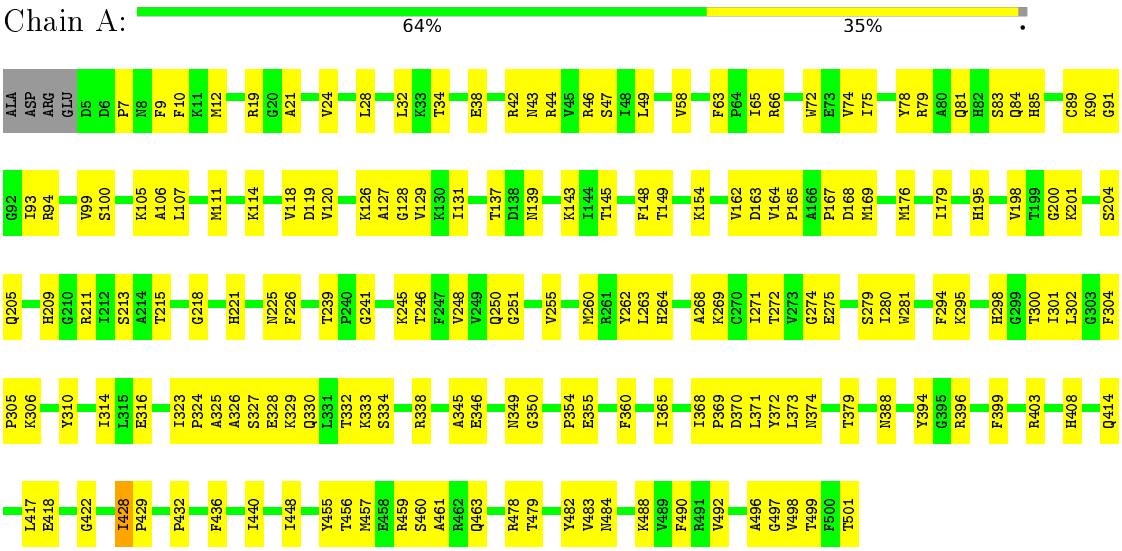
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	F	1	Total	C	N	O	P	0
			32	10	5	14	3	

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. 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.

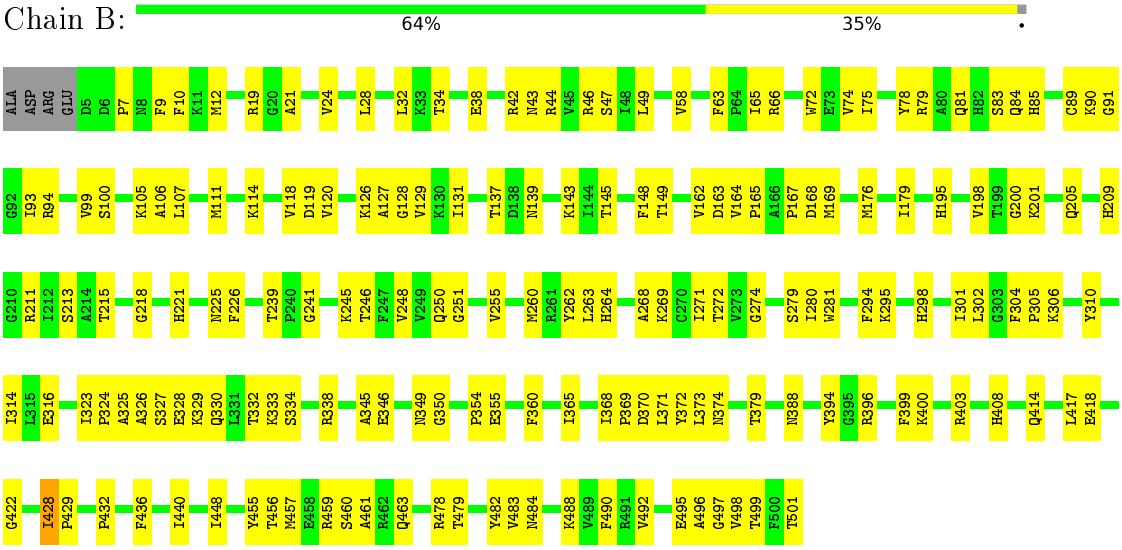
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain A:



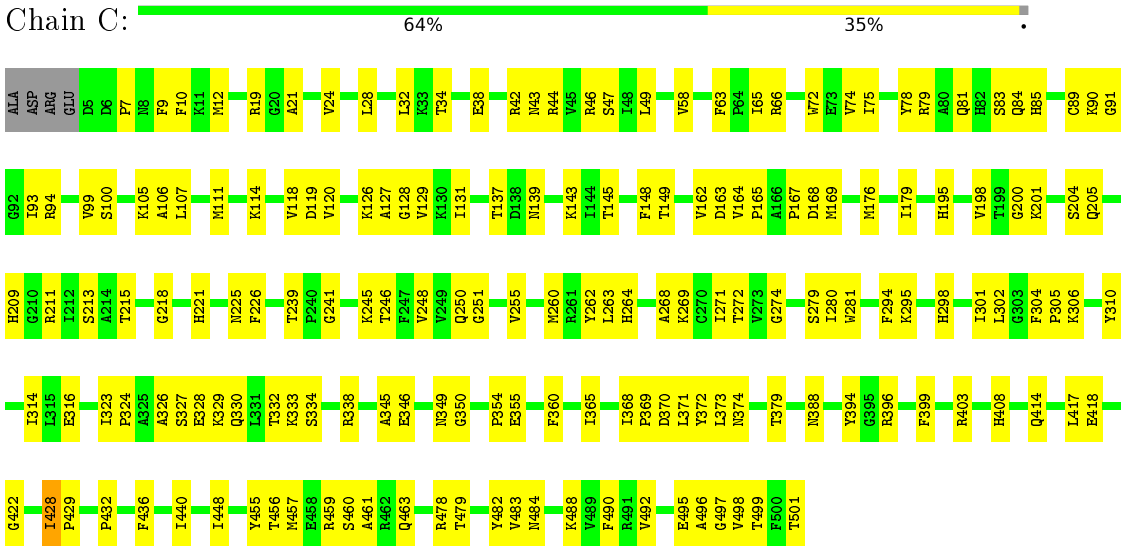
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain B:



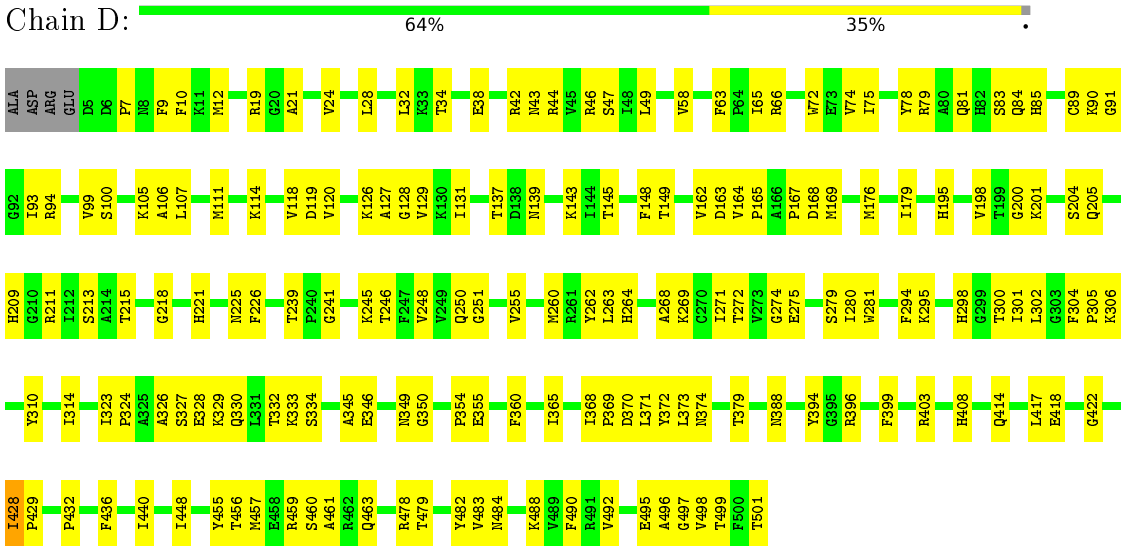
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:



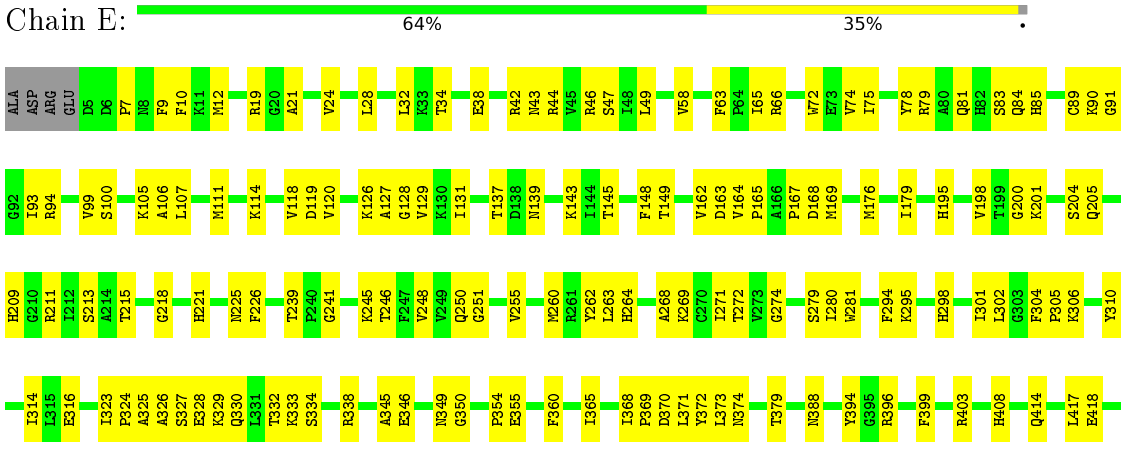
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D:



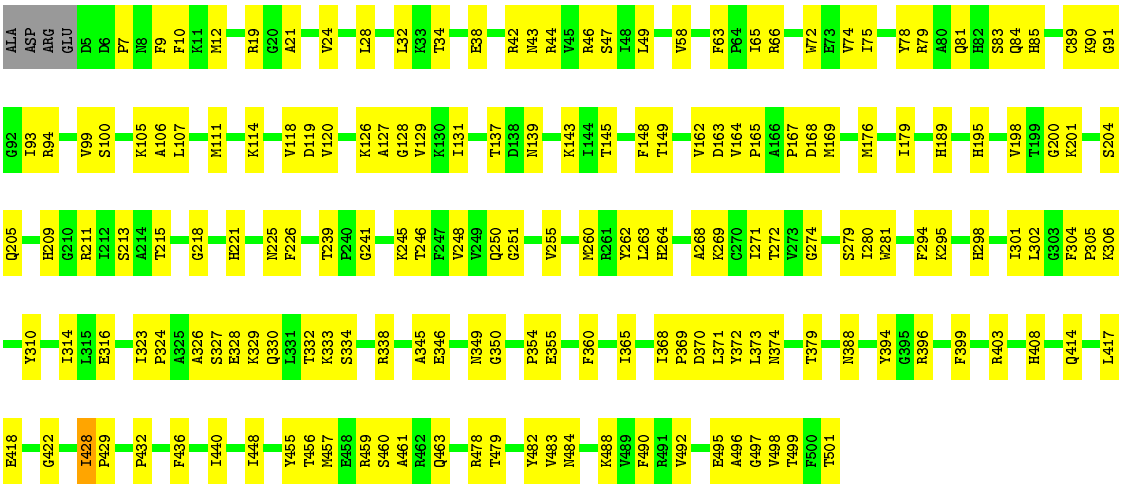
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain E:



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	20429	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, NAI

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	A	0.42	0/3972	0.49	1/5362 (0.0%)
1	B	0.41	0/3972	0.49	1/5362 (0.0%)
1	C	0.41	0/3972	0.49	1/5362 (0.0%)
1	D	0.41	0/3972	0.49	1/5362 (0.0%)
1	E	0.41	0/3972	0.49	1/5362 (0.0%)
1	F	0.41	0/3972	0.49	1/5362 (0.0%)
All	All	0.41	0/23832	0.49	6/32172 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	ILE	C-N-CD	5.20	139.32	128.40
1	D	428	ILE	C-N-CD	5.20	139.31	128.40
1	B	428	ILE	C-N-CD	5.18	139.29	128.40
1	C	428	ILE	C-N-CD	5.18	139.27	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	428	ILE	C-N-CD	5.17	139.26	128.40
1	F	428	ILE	C-N-CD	5.17	139.26	128.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	497	GLY	Peptide
1	B	497	GLY	Peptide
1	C	497	GLY	Peptide
1	D	497	GLY	Peptide
1	E	497	GLY	Peptide
1	F	497	GLY	Peptide

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	3889	0	3852	132	0
1	B	3889	0	3852	127	0
1	C	3889	0	3852	125	0
1	D	3889	0	3852	129	0
1	E	3889	0	3852	127	0
1	F	3889	0	3852	127	0
2	A	88	0	54	3	0
2	B	88	0	54	3	0
2	C	88	0	54	2	0
2	D	88	0	54	2	0
2	E	88	0	54	3	0
2	F	88	0	54	2	0
3	A	32	0	12	2	0
3	B	32	0	12	2	0
3	C	32	0	12	1	0
3	D	32	0	12	2	0
3	E	32	0	12	2	0
3	F	32	0	12	1	0
All	All	24054	0	23508	718	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 15.

All (718) 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:47:SER:HB2	1:E:72:TRP:HB2	1.63	0.80
1:B:326:ALA:HB3	1:B:330:GLN:HE22	1.47	0.80
1:E:326:ALA:HB3	1:E:330:GLN:HE22	1.47	0.80
1:A:326:ALA:HB3	1:A:330:GLN:HE22	1.47	0.79
1:C:195:HIS:O	1:C:201:LYS:NZ	2.16	0.79
1:F:195:HIS:O	1:F:201:LYS:NZ	2.16	0.79
1:D:326:ALA:HB3	1:D:330:GLN:HE22	1.47	0.79
1:C:326:ALA:HB3	1:C:330:GLN:HE22	1.47	0.79
1:F:326:ALA:HB3	1:F:330:GLN:HE22	1.47	0.79
1:B:72:TRP:HB2	1:D:47:SER:HB2	1.65	0.79
1:C:47:SER:HB2	1:F:72:TRP:HB2	1.65	0.79
1:D:195:HIS:O	1:D:201:LYS:NZ	2.16	0.78
1:A:195:HIS:O	1:A:201:LYS:NZ	2.16	0.78
1:C:72:TRP:HB2	1:F:47:SER:HB2	1.65	0.78
1:B:47:SER:HB2	1:D:72:TRP:HB2	1.65	0.78
1:E:195:HIS:O	1:E:201:LYS:NZ	2.16	0.78
1:B:195:HIS:O	1:B:201:LYS:NZ	2.16	0.78
1:A:72:TRP:HB2	1:E:47:SER:HB2	1.66	0.78
1:B:137:THR:HG22	1:B:139:ASN:H	1.56	0.71
1:E:137:THR:HG22	1:E:139:ASN:H	1.56	0.71
1:D:137:THR:HG22	1:D:139:ASN:H	1.56	0.71
1:A:137:THR:HG22	1:A:139:ASN:H	1.56	0.70
1:C:137:THR:HG22	1:C:139:ASN:H	1.56	0.70
1:F:137:THR:HG22	1:F:139:ASN:H	1.56	0.70
1:B:119:ASP:OD1	1:B:488:LYS:NZ	2.23	0.69
1:E:119:ASP:OD1	1:E:488:LYS:NZ	2.23	0.69
1:E:241:GLY:O	1:E:245:LYS:NZ	2.25	0.68
1:B:241:GLY:O	1:B:245:LYS:NZ	2.25	0.68
1:D:417:LEU:HB2	1:D:428:ILE:HD12	1.75	0.68
1:A:241:GLY:O	1:A:245:LYS:NZ	2.25	0.68
1:C:246:THR:HG22	1:C:269:LYS:HB3	1.76	0.68
1:F:246:THR:HG22	1:F:269:LYS:HB3	1.76	0.68
1:B:65:ILE:HD13	1:B:75:ILE:HD11	1.75	0.68
1:D:241:GLY:O	1:D:245:LYS:NZ	2.25	0.68
1:E:65:ILE:HD13	1:E:75:ILE:HD11	1.75	0.68
1:A:417:LEU:HB2	1:A:428:ILE:HD12	1.75	0.68
1:C:65:ILE:HD13	1:C:75:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ILE:HD13	1:F:75:ILE:HD11	1.75	0.68
1:D:94:ARG:HG3	1:D:169:MET:HB3	1.75	0.68
1:D:246:THR:HG22	1:D:269:LYS:HB3	1.76	0.68
1:A:94:ARG:HG3	1:A:169:MET:HB3	1.75	0.68
1:A:246:THR:HG22	1:A:269:LYS:HB3	1.76	0.68
1:C:417:LEU:HB2	1:C:428:ILE:HD12	1.76	0.68
1:E:94:ARG:NH1	1:E:328:GLU:OE2	2.27	0.68
1:B:94:ARG:NH1	1:B:328:GLU:OE2	2.27	0.68
1:F:417:LEU:HB2	1:F:428:ILE:HD12	1.76	0.68
1:F:94:ARG:HG3	1:F:169:MET:HB3	1.75	0.68
1:C:94:ARG:HG3	1:C:169:MET:HB3	1.75	0.67
1:B:94:ARG:HG3	1:B:169:MET:HB3	1.75	0.67
1:A:65:ILE:HD13	1:A:75:ILE:HD11	1.75	0.67
1:E:94:ARG:HG3	1:E:169:MET:HB3	1.75	0.67
1:A:346:GLU:H	1:A:373:LEU:HD12	1.60	0.67
1:D:65:ILE:HD13	1:D:75:ILE:HD11	1.75	0.67
1:E:246:THR:HG22	1:E:269:LYS:HB3	1.76	0.67
1:B:246:THR:HG22	1:B:269:LYS:HB3	1.76	0.67
1:F:94:ARG:NH1	1:F:328:GLU:OE2	2.27	0.67
1:C:119:ASP:OD1	1:C:488:LYS:NZ	2.23	0.67
1:C:94:ARG:NH1	1:C:328:GLU:OE2	2.27	0.67
1:D:346:GLU:H	1:D:373:LEU:HD12	1.60	0.67
1:A:408:HIS:HB3	1:C:436:PHE:HB2	1.77	0.67
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.77	0.67
1:E:417:LEU:HB2	1:E:428:ILE:HD12	1.77	0.66
1:F:119:ASP:OD1	1:F:488:LYS:NZ	2.23	0.66
1:B:417:LEU:HB2	1:B:428:ILE:HD12	1.77	0.66
1:A:143:LYS:HB3	1:E:501:THR:HG23	1.78	0.66
1:A:436:PHE:HB2	1:B:408:HIS:HB3	1.78	0.66
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.60	0.66
1:B:436:PHE:HB2	1:C:408:HIS:HB3	1.77	0.66
1:E:436:PHE:HB2	1:F:408:HIS:HB3	1.77	0.66
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.60	0.66
1:D:119:ASP:OD1	1:D:488:LYS:NZ	2.23	0.66
1:B:501:THR:HG23	1:D:143:LYS:HB3	1.78	0.66
1:D:94:ARG:NH1	1:D:328:GLU:OE2	2.27	0.66
1:D:408:HIS:HB3	1:F:436:PHE:HB2	1.77	0.66
1:A:94:ARG:NH1	1:A:328:GLU:OE2	2.27	0.66
1:C:241:GLY:O	1:C:245:LYS:NZ	2.25	0.66
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.60	0.66
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:GLY:O	1:F:245:LYS:NZ	2.25	0.66
1:B:346:GLU:H	1:B:373:LEU:HD12	1.60	0.66
1:D:349:ASN:OD1	1:D:374:ASN:ND2	2.28	0.66
1:A:501:THR:HG23	1:E:143:LYS:HB3	1.77	0.66
1:C:346:GLU:H	1:C:373:LEU:HD12	1.60	0.66
1:E:346:GLU:H	1:E:373:LEU:HD12	1.60	0.66
1:F:346:GLU:H	1:F:373:LEU:HD12	1.60	0.66
1:A:349:ASN:OD1	1:A:374:ASN:ND2	2.28	0.66
1:B:349:ASN:OD1	1:B:374:ASN:ND2	2.28	0.65
1:E:349:ASN:OD1	1:E:374:ASN:ND2	2.28	0.65
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.60	0.65
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.60	0.65
1:C:143:LYS:HB3	1:F:501:THR:HG23	1.78	0.65
1:C:501:THR:HG23	1:F:143:LYS:HB3	1.78	0.65
1:B:143:LYS:HB3	1:D:501:THR:HG23	1.78	0.65
1:A:119:ASP:O	1:B:396:ARG:NH1	2.28	0.65
1:D:119:ASP:O	1:E:396:ARG:NH1	2.28	0.64
1:B:260:MET:O	1:B:264:HIS:N	2.31	0.64
1:D:260:MET:O	1:D:264:HIS:N	2.31	0.64
1:E:260:MET:O	1:E:264:HIS:N	2.31	0.64
1:F:349:ASN:OD1	1:F:374:ASN:ND2	2.28	0.64
1:A:260:MET:O	1:A:264:HIS:N	2.31	0.64
1:C:260:MET:O	1:C:264:HIS:N	2.30	0.64
1:C:349:ASN:OD1	1:C:374:ASN:ND2	2.28	0.64
1:F:260:MET:O	1:F:264:HIS:N	2.31	0.64
1:D:396:ARG:NH1	1:F:119:ASP:O	2.29	0.64
1:A:396:ARG:NH1	1:C:119:ASP:O	2.29	0.64
1:A:274:GLY:HA3	1:A:314:ILE:HD11	1.79	0.63
1:D:274:GLY:HA3	1:D:314:ILE:HD11	1.79	0.63
1:E:350:GLY:N	1:E:370:ASP:OD2	2.28	0.63
1:A:119:ASP:OD1	1:A:488:LYS:NZ	2.23	0.63
1:B:350:GLY:N	1:B:370:ASP:OD2	2.28	0.63
1:B:274:GLY:HA3	1:B:314:ILE:HD11	1.80	0.63
1:C:274:GLY:HA3	1:C:314:ILE:HD11	1.79	0.63
1:E:274:GLY:HA3	1:E:314:ILE:HD11	1.80	0.63
1:F:274:GLY:HA3	1:F:314:ILE:HD11	1.80	0.63
1:F:213:SER:HB3	1:F:262:TYR:HE2	1.65	0.62
1:C:213:SER:HB3	1:C:262:TYR:HE2	1.65	0.62
1:A:32:LEU:HD21	1:A:44:ARG:HD3	1.82	0.62
1:D:32:LEU:HD21	1:D:44:ARG:HD3	1.82	0.62
1:C:323:ILE:HG12	1:C:345:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:ILE:HG12	1:D:345:ALA:HB3	1.81	0.62
1:F:323:ILE:HG12	1:F:345:ALA:HB3	1.81	0.62
1:A:323:ILE:HG12	1:A:345:ALA:HB3	1.81	0.62
1:E:213:SER:HB3	1:E:262:TYR:HE2	1.65	0.62
1:B:213:SER:HB3	1:B:262:TYR:HE2	1.65	0.61
1:B:323:ILE:HG12	1:B:345:ALA:HB3	1.81	0.61
1:B:32:LEU:HD21	1:B:44:ARG:HD3	1.82	0.61
1:B:119:ASP:O	1:C:396:ARG:NH1	2.29	0.61
1:E:323:ILE:HG12	1:E:345:ALA:HB3	1.81	0.61
1:E:32:LEU:HD21	1:E:44:ARG:HD3	1.82	0.61
1:D:58:VAL:HG21	1:D:105:LYS:HE2	1.83	0.61
1:F:350:GLY:N	1:F:370:ASP:OD2	2.28	0.61
1:A:58:VAL:HG21	1:A:105:LYS:HE2	1.83	0.61
1:E:119:ASP:O	1:F:396:ARG:NH1	2.29	0.61
1:C:350:GLY:N	1:C:370:ASP:OD2	2.28	0.61
1:D:213:SER:HB3	1:D:262:TYR:HE2	1.65	0.60
1:C:32:LEU:HD21	1:C:44:ARG:HD3	1.82	0.60
1:A:213:SER:HB3	1:A:262:TYR:HE2	1.65	0.60
1:F:32:LEU:HD21	1:F:44:ARG:HD3	1.82	0.60
1:C:99:VAL:HG21	1:C:128:GLY:HA3	1.83	0.60
1:F:99:VAL:HG21	1:F:128:GLY:HA3	1.83	0.60
1:C:280:ILE:HD11	1:C:302:LEU:HA	1.84	0.60
1:C:58:VAL:HG21	1:C:105:LYS:HE2	1.83	0.60
1:E:99:VAL:HG21	1:E:128:GLY:HA3	1.83	0.59
1:F:280:ILE:HD11	1:F:302:LEU:HA	1.84	0.59
1:B:99:VAL:HG21	1:B:128:GLY:HA3	1.83	0.59
1:F:58:VAL:HG21	1:F:105:LYS:HE2	1.83	0.59
1:E:58:VAL:HG21	1:E:105:LYS:HE2	1.83	0.59
1:B:58:VAL:HG21	1:B:105:LYS:HE2	1.83	0.59
1:A:280:ILE:HD11	1:A:302:LEU:HA	1.84	0.59
1:A:417:LEU:CB	1:A:428:ILE:HD12	2.33	0.59
1:D:417:LEU:CB	1:D:428:ILE:HD12	2.33	0.59
1:D:280:ILE:HD11	1:D:302:LEU:HA	1.84	0.59
1:D:414:GLN:NE2	1:D:428:ILE:O	2.35	0.59
1:A:99:VAL:HG21	1:A:128:GLY:HA3	1.83	0.59
1:B:414:GLN:NE2	1:B:428:ILE:O	2.36	0.59
1:D:99:VAL:HG21	1:D:128:GLY:HA3	1.83	0.59
1:E:414:GLN:NE2	1:E:428:ILE:O	2.36	0.59
1:A:414:GLN:NE2	1:A:428:ILE:O	2.36	0.58
1:A:350:GLY:N	1:A:370:ASP:OD2	2.28	0.58
1:D:350:GLY:N	1:D:370:ASP:OD2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ILE:HD11	1:B:302:LEU:HA	1.84	0.58
1:E:280:ILE:HD11	1:E:302:LEU:HA	1.84	0.58
1:C:414:GLN:NE2	1:C:428:ILE:O	2.36	0.58
1:A:81:GLN:NE2	1:A:163:ASP:OD2	2.34	0.58
1:D:81:GLN:NE2	1:D:163:ASP:OD2	2.34	0.58
1:B:417:LEU:CB	1:B:428:ILE:HD12	2.34	0.58
1:E:417:LEU:CB	1:E:428:ILE:HD12	2.34	0.58
1:F:414:GLN:NE2	1:F:428:ILE:O	2.36	0.57
1:F:81:GLN:NE2	1:F:163:ASP:OD2	2.34	0.57
1:B:81:GLN:NE2	1:B:163:ASP:OD2	2.34	0.57
1:E:81:GLN:NE2	1:E:163:ASP:OD2	2.34	0.57
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.86	0.57
1:C:81:GLN:NE2	1:C:163:ASP:OD2	2.34	0.57
1:B:200:GLY:HA2	1:B:211:ARG:HG2	1.87	0.57
1:E:12:MET:HG3	1:E:354:PRO:HD3	1.86	0.57
1:E:200:GLY:HA2	1:E:211:ARG:HG2	1.87	0.57
1:E:239:THR:O	1:E:245:LYS:NZ	2.32	0.57
1:C:417:LEU:CB	1:C:428:ILE:HD12	2.34	0.57
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.86	0.57
1:F:12:MET:HG3	1:F:354:PRO:HD3	1.86	0.57
2:D:601:NAI:N7N	2:D:601:NAI:O2N	2.38	0.56
1:F:417:LEU:CB	1:F:428:ILE:HD12	2.34	0.56
2:A:601:NAI:O2N	2:A:601:NAI:N7N	2.38	0.56
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.86	0.56
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.86	0.56
1:C:200:GLY:HA2	1:C:211:ARG:HG2	1.87	0.56
1:C:24:VAL:HG22	1:C:483:VAL:HG13	1.88	0.56
1:F:24:VAL:HG22	1:F:483:VAL:HG13	1.88	0.56
1:B:10:PHE:HA	1:B:106:ALA:HB2	1.88	0.56
1:F:200:GLY:HA2	1:F:211:ARG:HG2	1.87	0.56
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.88	0.56
1:A:200:GLY:HA2	1:A:211:ARG:HG2	1.87	0.56
1:D:200:GLY:HA2	1:D:211:ARG:HG2	1.87	0.56
1:A:149:THR:HG21	1:A:179:ILE:HG23	1.88	0.56
1:D:149:THR:HG21	1:D:179:ILE:HG23	1.88	0.56
1:D:10:PHE:HA	1:D:106:ALA:HB2	1.88	0.55
1:A:10:PHE:HA	1:A:106:ALA:HB2	1.88	0.55
1:B:24:VAL:HG22	1:B:483:VAL:HG13	1.88	0.55
1:E:24:VAL:HG22	1:E:483:VAL:HG13	1.88	0.55
1:D:43:ASN:OD1	1:D:46:ARG:NH2	2.38	0.55
1:A:43:ASN:OD1	1:A:46:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HB3	1:B:46:ARG:HH12	1.72	0.55
1:E:42:ARG:HB3	1:E:46:ARG:HH12	1.72	0.55
1:C:42:ARG:HB3	1:C:46:ARG:HH12	1.72	0.55
1:F:10:PHE:HA	1:F:106:ALA:HB2	1.88	0.55
1:F:42:ARG:HB3	1:F:46:ARG:HH12	1.72	0.55
1:A:24:VAL:HG22	1:A:483:VAL:HG13	1.88	0.54
1:D:24:VAL:HG22	1:D:483:VAL:HG13	1.88	0.54
1:E:149:THR:HG21	1:E:179:ILE:HG23	1.89	0.54
1:B:149:THR:HG21	1:B:179:ILE:HG23	1.89	0.54
1:C:10:PHE:HA	1:C:106:ALA:HB2	1.88	0.54
1:C:149:THR:HG21	1:C:179:ILE:HG23	1.88	0.54
1:D:279:SER:HB2	1:D:310:TYR:HB3	1.89	0.54
1:F:149:THR:HG21	1:F:179:ILE:HG23	1.89	0.54
1:A:279:SER:HB2	1:A:310:TYR:HB3	1.89	0.54
1:D:42:ARG:HB3	1:D:46:ARG:HH12	1.72	0.54
1:A:42:ARG:HB3	1:A:46:ARG:HH12	1.72	0.54
1:B:327:SER:HB3	1:B:330:GLN:HE21	1.73	0.54
1:E:495:GLU:OE1	1:F:204:SER:OG	2.21	0.54
1:C:43:ASN:OD1	1:C:46:ARG:NH2	2.38	0.54
1:E:327:SER:HB3	1:E:330:GLN:HE21	1.73	0.54
1:C:333:LYS:HD2	1:C:355:GLU:HG2	1.90	0.53
2:C:602:NAI:O2N	2:C:602:NAI:N7N	2.42	0.53
1:F:43:ASN:OD1	1:F:46:ARG:NH2	2.38	0.53
2:F:602:NAI:N7N	2:F:602:NAI:O2N	2.42	0.53
1:B:495:GLU:OE1	1:C:204:SER:OG	2.21	0.53
1:F:333:LYS:HD2	1:F:355:GLU:HG2	1.90	0.53
1:A:327:SER:HB3	1:A:330:GLN:HE21	1.73	0.53
1:D:327:SER:HB3	1:D:330:GLN:HE21	1.73	0.53
1:E:279:SER:HB2	1:E:310:TYR:HB3	1.89	0.53
1:F:239:THR:O	1:F:245:LYS:NZ	2.32	0.53
1:B:333:LYS:HD2	1:B:355:GLU:HG2	1.90	0.53
1:E:43:ASN:OD1	1:E:46:ARG:NH2	2.38	0.53
1:A:333:LYS:HD2	1:A:355:GLU:HG2	1.90	0.53
1:E:213:SER:HB3	1:E:262:TYR:CE2	2.44	0.53
1:E:250:GLN:HB3	1:E:324:PRO:HA	1.91	0.53
1:E:333:LYS:HD2	1:E:355:GLU:HG2	1.90	0.53
1:F:42:ARG:HB3	1:F:46:ARG:NH1	2.24	0.53
1:B:213:SER:HB3	1:B:262:TYR:CE2	2.44	0.53
1:B:279:SER:HB2	1:B:310:TYR:HB3	1.90	0.53
1:B:250:GLN:HB3	1:B:324:PRO:HA	1.91	0.53
1:C:42:ARG:HB3	1:C:46:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ASN:OD1	1:B:46:ARG:NH2	2.38	0.53
1:B:85:HIS:HB2	1:B:492:VAL:HG11	1.90	0.53
1:D:333:LYS:HD2	1:D:355:GLU:HG2	1.90	0.53
1:E:42:ARG:HB3	1:E:46:ARG:NH1	2.24	0.53
1:B:42:ARG:HB3	1:B:46:ARG:NH1	2.24	0.52
2:B:602:NAI:O2N	2:B:602:NAI:N7N	2.42	0.52
1:C:239:THR:O	1:C:245:LYS:NZ	2.32	0.52
1:C:327:SER:HB3	1:C:330:GLN:HE21	1.73	0.52
1:C:85:HIS:HB2	1:C:492:VAL:HG11	1.90	0.52
1:F:279:SER:HB2	1:F:310:TYR:HB3	1.89	0.52
1:C:279:SER:HB2	1:C:310:TYR:HB3	1.89	0.52
1:E:85:HIS:HB2	1:E:492:VAL:HG11	1.90	0.52
1:F:85:HIS:HB2	1:F:492:VAL:HG11	1.90	0.52
1:F:327:SER:HB3	1:F:330:GLN:HE21	1.73	0.52
1:A:42:ARG:HB3	1:A:46:ARG:NH1	2.24	0.52
2:E:602:NAI:O2N	2:E:602:NAI:N7N	2.42	0.52
1:A:85:HIS:HB2	1:A:492:VAL:HG11	1.90	0.52
1:D:213:SER:HB3	1:D:262:TYR:CE2	2.44	0.52
1:D:42:ARG:HB3	1:D:46:ARG:NH1	2.24	0.52
1:A:213:SER:HB3	1:A:262:TYR:CE2	2.44	0.52
1:D:85:HIS:HB2	1:D:492:VAL:HG11	1.90	0.52
1:F:250:GLN:HB3	1:F:324:PRO:HA	1.91	0.52
1:C:213:SER:HB3	1:C:262:TYR:CE2	2.44	0.52
1:D:349:ASN:ND2	2:D:601:NAI:O2D	2.43	0.52
1:F:213:SER:HB3	1:F:262:TYR:CE2	2.44	0.52
1:A:455:TYR:OH	1:A:459:ARG:HD2	2.10	0.52
1:C:250:GLN:HB3	1:C:324:PRO:HA	1.91	0.52
1:D:455:TYR:OH	1:D:459:ARG:HD2	2.10	0.51
1:E:360:PHE:CD1	1:E:365:ILE:HD11	2.45	0.51
1:B:360:PHE:CD1	1:B:365:ILE:HD11	2.46	0.51
1:D:250:GLN:HB3	1:D:324:PRO:HA	1.91	0.51
1:D:360:PHE:CD1	1:D:365:ILE:HD11	2.46	0.51
1:E:455:TYR:OH	1:E:459:ARG:HD2	2.10	0.51
1:A:250:GLN:HB3	1:A:324:PRO:HA	1.91	0.51
1:A:360:PHE:CD1	1:A:365:ILE:HD11	2.46	0.51
1:B:455:TYR:OH	1:B:459:ARG:HD2	2.10	0.51
1:F:360:PHE:CD1	1:F:365:ILE:HD11	2.46	0.51
1:C:162:VAL:HG23	1:C:163:ASP:H	1.75	0.51
1:C:360:PHE:CD1	1:C:365:ILE:HD11	2.46	0.51
1:F:162:VAL:HG23	1:F:163:ASP:H	1.75	0.51
1:A:162:VAL:HG23	1:A:163:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:HG23	1:D:163:ASP:H	1.75	0.51
1:E:349:ASN:ND2	2:E:602:NAI:O2D	2.45	0.50
1:F:455:TYR:OH	1:F:459:ARG:HD2	2.10	0.50
1:B:349:ASN:ND2	2:B:602:NAI:O2D	2.45	0.50
1:C:455:TYR:OH	1:C:459:ARG:HD2	2.10	0.50
1:A:372:TYR:HD1	1:A:460:SER:HG	1.57	0.50
1:B:63:PHE:HB2	1:B:75:ILE:HB	1.94	0.50
1:E:162:VAL:HG23	1:E:163:ASP:H	1.75	0.50
1:F:7:PRO:O	1:F:329:LYS:NZ	2.30	0.50
1:E:63:PHE:HB2	1:E:75:ILE:HB	1.94	0.50
1:D:372:TYR:HD1	1:D:460:SER:HG	1.57	0.50
1:B:162:VAL:HG23	1:B:163:ASP:H	1.75	0.50
1:A:349:ASN:ND2	2:A:601:NAI:O2D	2.45	0.50
1:C:7:PRO:O	1:C:329:LYS:NZ	2.30	0.50
1:F:63:PHE:HB2	1:F:75:ILE:HB	1.93	0.50
1:E:165:PRO:HD2	1:E:198:VAL:HG12	1.94	0.49
1:A:295:LYS:HD3	1:A:301:ILE:HG23	1.95	0.49
1:B:165:PRO:HD2	1:B:198:VAL:HG12	1.94	0.49
1:C:165:PRO:HD2	1:C:198:VAL:HG12	1.94	0.49
1:C:63:PHE:HB2	1:C:75:ILE:HB	1.94	0.49
1:F:295:LYS:HD3	1:F:301:ILE:HG23	1.94	0.49
1:F:349:ASN:ND2	2:F:602:NAI:O2D	2.45	0.49
1:C:295:LYS:HD3	1:C:301:ILE:HG23	1.95	0.49
1:D:295:LYS:HD3	1:D:301:ILE:HG23	1.95	0.49
1:F:165:PRO:HD2	1:F:198:VAL:HG12	1.94	0.49
1:C:372:TYR:HD1	1:C:460:SER:HG	1.59	0.49
1:C:349:ASN:ND2	2:C:602:NAI:O2D	2.46	0.49
1:D:165:PRO:HD2	1:D:198:VAL:HG12	1.94	0.49
1:A:165:PRO:HD2	1:A:198:VAL:HG12	1.94	0.49
1:A:455:TYR:HH	1:B:399:PHE:HD2	1.61	0.49
1:F:372:TYR:HD1	1:F:460:SER:HG	1.59	0.49
1:D:63:PHE:HB2	1:D:75:ILE:HB	1.94	0.49
1:D:495:GLU:OE1	1:E:204:SER:OG	2.21	0.49
1:A:63:PHE:HB2	1:A:75:ILE:HB	1.94	0.49
1:B:372:TYR:HD1	1:B:460:SER:HG	1.60	0.48
1:E:372:TYR:HD1	1:E:460:SER:HG	1.60	0.48
1:C:63:PHE:O	1:C:74:VAL:HA	2.14	0.48
1:D:7:PRO:O	1:D:329:LYS:NZ	2.30	0.48
1:F:63:PHE:O	1:F:74:VAL:HA	2.14	0.48
1:E:63:PHE:O	1:E:74:VAL:HA	2.14	0.48
1:A:38:GLU:OE2	1:A:42:ARG:NE	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:THR:HB	1:B:281:TRP:HD1	1.79	0.48
1:B:295:LYS:HD3	1:B:301:ILE:HG23	1.94	0.48
1:A:7:PRO:O	1:A:329:LYS:NZ	2.30	0.48
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.96	0.48
1:B:63:PHE:O	1:B:74:VAL:HA	2.14	0.48
1:E:107:LEU:HB3	1:E:126:LYS:HE3	1.96	0.48
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.96	0.48
1:E:272:THR:HB	1:E:281:TRP:HD1	1.79	0.48
1:A:107:LEU:HB3	1:A:126:LYS:HE3	1.96	0.48
1:A:314:ILE:H	1:A:314:ILE:HD12	1.78	0.48
1:D:314:ILE:H	1:D:314:ILE:HD12	1.79	0.48
1:D:38:GLU:OE2	1:D:42:ARG:NE	2.40	0.48
1:B:239:THR:O	1:B:245:LYS:NZ	2.32	0.48
1:B:304:PHE:CE2	1:B:306:LYS:HB2	2.49	0.48
1:C:314:ILE:HD12	1:C:314:ILE:H	1.79	0.48
1:E:295:LYS:HD3	1:E:301:ILE:HG23	1.95	0.48
1:C:107:LEU:HB3	1:C:126:LYS:HE3	1.96	0.48
1:D:272:THR:HB	1:D:281:TRP:HD1	1.79	0.47
1:D:304:PHE:CE2	1:D:306:LYS:HB2	2.49	0.47
1:E:304:PHE:CE2	1:E:306:LYS:HB2	2.49	0.47
1:E:314:ILE:H	1:E:314:ILE:HD12	1.78	0.47
1:F:107:LEU:HB3	1:F:126:LYS:HE3	1.96	0.47
1:F:314:ILE:H	1:F:314:ILE:HD12	1.79	0.47
1:A:272:THR:HB	1:A:281:TRP:HD1	1.79	0.47
1:B:314:ILE:HD12	1:B:314:ILE:H	1.78	0.47
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.15	0.47
1:F:372:TYR:OH	1:F:461:ALA:HB2	2.15	0.47
1:A:304:PHE:CE2	1:A:306:LYS:HB2	2.49	0.47
1:C:324:PRO:HD2	1:C:345:ALA:O	2.14	0.47
1:F:324:PRO:HD2	1:F:345:ALA:O	2.14	0.47
1:A:294:PHE:HE2	1:A:305:PRO:HD2	1.79	0.47
1:C:32:LEU:HG	1:C:34:THR:HG22	1.96	0.47
1:D:294:PHE:HE2	1:D:305:PRO:HD2	1.79	0.47
1:E:324:PRO:HD2	1:E:345:ALA:O	2.14	0.47
1:B:248:VAL:HG12	1:B:271:ILE:HB	1.96	0.47
1:B:324:PRO:HD2	1:B:345:ALA:O	2.14	0.47
1:C:248:VAL:HG12	1:C:271:ILE:HB	1.96	0.47
1:A:66:ARG:H	1:E:501:THR:HG22	1.79	0.47
1:F:32:LEU:HG	1:F:34:THR:HG22	1.97	0.47
1:A:371:LEU:HD11	1:A:482:TYR:CZ	2.50	0.47
1:D:371:LEU:HD11	1:D:482:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:VAL:HG12	1:F:271:ILE:HB	1.96	0.47
1:B:372:TYR:OH	1:B:461:ALA:HB2	2.15	0.47
1:D:455:TYR:HH	1:E:399:PHE:HD2	1.63	0.47
1:E:248:VAL:HG12	1:E:271:ILE:HB	1.96	0.47
1:B:38:GLU:OE2	1:B:42:ARG:NE	2.40	0.47
1:E:372:TYR:OH	1:E:461:ALA:HB2	2.15	0.47
1:A:372:TYR:OH	1:A:461:ALA:HB2	2.15	0.47
1:C:272:THR:HB	1:C:281:TRP:HD1	1.79	0.47
1:C:304:PHE:CE2	1:C:306:LYS:HB2	2.49	0.47
1:D:324:PRO:HD2	1:D:345:ALA:O	2.14	0.47
1:F:304:PHE:CE2	1:F:306:LYS:HB2	2.49	0.47
1:A:324:PRO:HD2	1:A:345:ALA:O	2.14	0.47
1:A:63:PHE:O	1:A:74:VAL:HA	2.14	0.47
1:C:294:PHE:HE2	1:C:305:PRO:HD2	1.79	0.47
1:F:272:THR:HB	1:F:281:TRP:HD1	1.79	0.47
1:A:399:PHE:HD2	1:C:455:TYR:HH	1.63	0.47
1:C:91:GLY:HA2	1:C:111:MET:SD	2.55	0.47
1:D:372:TYR:OH	1:D:461:ALA:HB2	2.15	0.47
1:D:63:PHE:O	1:D:74:VAL:HA	2.14	0.47
1:E:38:GLU:OE2	1:E:42:ARG:NE	2.40	0.47
1:E:7:PRO:O	1:E:329:LYS:NZ	2.30	0.47
1:F:316:GLU:OE2	1:F:338:ARG:NE	2.28	0.47
1:F:371:LEU:HD11	1:F:482:TYR:CZ	2.50	0.47
1:F:209:HIS:HE1	3:F:603:GTP:H5"	1.80	0.47
1:A:91:GLY:HA2	1:A:111:MET:SD	2.55	0.46
1:B:221:HIS:O	1:B:225:ASN:ND2	2.48	0.46
1:B:294:PHE:HE2	1:B:305:PRO:HD2	1.79	0.46
1:B:371:LEU:HD11	1:B:482:TYR:CZ	2.50	0.46
1:C:209:HIS:HE1	3:C:603:GTP:H5"	1.80	0.46
1:C:371:LEU:HD11	1:C:482:TYR:CZ	2.50	0.46
1:D:21:ALA:HB1	1:D:49:LEU:HD13	1.97	0.46
1:B:501:THR:HG22	1:D:66:ARG:H	1.79	0.46
1:E:221:HIS:O	1:E:225:ASN:ND2	2.48	0.46
1:E:294:PHE:HE2	1:E:305:PRO:HD2	1.79	0.46
1:F:21:ALA:HB1	1:F:49:LEU:HD13	1.97	0.46
1:F:294:PHE:HE2	1:F:305:PRO:HD2	1.79	0.46
1:F:195:HIS:CD2	1:F:388:ASN:HB2	2.50	0.46
1:F:91:GLY:HA2	1:F:111:MET:SD	2.55	0.46
1:A:21:ALA:HB1	1:A:49:LEU:HD13	1.97	0.46
1:B:66:ARG:H	1:D:501:THR:HG22	1.80	0.46
1:C:21:ALA:HB1	1:C:49:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:HIS:CD2	1:C:388:ASN:HB2	2.51	0.46
1:C:403:ARG:HA	1:C:440:ILE:HG22	1.97	0.46
1:D:91:GLY:HA2	1:D:111:MET:SD	2.55	0.46
1:E:371:LEU:HD11	1:E:482:TYR:CZ	2.50	0.46
1:E:195:HIS:CD2	1:E:388:ASN:HB2	2.51	0.46
1:E:91:GLY:HA2	1:E:111:MET:SD	2.55	0.46
1:A:63:PHE:CZ	1:A:148:PHE:HD1	2.34	0.46
1:A:248:VAL:HG12	1:A:271:ILE:HB	1.96	0.46
1:B:21:ALA:HB1	1:B:49:LEU:HD13	1.97	0.46
1:B:195:HIS:CD2	1:B:388:ASN:HB2	2.51	0.46
1:D:63:PHE:CZ	1:D:148:PHE:HD1	2.34	0.46
1:A:195:HIS:CD2	1:A:388:ASN:HB2	2.51	0.46
1:B:91:GLY:HA2	1:B:111:MET:SD	2.55	0.46
1:C:19:ARG:NH1	1:C:479:THR:OG1	2.48	0.46
1:D:248:VAL:HG12	1:D:271:ILE:HB	1.96	0.46
1:E:21:ALA:HB1	1:E:49:LEU:HD13	1.97	0.46
1:E:417:LEU:HB3	1:E:428:ILE:CD1	2.46	0.46
1:F:403:ARG:HA	1:F:440:ILE:HG22	1.98	0.46
1:A:463:GLN:O	1:A:484:ASN:ND2	2.46	0.46
1:C:316:GLU:OE2	1:C:338:ARG:NE	2.28	0.46
1:D:195:HIS:CD2	1:D:388:ASN:HB2	2.51	0.46
1:E:403:ARG:HA	1:E:440:ILE:HG22	1.98	0.46
1:C:66:ARG:H	1:F:501:THR:HG22	1.80	0.46
1:B:403:ARG:HA	1:B:440:ILE:HG22	1.97	0.46
1:D:221:HIS:O	1:D:225:ASN:ND2	2.48	0.46
1:F:19:ARG:NH1	1:F:479:THR:OG1	2.48	0.46
1:B:417:LEU:HB3	1:B:428:ILE:CD1	2.46	0.46
1:B:209:HIS:HE1	3:B:603:GTP:H5"	1.80	0.46
1:B:7:PRO:O	1:B:329:LYS:NZ	2.30	0.46
1:D:463:GLN:O	1:D:484:ASN:ND2	2.46	0.46
1:A:221:HIS:O	1:A:225:ASN:ND2	2.48	0.46
1:A:32:LEU:HG	1:A:34:THR:HG22	1.97	0.46
1:D:19:ARG:NH1	1:D:479:THR:OG1	2.48	0.46
1:E:209:HIS:HE1	3:E:603:GTP:H5"	1.80	0.46
1:C:501:THR:HG22	1:F:66:ARG:H	1.80	0.46
1:D:32:LEU:HG	1:D:34:THR:HG22	1.97	0.46
1:A:19:ARG:NH1	1:A:479:THR:OG1	2.48	0.46
1:B:63:PHE:CZ	1:B:148:PHE:HD1	2.34	0.46
1:C:221:HIS:O	1:C:225:ASN:ND2	2.48	0.46
1:C:379:THR:HG21	1:C:456:THR:HG21	1.98	0.46
1:D:417:LEU:HB3	1:D:428:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:LEU:HB3	1:F:428:ILE:CD1	2.46	0.46
1:A:316:GLU:OE2	1:A:338:ARG:NE	2.28	0.45
1:C:417:LEU:HB3	1:C:428:ILE:CD1	2.46	0.45
1:E:63:PHE:CZ	1:E:148:PHE:HD1	2.34	0.45
1:F:221:HIS:O	1:F:225:ASN:ND2	2.48	0.45
1:F:379:THR:HG21	1:F:456:THR:HG21	1.98	0.45
1:B:32:LEU:HG	1:B:34:THR:HG22	1.97	0.45
1:C:63:PHE:CZ	1:C:148:PHE:HD1	2.34	0.45
1:D:168:ASP:OD1	1:D:169:MET:N	2.49	0.45
1:A:294:PHE:O	1:A:298:HIS:N	2.47	0.45
1:B:379:THR:HG21	1:B:456:THR:HG21	1.98	0.45
1:B:455:TYR:HH	1:C:399:PHE:HD2	1.63	0.45
1:D:294:PHE:O	1:D:298:HIS:N	2.47	0.45
1:E:32:LEU:HG	1:E:34:THR:HG22	1.96	0.45
1:E:379:THR:HG21	1:E:456:THR:HG21	1.98	0.45
1:A:209:HIS:HE1	3:A:602:GTP:H5"	1.80	0.45
1:B:168:ASP:OD1	1:B:169:MET:N	2.49	0.45
1:E:168:ASP:OD1	1:E:169:MET:N	2.49	0.45
1:F:63:PHE:CZ	1:F:148:PHE:HD1	2.34	0.45
1:A:417:LEU:HB3	1:A:428:ILE:CD1	2.47	0.45
1:A:403:ARG:HA	1:A:440:ILE:HG22	1.98	0.45
1:C:81:GLN:OE1	1:C:84:GLN:NE2	2.50	0.45
1:D:209:HIS:HE1	3:D:602:GTP:H5"	1.81	0.45
1:E:81:GLN:OE1	1:E:84:GLN:NE2	2.50	0.45
1:C:463:GLN:O	1:C:484:ASN:ND2	2.46	0.45
1:F:81:GLN:OE1	1:F:84:GLN:NE2	2.50	0.45
1:B:81:GLN:OE1	1:B:84:GLN:NE2	2.50	0.45
1:C:218:GLY:HA2	1:C:457:MET:SD	2.57	0.45
1:D:399:PHE:HD2	1:F:455:TYR:HH	1.65	0.45
1:D:403:ARG:HA	1:D:440:ILE:HG22	1.98	0.45
1:E:12:MET:SD	1:E:354:PRO:HD3	2.57	0.45
1:B:12:MET:SD	1:B:354:PRO:HD3	2.57	0.45
1:D:12:MET:SD	1:D:354:PRO:HD3	2.57	0.45
1:F:218:GLY:HA2	1:F:457:MET:SD	2.57	0.45
1:A:12:MET:SD	1:A:354:PRO:HD3	2.57	0.44
1:C:78:TYR:HE2	1:C:100:SER:HA	1.83	0.44
1:F:78:TYR:HE2	1:F:100:SER:HA	1.83	0.44
1:F:463:GLN:O	1:F:484:ASN:ND2	2.46	0.44
1:A:78:TYR:HE2	1:A:100:SER:HA	1.82	0.44
1:D:379:THR:HG21	1:D:456:THR:HG21	1.98	0.44
1:A:379:THR:HG21	1:A:456:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:TYR:HE2	1:D:100:SER:HA	1.83	0.44
1:A:9:PHE:CD2	1:A:106:ALA:HB3	2.53	0.44
1:B:78:TYR:HE2	1:B:100:SER:HA	1.82	0.44
1:B:19:ARG:NH1	1:B:479:THR:OG1	2.48	0.44
1:C:93:ILE:HG12	1:C:127:ALA:HB3	2.00	0.44
1:C:9:PHE:CD2	1:C:106:ALA:HB3	2.53	0.44
1:D:9:PHE:CD2	1:D:106:ALA:HB3	2.53	0.44
1:D:263:LEU:O	1:D:268:ALA:HB3	2.18	0.44
1:D:81:GLN:OE1	1:D:84:GLN:NE2	2.50	0.44
1:E:218:GLY:HA2	1:E:457:MET:SD	2.57	0.44
1:F:93:ILE:HG12	1:F:127:ALA:HB3	2.00	0.44
1:F:9:PHE:CD2	1:F:106:ALA:HB3	2.53	0.44
1:A:263:LEU:O	1:A:268:ALA:HB3	2.18	0.44
1:B:218:GLY:HA2	1:B:457:MET:SD	2.57	0.44
1:D:90:LYS:HG2	1:D:164:VAL:HB	2.00	0.44
1:E:78:TYR:HE2	1:E:100:SER:HA	1.83	0.44
1:A:90:LYS:HG2	1:A:164:VAL:HB	2.00	0.44
1:A:81:GLN:OE1	1:A:84:GLN:NE2	2.50	0.44
1:B:118:VAL:HG23	1:B:120:VAL:HG23	2.00	0.44
1:C:118:VAL:HG23	1:C:120:VAL:HG23	2.00	0.44
1:C:12:MET:SD	1:C:354:PRO:HD3	2.57	0.44
1:E:19:ARG:NH1	1:E:479:THR:OG1	2.48	0.44
1:F:118:VAL:HG23	1:F:120:VAL:HG23	2.00	0.44
1:B:418:GLU:O	1:B:422:GLY:HA3	2.18	0.44
1:E:118:VAL:HG23	1:E:120:VAL:HG23	2.00	0.44
1:E:418:GLU:O	1:E:422:GLY:HA3	2.18	0.44
1:E:9:PHE:CD2	1:E:106:ALA:HB3	2.53	0.44
1:F:12:MET:SD	1:F:354:PRO:HD3	2.57	0.44
1:F:263:LEU:O	1:F:268:ALA:HB3	2.18	0.44
1:F:418:GLU:O	1:F:422:GLY:HA3	2.18	0.44
1:B:9:PHE:CD2	1:B:106:ALA:HB3	2.53	0.44
1:C:263:LEU:O	1:C:268:ALA:HB3	2.18	0.44
1:D:93:ILE:HG12	1:D:127:ALA:HB3	2.00	0.44
1:E:209:HIS:NE2	3:E:603:GTP:O2B	2.35	0.44
1:A:93:ILE:HG12	1:A:127:ALA:HB3	2.00	0.44
1:A:272:THR:HG1	1:A:280:ILE:C	2.22	0.44
1:B:294:PHE:O	1:B:298:HIS:N	2.47	0.44
1:C:418:GLU:O	1:C:422:GLY:HA3	2.18	0.44
1:C:455:TYR:CZ	1:C:459:ARG:HD2	2.53	0.44
1:A:218:GLY:HA2	1:A:457:MET:SD	2.57	0.43
1:A:501:THR:HG22	1:E:66:ARG:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLY:HA2	1:D:457:MET:SD	2.57	0.43
1:F:455:TYR:CZ	1:F:459:ARG:HD2	2.53	0.43
1:A:118:VAL:HG23	1:A:120:VAL:HG23	2.00	0.43
1:A:455:TYR:CZ	1:A:459:ARG:HD2	2.53	0.43
1:C:38:GLU:OE2	1:C:42:ARG:NE	2.40	0.43
1:D:118:VAL:HG23	1:D:120:VAL:HG23	2.00	0.43
1:E:294:PHE:O	1:E:298:HIS:N	2.47	0.43
1:F:90:LYS:HG2	1:F:164:VAL:HB	2.00	0.43
1:D:455:TYR:CZ	1:D:459:ARG:HD2	2.53	0.43
1:A:239:THR:O	1:A:245:LYS:NZ	2.32	0.43
1:C:90:LYS:HG2	1:C:164:VAL:HB	2.00	0.43
1:D:369:PRO:HB3	1:D:478:ARG:HA	2.01	0.43
1:E:369:PRO:HB3	1:E:478:ARG:HA	2.01	0.43
1:A:369:PRO:HB3	1:A:478:ARG:HA	2.01	0.43
1:D:209:HIS:NE2	3:D:602:GTP:O2B	2.36	0.43
1:F:38:GLU:OE2	1:F:42:ARG:NE	2.40	0.43
1:E:455:TYR:HH	1:F:399:PHE:HD2	1.65	0.43
1:B:263:LEU:O	1:B:268:ALA:HB3	2.18	0.43
1:B:369:PRO:HB3	1:B:478:ARG:HA	2.01	0.43
1:B:209:HIS:NE2	3:B:603:GTP:O2B	2.36	0.43
1:C:369:PRO:HB3	1:C:478:ARG:HA	2.01	0.43
1:D:239:THR:O	1:D:245:LYS:NZ	2.33	0.43
1:A:72:TRP:CH2	1:E:498:VAL:HB	2.54	0.43
1:A:83:SER:OG	1:A:85:HIS:HD2	2.02	0.43
1:D:272:THR:HG1	1:D:280:ILE:C	2.22	0.43
1:D:83:SER:OG	1:D:85:HIS:HD2	2.02	0.43
1:E:215:THR:HG21	1:E:255:VAL:HG22	2.01	0.43
1:E:226:PHE:HE2	1:E:368:ILE:HG23	1.84	0.43
1:E:263:LEU:O	1:E:268:ALA:HB3	2.18	0.43
1:B:215:THR:HG21	1:B:255:VAL:HG22	2.01	0.43
1:B:226:PHE:HE2	1:B:368:ILE:HG23	1.84	0.43
1:F:369:PRO:HB3	1:F:478:ARG:HA	2.01	0.43
1:A:418:GLU:O	1:A:422:GLY:HA3	2.18	0.43
1:B:90:LYS:HG2	1:B:164:VAL:HB	2.00	0.43
1:A:226:PHE:HE2	1:A:368:ILE:HG23	1.84	0.43
1:C:215:THR:HG21	1:C:255:VAL:HG22	2.01	0.43
1:D:226:PHE:HE2	1:D:368:ILE:HG23	1.84	0.43
1:D:418:GLU:O	1:D:422:GLY:HA3	2.18	0.43
1:D:418:GLU:HG2	1:D:428:ILE:HG13	2.00	0.43
1:E:90:LYS:HG2	1:E:164:VAL:HB	2.00	0.43
1:F:215:THR:HG21	1:F:255:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:O	1:B:149:THR:HG23	2.19	0.42
1:B:455:TYR:CZ	1:B:459:ARG:HD2	2.53	0.42
1:C:145:THR:O	1:C:149:THR:HG23	2.19	0.42
1:F:145:THR:O	1:F:149:THR:HG23	2.19	0.42
1:A:215:THR:HG21	1:A:255:VAL:HG22	2.01	0.42
1:C:83:SER:OG	1:C:85:HIS:HD2	2.02	0.42
1:D:215:THR:HG21	1:D:255:VAL:HG22	2.01	0.42
1:E:145:THR:O	1:E:149:THR:HG23	2.19	0.42
1:E:455:TYR:CZ	1:E:459:ARG:HD2	2.53	0.42
1:E:93:ILE:HG12	1:E:127:ALA:HB3	2.00	0.42
1:A:145:THR:O	1:A:149:THR:HG23	2.19	0.42
1:E:83:SER:OG	1:E:85:HIS:HD2	2.02	0.42
1:F:418:GLU:HG2	1:F:428:ILE:HG13	2.01	0.42
1:F:417:LEU:CB	1:F:428:ILE:CD1	2.97	0.42
1:F:83:SER:OG	1:F:85:HIS:HD2	2.02	0.42
1:B:93:ILE:HG12	1:B:127:ALA:HB3	2.00	0.42
1:D:145:THR:O	1:D:149:THR:HG23	2.19	0.42
1:B:463:GLN:O	1:B:484:ASN:ND2	2.46	0.42
1:B:83:SER:OG	1:B:85:HIS:HD2	2.02	0.42
1:C:417:LEU:CB	1:C:428:ILE:CD1	2.97	0.42
1:E:316:GLU:OE2	1:E:338:ARG:NE	2.28	0.42
1:E:417:LEU:CB	1:E:428:ILE:CD1	2.98	0.42
1:A:209:HIS:NE2	3:A:602:GTP:O2B	2.36	0.42
1:C:418:GLU:HG2	1:C:428:ILE:HG13	2.02	0.42
1:D:28:LEU:HD21	1:D:490:PHE:CG	2.55	0.42
1:B:72:TRP:CH2	1:D:498:VAL:HB	2.55	0.42
1:B:498:VAL:HB	1:D:72:TRP:CH2	2.55	0.42
1:A:498:VAL:HB	1:E:72:TRP:CH2	2.55	0.42
1:A:129:VAL:O	1:A:131:ILE:HG22	2.20	0.42
1:A:28:LEU:HD21	1:A:490:PHE:CG	2.55	0.42
1:B:394:TYR:CE2	1:B:448:ILE:HG21	2.55	0.42
1:C:72:TRP:CH2	1:F:498:VAL:HB	2.55	0.42
1:D:129:VAL:O	1:D:131:ILE:HG22	2.20	0.42
1:E:463:GLN:O	1:E:484:ASN:ND2	2.46	0.42
1:D:498:VAL:HG12	1:D:499:THR:HG23	2.01	0.42
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.85	0.42
1:E:394:TYR:CE2	1:E:448:ILE:HG21	2.55	0.42
1:A:372:TYR:OH	1:A:457:MET:O	2.36	0.42
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.85	0.42
1:B:498:VAL:HG12	1:B:499:THR:HG23	2.01	0.42
1:C:167:PRO:HG3	1:C:176:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ASN:ND2	1:E:457:MET:O	2.53	0.42
1:A:44:ARG:O	1:A:47:SER:OG	2.35	0.42
1:A:498:VAL:HG12	1:A:499:THR:HG23	2.01	0.42
1:B:129:VAL:O	1:B:131:ILE:HG22	2.20	0.42
1:B:417:LEU:CB	1:B:428:ILE:CD1	2.98	0.42
1:B:225:ASN:ND2	1:B:457:MET:O	2.53	0.42
1:C:28:LEU:HD21	1:C:490:PHE:CG	2.55	0.42
1:E:129:VAL:O	1:E:131:ILE:HG22	2.20	0.42
1:E:251:GLY:HA3	1:E:326:ALA:HB2	2.02	0.42
1:E:498:VAL:HG12	1:E:499:THR:HG23	2.01	0.42
1:F:114:LYS:O	1:F:118:VAL:HG22	2.20	0.42
1:F:332:THR:HG23	1:F:334:SER:H	1.85	0.42
1:C:498:VAL:HB	1:F:72:TRP:CH2	2.55	0.42
1:A:418:GLU:HG2	1:A:428:ILE:HG13	2.01	0.41
1:A:225:ASN:ND2	1:A:457:MET:O	2.53	0.41
1:B:251:GLY:HA3	1:B:326:ALA:HB2	2.02	0.41
1:B:316:GLU:OE2	1:B:338:ARG:NE	2.28	0.41
1:C:114:LYS:O	1:C:118:VAL:HG22	2.20	0.41
1:C:332:THR:HG23	1:C:334:SER:H	1.85	0.41
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.85	0.41
1:D:417:LEU:CB	1:D:428:ILE:CD1	2.97	0.41
1:D:44:ARG:O	1:D:47:SER:OG	2.35	0.41
1:D:225:ASN:ND2	1:D:457:MET:O	2.53	0.41
1:E:346:GLU:H	1:E:373:LEU:CD1	2.31	0.41
1:F:167:PRO:HG3	1:F:176:MET:HG3	2.02	0.41
1:F:28:LEU:HD21	1:F:490:PHE:CG	2.55	0.41
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.85	0.41
1:B:89:CYS:HB2	1:B:163:ASP:OD1	2.20	0.41
1:B:90:LYS:NZ	1:B:90:LYS:HB3	2.36	0.41
1:D:372:TYR:OH	1:D:457:MET:O	2.36	0.41
1:E:90:LYS:HB3	1:E:90:LYS:NZ	2.36	0.41
1:B:372:TYR:OH	1:B:457:MET:O	2.36	0.41
1:C:226:PHE:HE2	1:C:368:ILE:HG23	1.84	0.41
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.85	0.41
1:E:89:CYS:HB2	1:E:163:ASP:OD1	2.20	0.41
1:F:226:PHE:HE2	1:F:368:ILE:HG23	1.84	0.41
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.85	0.41
1:A:496:ALA:HB2	1:B:205:GLN:NE2	2.36	0.41
1:B:346:GLU:H	1:B:373:LEU:CD1	2.31	0.41
1:B:28:LEU:HD21	1:B:490:PHE:CG	2.55	0.41
1:D:275:GLU:OE2	1:D:300:THR:OG1	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:PHE:O	1:F:298:HIS:N	2.47	0.41
1:F:394:TYR:CE2	1:F:448:ILE:HG21	2.55	0.41
1:D:204:SER:OG	1:F:495:GLU:OE1	2.21	0.41
1:A:89:CYS:HB2	1:A:163:ASP:OD1	2.20	0.41
1:C:294:PHE:O	1:C:298:HIS:N	2.47	0.41
1:C:394:TYR:CE2	1:C:448:ILE:HG21	2.55	0.41
1:C:225:ASN:ND2	1:C:457:MET:O	2.53	0.41
1:D:90:LYS:NZ	1:D:90:LYS:HB3	2.36	0.41
1:E:114:LYS:O	1:E:118:VAL:HG22	2.20	0.41
1:D:496:ALA:HB2	1:E:205:GLN:NE2	2.36	0.41
1:E:372:TYR:OH	1:E:457:MET:O	2.36	0.41
1:A:167:PRO:HG3	1:A:176:MET:HG3	2.02	0.41
1:A:394:TYR:CE2	1:A:448:ILE:HG21	2.55	0.41
1:A:90:LYS:HB3	1:A:90:LYS:NZ	2.36	0.41
1:B:114:LYS:O	1:B:118:VAL:HG22	2.20	0.41
1:C:498:VAL:HG12	1:C:499:THR:HG23	2.01	0.41
1:C:89:CYS:HB2	1:C:163:ASP:OD1	2.20	0.41
1:D:394:TYR:CE2	1:D:448:ILE:HG21	2.55	0.41
1:E:28:LEU:HD21	1:E:490:PHE:CG	2.55	0.41
1:F:225:ASN:ND2	1:F:457:MET:O	2.53	0.41
1:F:89:CYS:HB2	1:F:163:ASP:OD1	2.20	0.41
1:A:251:GLY:HA3	1:A:326:ALA:HB2	2.02	0.41
1:D:167:PRO:HG3	1:D:176:MET:HG3	2.02	0.41
1:D:251:GLY:HA3	1:D:326:ALA:HB2	2.02	0.41
1:D:89:CYS:HB2	1:D:163:ASP:OD1	2.20	0.41
1:A:114:LYS:O	1:A:118:VAL:HG22	2.20	0.41
1:C:251:GLY:HA3	1:C:326:ALA:HB2	2.02	0.41
1:C:90:LYS:HB3	1:C:90:LYS:NZ	2.36	0.41
1:D:114:LYS:O	1:D:118:VAL:HG22	2.20	0.41
1:D:414:GLN:CD	1:D:428:ILE:O	2.59	0.41
1:E:167:PRO:HG3	1:E:176:MET:HG3	2.02	0.41
1:A:346:GLU:H	1:A:373:LEU:CD1	2.31	0.41
1:B:325:ALA:O	2:B:602:NAI:H51N	2.21	0.41
1:E:325:ALA:O	2:E:602:NAI:H51N	2.21	0.41
1:E:496:ALA:HB2	1:F:205:GLN:NE2	2.36	0.41
1:F:498:VAL:HG12	1:F:499:THR:HG23	2.01	0.41
1:F:90:LYS:NZ	1:F:90:LYS:HB3	2.36	0.41
1:A:325:ALA:O	2:A:601:NAI:H51N	2.21	0.41
1:A:332:THR:HG23	1:A:334:SER:H	1.85	0.41
1:B:167:PRO:HG3	1:B:176:MET:HG3	2.02	0.41
1:B:496:ALA:HB2	1:C:205:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:GLN:NE2	1:F:496:ALA:HB2	2.36	0.41
1:A:275:GLU:OE2	1:A:300:THR:OG1	2.26	0.41
1:A:414:GLN:CD	1:A:428:ILE:O	2.60	0.41
1:A:455:TYR:HB2	1:B:400:LYS:HB2	2.03	0.41
1:F:251:GLY:HA3	1:F:326:ALA:HB2	2.02	0.41
1:A:168:ASP:OD1	1:A:169:MET:N	2.49	0.40
1:C:168:ASP:OD1	1:C:169:MET:N	2.49	0.40
1:A:205:GLN:NE2	1:C:496:ALA:HB2	2.36	0.40
1:E:332:THR:HG23	1:E:334:SER:H	1.85	0.40
1:F:129:VAL:O	1:F:131:ILE:HG22	2.20	0.40
1:A:417:LEU:CB	1:A:428:ILE:CD1	2.98	0.40
1:B:332:THR:HG23	1:B:334:SER:H	1.85	0.40
1:C:129:VAL:O	1:C:131:ILE:HG22	2.20	0.40
1:C:372:TYR:OH	1:C:457:MET:O	2.36	0.40
1:A:204:SER:OG	1:C:495:GLU:OE1	2.22	0.40
1:D:332:THR:HG23	1:D:334:SER:H	1.85	0.40
1:A:154:LYS:HD3	1:F:189:HIS:CE1	2.56	0.40
1:F:372:TYR:OH	1:F:457:MET:O	2.36	0.40
1:B:414:GLN:HG3	1:B:428:ILE:O	2.21	0.40
1:D:346:GLU:H	1:D:373:LEU:CD1	2.31	0.40
1:E:414:GLN:HG3	1:E:428:ILE:O	2.21	0.40
1:C:414:GLN:HG3	1:C:428:ILE:O	2.21	0.40
1:F:168:ASP:OD1	1:F:169:MET:N	2.49	0.40
1:F:346:GLU:H	1:F:373:LEU:CD1	2.31	0.40
1:F:414:GLN:HG3	1:F:428:ILE: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	A	495/501 (99%)	460 (93%)	34 (7%)	1 (0%)	52 87

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	495/501 (99%)	460 (93%)	34 (7%)	1 (0%)	52 87
1	C	495/501 (99%)	460 (93%)	34 (7%)	1 (0%)	52 87
1	D	495/501 (99%)	461 (93%)	33 (7%)	1 (0%)	52 87
1	E	495/501 (99%)	460 (93%)	34 (7%)	1 (0%)	52 87
1	F	495/501 (99%)	460 (93%)	34 (7%)	1 (0%)	52 87
All	All	2970/3006 (99%)	2761 (93%)	203 (7%)	6 (0%)	56 87

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	PRO
1	B	429	PRO
1	C	429	PRO
1	D	429	PRO
1	E	429	PRO
1	F	429	PRO

5.3.2 Protein sidechains (i)

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	A	417/420 (99%)	417 (100%)	0	100 100
1	B	417/420 (99%)	417 (100%)	0	100 100
1	C	417/420 (99%)	417 (100%)	0	100 100
1	D	417/420 (99%)	417 (100%)	0	100 100
1	E	417/420 (99%)	417 (100%)	0	100 100
1	F	417/420 (99%)	417 (100%)	0	100 100
All	All	2502/2520 (99%)	2502 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	85	HIS
1	A	189	HIS
1	A	205	GLN
1	A	225	ASN
1	A	330	GLN
1	A	388	ASN
1	A	391	HIS
1	B	84	GLN
1	B	85	HIS
1	B	189	HIS
1	B	205	GLN
1	B	225	ASN
1	B	330	GLN
1	B	388	ASN
1	B	391	HIS
1	C	84	GLN
1	C	85	HIS
1	C	189	HIS
1	C	205	GLN
1	C	225	ASN
1	C	330	GLN
1	C	388	ASN
1	C	391	HIS
1	D	84	GLN
1	D	85	HIS
1	D	189	HIS
1	D	205	GLN
1	D	225	ASN
1	D	330	GLN
1	D	388	ASN
1	D	391	HIS
1	E	84	GLN
1	E	85	HIS
1	E	189	HIS
1	E	205	GLN
1	E	225	ASN
1	E	330	GLN
1	E	388	ASN
1	E	391	HIS
1	F	84	GLN
1	F	85	HIS
1	F	189	HIS

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Mol	Chain	Res	Type
1	F	205	GLN
1	F	225	ASN
1	F	330	GLN
1	F	388	ASN
1	F	391	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

18 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	NAI	A	601	-	41,48,48	1.05	3 (7%)	46,73,73	1.30	2 (4%)
3	GTP	A	602	-	26,34,34	0.95	1 (3%)	29,54,54	1.53	3 (10%)
2	NAI	A	603	-	41,48,48	1.05	3 (7%)	46,73,73	1.40	2 (4%)
2	NAI	B	601	-	41,48,48	1.04	3 (7%)	46,73,73	1.39	2 (4%)
2	NAI	B	602	-	41,48,48	1.05	3 (7%)	46,73,73	1.31	2 (4%)
3	GTP	B	603	-	26,34,34	0.96	1 (3%)	29,54,54	1.54	4 (13%)
2	NAI	C	601	-	41,48,48	1.05	3 (7%)	46,73,73	1.38	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAI	C	602	-	41,48,48	1.05	3 (7%)	46,73,73	1.30	1 (2%)
3	GTP	C	603	-	26,34,34	0.95	1 (3%)	29,54,54	1.54	4 (13%)
2	NAI	D	601	-	41,48,48	1.05	3 (7%)	46,73,73	1.30	2 (4%)
3	GTP	D	602	-	26,34,34	0.95	1 (3%)	29,54,54	1.53	3 (10%)
2	NAI	D	603	-	41,48,48	1.04	3 (7%)	46,73,73	1.39	2 (4%)
2	NAI	E	601	-	41,48,48	1.04	3 (7%)	46,73,73	1.40	2 (4%)
2	NAI	E	602	-	41,48,48	1.04	3 (7%)	46,73,73	1.31	2 (4%)
3	GTP	E	603	-	26,34,34	0.96	1 (3%)	29,54,54	1.54	4 (13%)
2	NAI	F	601	-	41,48,48	1.04	3 (7%)	46,73,73	1.39	2 (4%)
2	NAI	F	602	-	41,48,48	1.04	3 (7%)	46,73,73	1.31	1 (2%)
3	GTP	F	603	-	26,34,34	0.95	1 (3%)	29,54,54	1.55	4 (13%)

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	NAI	A	601	-	-	0/25/72/72	0/5/5/5
3	GTP	A	602	-	-	0/18/38/38	0/3/3/3
2	NAI	A	603	-	-	0/25/72/72	0/5/5/5
2	NAI	B	601	-	-	0/25/72/72	0/5/5/5
2	NAI	B	602	-	-	0/25/72/72	0/5/5/5
3	GTP	B	603	-	-	0/18/38/38	0/3/3/3
2	NAI	C	601	-	-	0/25/72/72	0/5/5/5
2	NAI	C	602	-	-	0/25/72/72	0/5/5/5
3	GTP	C	603	-	-	0/18/38/38	0/3/3/3
2	NAI	D	601	-	-	0/25/72/72	0/5/5/5
3	GTP	D	602	-	-	0/18/38/38	0/3/3/3
2	NAI	D	603	-	-	0/25/72/72	0/5/5/5
2	NAI	E	601	-	-	0/25/72/72	0/5/5/5
2	NAI	E	602	-	-	0/25/72/72	0/5/5/5
3	GTP	E	603	-	-	0/18/38/38	0/3/3/3
2	NAI	F	601	-	-	0/25/72/72	0/5/5/5
2	NAI	F	602	-	-	0/25/72/72	0/5/5/5
3	GTP	F	603	-	-	0/18/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	NAI	C2N-N1N	-2.30	1.33	1.37
2	C	601	NAI	C2N-N1N	-2.30	1.33	1.37
2	A	603	NAI	C2N-N1N	-2.29	1.33	1.37
2	D	603	NAI	C2N-N1N	-2.28	1.33	1.37
2	F	602	NAI	C2N-N1N	-2.26	1.33	1.37
2	C	602	NAI	C2N-N1N	-2.25	1.33	1.37
2	A	601	NAI	C2N-N1N	-2.25	1.33	1.37
2	D	601	NAI	C2N-N1N	-2.25	1.33	1.37
2	B	602	NAI	C2N-N1N	-2.24	1.33	1.37
2	E	601	NAI	C2N-N1N	-2.24	1.33	1.37
2	B	601	NAI	C2N-N1N	-2.23	1.33	1.37
2	E	602	NAI	C2N-N1N	-2.22	1.33	1.37
2	D	603	NAI	C5A-C4A	2.56	1.46	1.40
2	B	601	NAI	C5A-C4A	2.59	1.46	1.40
2	A	603	NAI	C5A-C4A	2.60	1.46	1.40
2	E	601	NAI	C5A-C4A	2.61	1.46	1.40
2	F	601	NAI	C5A-C4A	2.62	1.46	1.40
2	C	601	NAI	C5A-C4A	2.63	1.46	1.40
3	A	602	GTP	C6-N1	2.82	1.38	1.33
3	E	603	GTP	C6-N1	2.84	1.38	1.33
3	C	603	GTP	C6-N1	2.85	1.38	1.33
3	F	603	GTP	C6-N1	2.85	1.38	1.33
3	B	603	GTP	C6-N1	2.86	1.38	1.33
2	D	601	NAI	C5A-C4A	2.86	1.47	1.40
3	D	602	GTP	C6-N1	2.87	1.38	1.33
2	F	602	NAI	C5A-C4A	2.88	1.47	1.40
2	E	602	NAI	C5A-C4A	2.89	1.47	1.40
2	C	602	NAI	C5A-C4A	2.89	1.47	1.40
2	B	602	NAI	C5A-C4A	2.90	1.47	1.40
2	A	601	NAI	C5A-C4A	2.92	1.47	1.40
2	C	601	NAI	C6N-C5N	3.01	1.38	1.33
2	F	601	NAI	C6N-C5N	3.01	1.38	1.33
2	E	601	NAI	C6N-C5N	3.01	1.38	1.33
2	B	601	NAI	C6N-C5N	3.01	1.38	1.33
2	F	602	NAI	C6N-C5N	3.02	1.38	1.33
2	D	603	NAI	C6N-C5N	3.03	1.38	1.33
2	A	603	NAI	C6N-C5N	3.04	1.38	1.33
2	C	602	NAI	C6N-C5N	3.08	1.38	1.33
2	A	601	NAI	C6N-C5N	3.08	1.38	1.33
2	D	601	NAI	C6N-C5N	3.08	1.38	1.33
2	B	602	NAI	C6N-C5N	3.10	1.39	1.33
2	E	602	NAI	C6N-C5N	3.10	1.39	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	603	NAI	N3A-C2A-N1A	-6.39	123.85	128.87
2	F	601	NAI	N3A-C2A-N1A	-6.36	123.87	128.87
2	C	601	NAI	N3A-C2A-N1A	-6.35	123.89	128.87
2	D	603	NAI	N3A-C2A-N1A	-6.32	123.91	128.87
2	E	601	NAI	N3A-C2A-N1A	-6.30	123.92	128.87
2	B	601	NAI	N3A-C2A-N1A	-6.27	123.95	128.87
2	B	602	NAI	N3A-C2A-N1A	-6.18	124.02	128.87
2	E	602	NAI	N3A-C2A-N1A	-6.10	124.08	128.87
2	D	601	NAI	N3A-C2A-N1A	-6.09	124.09	128.87
2	F	602	NAI	N3A-C2A-N1A	-6.09	124.09	128.87
2	A	601	NAI	N3A-C2A-N1A	-6.08	124.09	128.87
2	C	602	NAI	N3A-C2A-N1A	-6.04	124.13	128.87
3	F	603	GTP	N3-C2-N1	-5.22	120.46	127.56
3	C	603	GTP	N3-C2-N1	-5.18	120.52	127.56
3	E	603	GTP	N3-C2-N1	-5.17	120.52	127.56
3	B	603	GTP	N3-C2-N1	-5.17	120.53	127.56
3	A	602	GTP	N3-C2-N1	-5.17	120.53	127.56
3	D	602	GTP	N3-C2-N1	-5.16	120.54	127.56
3	B	603	GTP	C5-C6-N1	-3.06	119.53	123.52
3	C	603	GTP	C5-C6-N1	-3.03	119.56	123.52
3	F	603	GTP	C5-C6-N1	-3.03	119.56	123.52
3	A	602	GTP	C5-C6-N1	-3.03	119.57	123.52
3	D	602	GTP	C5-C6-N1	-3.01	119.59	123.52
3	E	603	GTP	C5-C6-N1	-3.00	119.60	123.52
2	E	602	NAI	C2B-C1B-N9A	-2.07	107.92	113.47
2	D	601	NAI	C2B-C1B-N9A	-2.06	107.96	113.47
2	A	601	NAI	C2B-C1B-N9A	-2.05	107.97	113.47
2	B	602	NAI	C2B-C1B-N9A	-2.05	107.97	113.47
3	E	603	GTP	C4'-O4'-C1'	2.05	111.82	109.64
3	C	603	GTP	C4'-O4'-C1'	2.05	111.82	109.64
3	B	603	GTP	C4'-O4'-C1'	2.07	111.83	109.64
3	F	603	GTP	C4'-O4'-C1'	2.07	111.83	109.64
2	D	603	NAI	C3D-C2D-C1D	2.40	106.26	101.44
2	C	601	NAI	C3D-C2D-C1D	2.41	106.28	101.44
2	F	601	NAI	C3D-C2D-C1D	2.41	106.28	101.44
2	A	603	NAI	C3D-C2D-C1D	2.42	106.31	101.44
2	B	601	NAI	C3D-C2D-C1D	2.43	106.31	101.44
2	E	601	NAI	C3D-C2D-C1D	2.45	106.37	101.44
3	D	602	GTP	C6-N1-C2	3.17	119.60	115.88
3	E	603	GTP	C6-N1-C2	3.18	119.61	115.88
3	A	602	GTP	C6-N1-C2	3.20	119.63	115.88
3	B	603	GTP	C6-N1-C2	3.21	119.64	115.88
3	C	603	GTP	C6-N1-C2	3.22	119.65	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	603	GTP	C6-N1-C2	3.23	119.67	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAI	3	0
3	A	602	GTP	2	0
2	B	602	NAI	3	0
3	B	603	GTP	2	0
2	C	602	NAI	2	0
3	C	603	GTP	1	0
2	D	601	NAI	2	0
3	D	602	GTP	2	0
2	E	602	NAI	3	0
3	E	603	GTP	2	0
2	F	602	NAI	2	0
3	F	603	GTP	1	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.