wwPDB EM Map/Model Validation Report (i)

Jun 20, 2016 – 11:56 AM EDT

PDB ID	:	5JCO
EMDB ID:	:	EMD-8150
Title	:	Structure and dynamics of single-isoform recombinant neuronal human tubulin
Authors	:	Vemu, A.; Atherton, J.; Spector, J.O.; Szyk, A.; Moores, C.A.; Roll-Mecak, A.
Deposited on	:	2016-04-15
Resolution	:	4.00 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

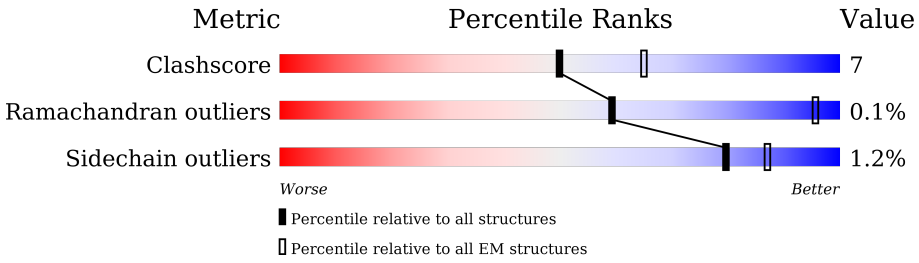
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 4.00 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	C	426	88% 12%
1	D	426	87% 13%
1	I	426	87% 13%
1	J	426	87% 13%
1	K	426	86% 14%
1	L	426	86% 14%
2	A	437	80% 17% ••
2	B	437	80% 18% ••
2	E	437	79% 18% ••

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Mol	Chain	Length	Quality of chain
2	F	437	79% 18%
2	G	437	78% 19%
2	H	437	79% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40512 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.

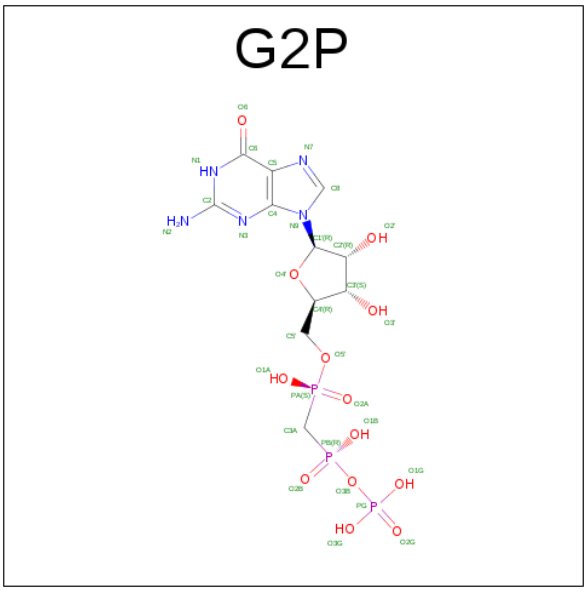
- Molecule 1 is a protein called Tubulin beta-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	426	Total	C	N	O	S	0	0
			3341	2103	571	642	25		
1	I	426	Total	C	N	O	S	0	0
			3341	2103	571	642	25		
1	J	426	Total	C	N	O	S	0	0
			3341	2103	571	642	25		
1	C	426	Total	C	N	O	S	0	0
			3341	2103	571	642	25		
1	D	426	Total	C	N	O	S	0	0
			3341	2103	571	642	25		
1	L	426	Total	C	N	O	S	0	0
			3341	2103	571	642	25		

- Molecule 2 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	428	Total	C	N	O	S	0	0
			3345	2124	571	629	21		
2	E	428	Total	C	N	O	S	0	0
			3345	2124	571	629	21		
2	F	428	Total	C	N	O	S	0	0
			3345	2124	571	629	21		
2	A	428	Total	C	N	O	S	0	0
			3345	2124	571	629	21		
2	B	428	Total	C	N	O	S	0	0
			3345	2124	571	629	21		
2	G	428	Total	C	N	O	S	0	0
			3345	2124	571	629	21		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	K	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	I	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	J	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	C	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	D	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	L	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	
4	J	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	H	1	Total	Mg	0
			1	1	

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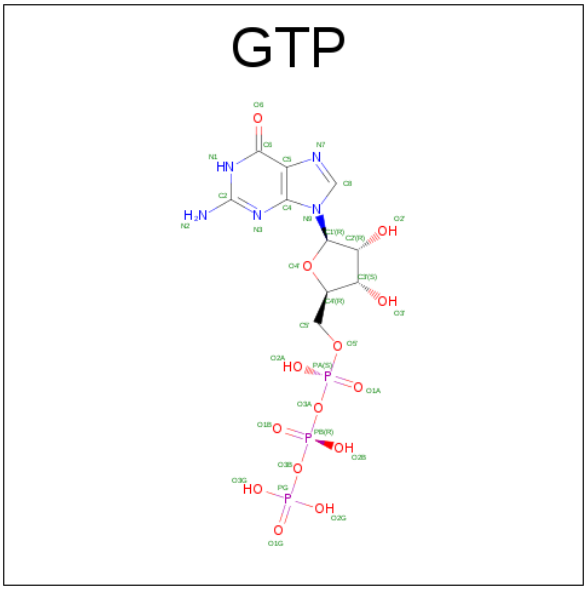
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Mg 1 1	0
4	I	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	A	1	Total Mg 1 1	0
4	L	1	Total Mg 1 1	0
4	F	1	Total Mg 1 1	0

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



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

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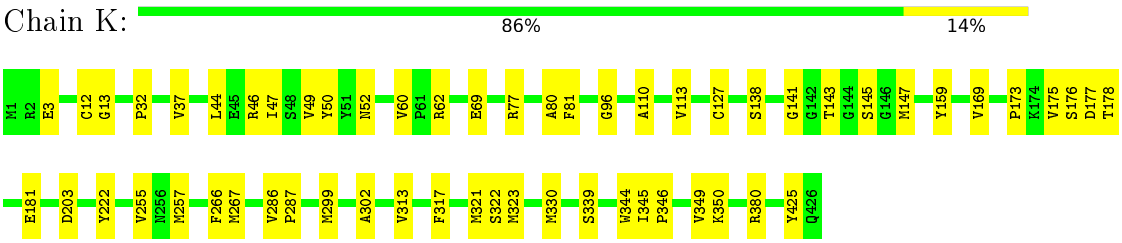
Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

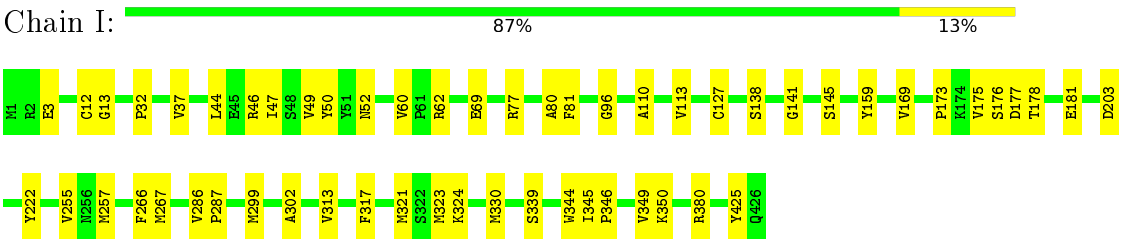
- Molecule 1: Tubulin beta-3 chain

Chain K:



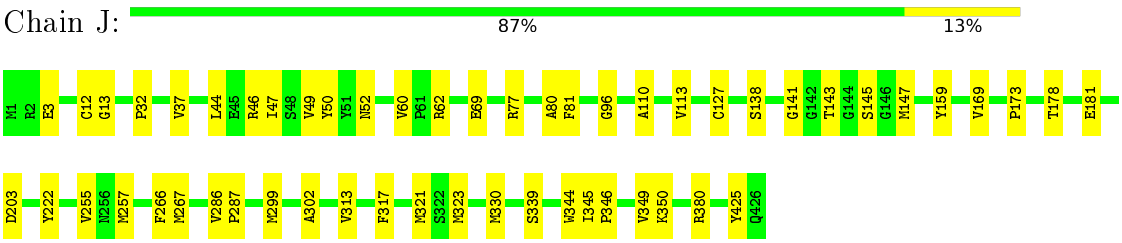
- Molecule 1: Tubulin beta-3 chain

Chain I:



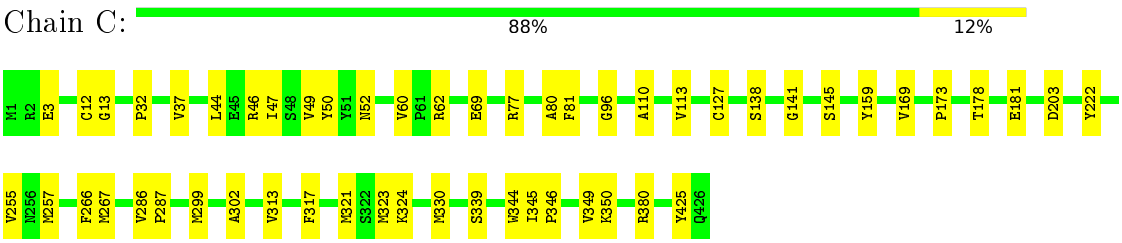
- Molecule 1: Tubulin beta-3 chain

Chain J:



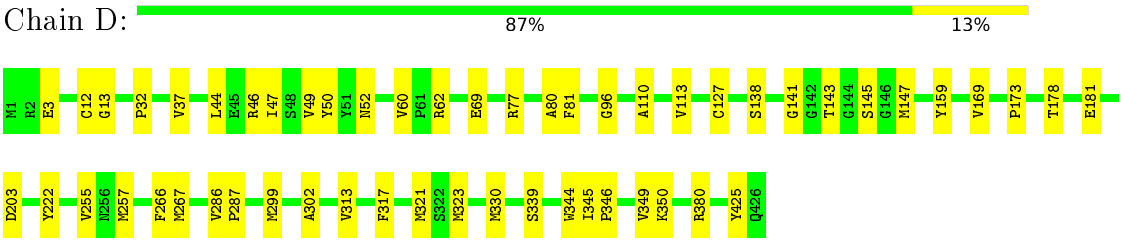
- Molecule 1: Tubulin beta-3 chain

Chain C:



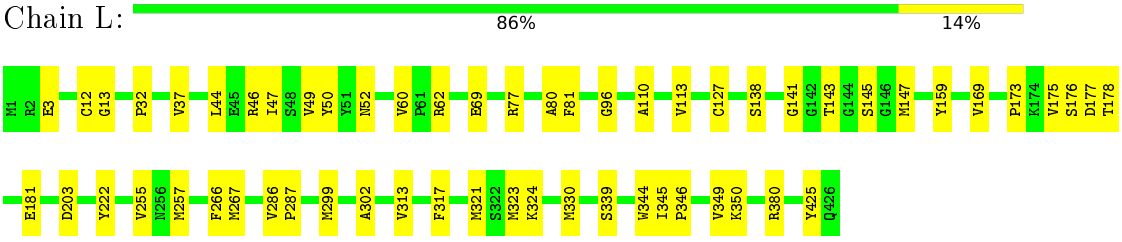
- Molecule 1: Tubulin beta-3 chain

Chain D:



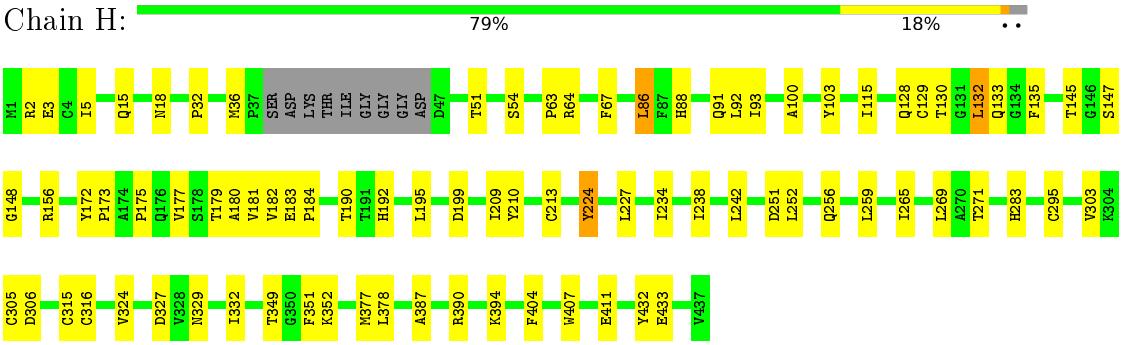
• Molecule 1: Tubulin beta-3 chain

Chain L:



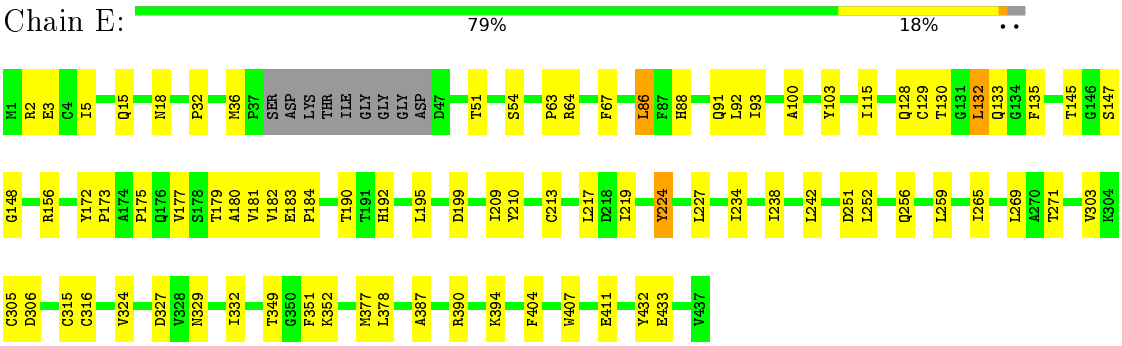
• Molecule 2: Tubulin alpha-1A chain

Chain H:



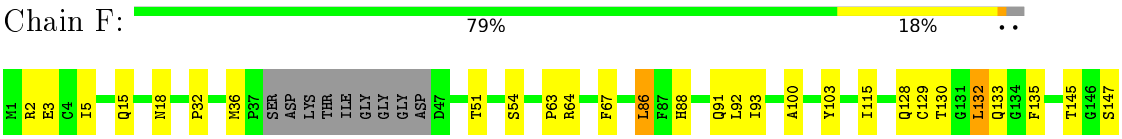
• Molecule 2: Tubulin alpha-1A chain

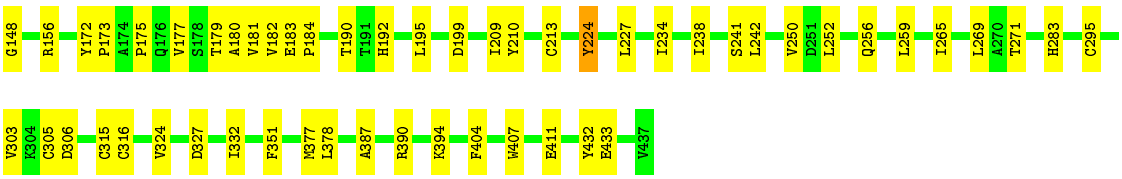
Chain E:



• Molecule 2: Tubulin alpha-1A chain

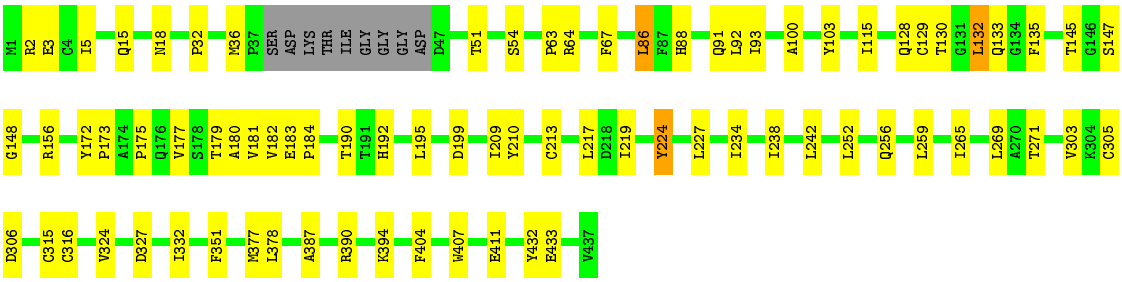
Chain F:





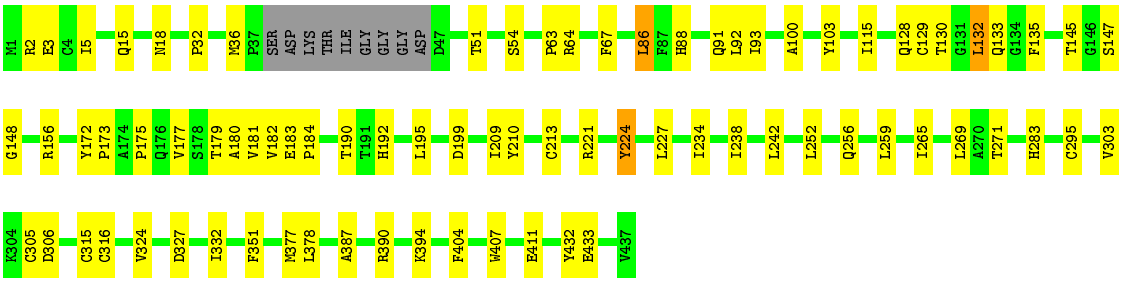
- Molecule 2: Tubulin alpha-1A chain

Chain A:



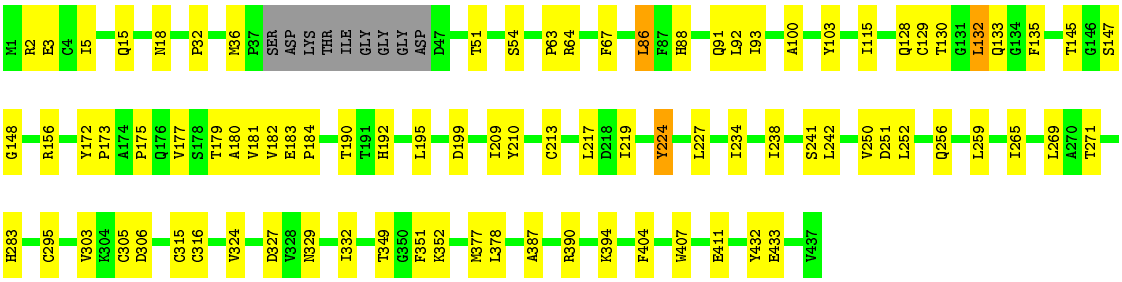
- Molecule 2: Tubulin alpha-1A chain

Chain B:



- Molecule 2: Tubulin alpha-1A chain

Chain G:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	10164	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, MG, G2P

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	C	0.48	0/3416	0.75	0/4628
1	D	0.48	0/3416	0.75	0/4628
1	I	0.49	0/3416	0.75	0/4628
1	J	0.48	0/3416	0.75	0/4628
1	K	0.49	0/3416	0.75	0/4628
1	L	0.49	0/3416	0.75	0/4628
2	A	0.49	0/3422	0.91	1/4647 (0.0%)
2	B	0.49	0/3422	0.85	1/4647 (0.0%)
2	E	0.49	0/3422	0.90	1/4647 (0.0%)
2	F	0.48	0/3422	0.85	1/4647 (0.0%)
2	G	0.48	0/3422	0.86	1/4647 (0.0%)
2	H	0.49	0/3422	0.86	1/4647 (0.0%)
All	All	0.49	0/41028	0.81	6/55650 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	36	MET	C-N-CD	-32.97	48.07	120.60
2	E	36	MET	C-N-CD	-30.94	52.53	120.60
2	H	36	MET	C-N-CD	-26.49	62.33	120.60
2	G	36	MET	C-N-CD	-25.84	63.75	120.60
2	B	36	MET	C-N-CD	-25.00	65.61	120.60
2	F	36	MET	C-N-CD	-24.94	65.73	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3341	0	3224	38	0
1	D	3341	0	3224	38	0
1	I	3341	0	3224	49	0
1	J	3341	0	3224	39	0
1	K	3341	0	3224	49	0
1	L	3341	0	3224	49	0
2	A	3345	0	3259	62	0
2	B	3345	0	3259	64	0
2	E	3345	0	3259	71	0
2	F	3345	0	3259	62	0
2	G	3345	0	3259	72	0
2	H	3345	0	3259	72	0
3	C	32	0	14	0	0
3	D	32	0	14	0	0
3	I	32	0	14	0	0
3	J	32	0	14	0	0
3	K	32	0	14	0	0
3	L	32	0	14	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	32	0	12	1	0
5	B	32	0	12	1	0
5	E	32	0	12	1	0
5	F	32	0	12	1	0
5	G	32	0	12	1	0
5	H	32	0	12	1	0
All	All	40512	0	39054	582	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 7.

All (582) 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)
2:G:324:VAL:HG23	2:G:327:ASP:HB2	1.60	0.84
2:H:324:VAL:HG23	2:H:327:ASP:HB2	1.60	0.84
2:F:324:VAL:HG23	2:F:327:ASP:HB2	1.60	0.84
2:B:324:VAL:HG23	2:B:327:ASP:HB2	1.60	0.83
2:E:324:VAL:HG23	2:E:327:ASP:HB2	1.60	0.83
2:A:324:VAL:HG23	2:A:327:ASP:HB2	1.60	0.83
1:C:317:PHE:HB3	1:C:321:MET:HE1	1.60	0.82
1:I:317:PHE:HB3	1:I:321:MET:HE1	1.60	0.82
1:J:317:PHE:HB3	1:J:321:MET:HE1	1.61	0.80
1:L:317:PHE:HB3	1:L:321:MET:HE1	1.61	0.80
1:D:317:PHE:HB3	1:D:321:MET:HE1	1.61	0.80
1:K:317:PHE:HB3	1:K:321:MET:HE1	1.61	0.80
1:L:177:ASP:O	2:G:352:LYS:HD2	1.84	0.78
1:I:177:ASP:O	2:E:352:LYS:HD2	1.84	0.78
1:K:177:ASP:O	2:H:352:LYS:HD2	1.84	0.75
1:K:175:VAL:HG11	2:H:329:ASN:ND2	2.01	0.75
1:I:175:VAL:HG11	2:E:329:ASN:ND2	2.02	0.74
1:L:175:VAL:HG11	2:G:329:ASN:ND2	2.02	0.74
1:C:317:PHE:HB3	1:C:321:MET:CE	2.20	0.72
1:I:317:PHE:HB3	1:I:321:MET:CE	2.20	0.72
1:D:317:PHE:HB3	1:D:321:MET:CE	2.20	0.71
1:K:317:PHE:HB3	1:K:321:MET:CE	2.20	0.71
2:G:242:LEU:HD11	2:G:252:LEU:HD13	1.73	0.71
2:A:242:LEU:HD11	2:A:252:LEU:HD13	1.73	0.71
2:E:242:LEU:HD11	2:E:252:LEU:HD13	1.73	0.71
2:F:242:LEU:HD11	2:F:252:LEU:HD13	1.73	0.71
2:H:242:LEU:HD11	2:H:252:LEU:HD13	1.73	0.71
1:J:317:PHE:HB3	1:J:321:MET:CE	2.20	0.71
2:B:242:LEU:HD11	2:B:252:LEU:HD13	1.73	0.71
1:L:317:PHE:HB3	1:L:321:MET:CE	2.20	0.71
2:E:259:LEU:HD11	2:E:316:CYS:SG	2.31	0.69
2:H:259:LEU:HD11	2:H:316:CYS:SG	2.31	0.69
2:B:259:LEU:HD11	2:B:316:CYS:SG	2.31	0.69
2:A:259:LEU:HD11	2:A:316:CYS:SG	2.31	0.69
2:G:259:LEU:HD11	2:G:316:CYS:SG	2.31	0.69
2:F:259:LEU:HD11	2:F:316:CYS:SG	2.31	0.69
1:L:178:THR:OG1	1:L:181:GLU:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:THR:OG1	1:J:181:GLU:HG3	1.93	0.68
1:I:178:THR:OG1	1:I:181:GLU:HG3	1.93	0.68
1:C:178:THR:OG1	1:C:181:GLU:HG3	1.93	0.68
1:K:178:THR:OG1	1:K:181:GLU:HG3	1.93	0.67
1:D:178:THR:OG1	1:D:181:GLU:HG3	1.93	0.67
2:G:210:TYR:O	2:G:213:CYS:SG	2.48	0.65
1:I:141:GLY:O	1:I:145:SER:OG	2.07	0.65
1:K:141:GLY:O	1:K:145:SER:OG	2.07	0.65
1:C:141:GLY:O	1:C:145:SER:OG	2.07	0.65
1:D:141:GLY:O	1:D:145:SER:OG	2.07	0.65
1:I:175:VAL:CG1	2:E:329:ASN:OD1	2.45	0.65
1:I:175:VAL:HG11	2:E:329:ASN:HD21	1.63	0.64
1:K:175:VAL:CG1	2:H:329:ASN:OD1	2.45	0.64
1:K:175:VAL:HG11	2:H:329:ASN:HD21	1.62	0.64
1:I:175:VAL:HG11	2:E:329:ASN:CG	2.17	0.64
1:L:175:VAL:HG11	2:G:329:ASN:OD1	1.97	0.64
1:L:175:VAL:CG1	2:G:329:ASN:OD1	2.45	0.64
1:K:175:VAL:HG11	2:H:329:ASN:OD1	1.98	0.64
1:I:175:VAL:HG11	2:E:329:ASN:OD1	1.97	0.64
2:F:394:LYS:HG3	1:L:346:PRO:HG3	1.79	0.64
1:K:175:VAL:HG11	2:H:329:ASN:CG	2.17	0.63
1:K:346:PRO:HG3	2:B:394:LYS:HG3	1.78	0.63
2:E:394:LYS:HG3	1:C:346:PRO:HG3	1.80	0.63
1:L:175:VAL:HG11	2:G:329:ASN:CG	2.17	0.63
2:F:407:TRP:O	2:F:411:GLU:HG2	1.99	0.63
2:G:407:TRP:O	2:G:411:GLU:HG2	1.99	0.63
1:I:346:PRO:HG3	2:A:394:LYS:HG3	1.81	0.62
2:A:407:TRP:O	2:A:411:GLU:HG2	1.99	0.62
2:E:407:TRP:O	2:E:411:GLU:HG2	1.99	0.62
2:B:407:TRP:O	2:B:411:GLU:HG2	1.99	0.62
2:H:407:TRP:O	2:H:411:GLU:HG2	1.99	0.62
1:L:175:VAL:HG11	2:G:329:ASN:HD21	1.63	0.61
2:H:394:LYS:HG3	1:D:346:PRO:HG3	1.81	0.60
2:E:3:GLU:O	2:E:132:LEU:HB2	2.01	0.59
1:J:346:PRO:HG3	2:G:394:LYS:HG3	1.83	0.59
2:A:3:GLU:O	2:A:132:LEU:HB2	2.02	0.59
2:H:3:GLU:O	2:H:132:LEU:HB2	2.01	0.59
2:B:3:GLU:O	2:B:132:LEU:HB2	2.02	0.59
2:G:3:GLU:O	2:G:132:LEU:HB2	2.01	0.59
2:F:3:GLU:O	2:F:132:LEU:HB2	2.02	0.59
2:E:324:VAL:HG23	2:E:327:ASP:CB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:VAL:HG23	2:H:327:ASP:CB	2.32	0.58
2:A:324:VAL:HG23	2:A:327:ASP:CB	2.33	0.58
2:F:129:CYS:SG	2:F:130:THR:N	2.76	0.58
2:G:129:CYS:SG	2:G:130:THR:N	2.76	0.58
2:G:324:VAL:HG23	2:G:327:ASP:CB	2.32	0.58
2:A:129:CYS:SG	2:A:130:THR:N	2.77	0.58
2:E:5:ILE:HG22	2:E:64:ARG:HB3	1.84	0.58
2:A:5:ILE:HG22	2:A:64:ARG:HB3	1.84	0.57
2:B:5:ILE:HG22	2:B:64:ARG:HB3	1.84	0.57
2:E:129:CYS:SG	2:E:130:THR:N	2.77	0.57
2:F:5:ILE:HG22	2:F:64:ARG:HB3	1.84	0.57
2:B:324:VAL:HG23	2:B:327:ASP:CB	2.33	0.57
2:G:5:ILE:HG22	2:G:64:ARG:HB3	1.84	0.57
2:H:5:ILE:HG22	2:H:64:ARG:HB3	1.84	0.57
2:F:324:VAL:HG23	2:F:327:ASP:CB	2.33	0.57
2:E:88:HIS:O	2:E:91:GLN:HG2	2.05	0.57
2:G:324:VAL:CG2	2:G:327:ASP:HB2	2.33	0.57
2:H:88:HIS:O	2:H:91:GLN:HG2	2.05	0.57
2:H:324:VAL:CG2	2:H:327:ASP:HB2	2.33	0.57
2:A:88:HIS:O	2:A:91:GLN:HG2	2.05	0.57
2:B:88:HIS:O	2:B:91:GLN:HG2	2.05	0.57
2:F:324:VAL:CG2	2:F:327:ASP:HB2	2.33	0.57
2:B:129:CYS:SG	2:B:130:THR:N	2.77	0.57
2:E:324:VAL:CG2	2:E:327:ASP:HB2	2.33	0.56
2:H:129:CYS:SG	2:H:130:THR:N	2.77	0.56
2:B:324:VAL:CG2	2:B:327:ASP:HB2	2.33	0.56
2:F:88:HIS:O	2:F:91:GLN:HG2	2.05	0.56
2:G:88:HIS:O	2:G:91:GLN:HG2	2.05	0.56
2:A:324:VAL:CG2	2:A:327:ASP:HB2	2.33	0.56
2:E:210:TYR:O	2:E:213:CYS:SG	2.48	0.56
2:A:210:TYR:O	2:A:213:CYS:SG	2.48	0.56
2:H:283:HIS:CB	2:E:88:HIS:HB3	2.36	0.56
2:F:394:LYS:HG3	1:L:346:PRO:CG	2.36	0.55
2:B:210:TYR:O	2:B:213:CYS:SG	2.48	0.55
2:G:63:PRO:HD3	2:G:86:LEU:HD12	1.89	0.55
2:H:210:TYR:O	2:H:213:CYS:SG	2.48	0.55
2:A:88:HIS:HB3	2:B:283:HIS:CB	2.37	0.55
2:F:63:PRO:HD3	2:F:86:LEU:HD12	1.89	0.55
2:B:63:PRO:HD3	2:B:86:LEU:HD12	1.89	0.55
2:G:173:PRO:HB3	2:G:183:GLU:OE1	2.07	0.55
2:B:147:SER:OG	2:B:190:THR:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:PRO:HB3	2:F:183:GLU:OE1	2.07	0.54
2:H:147:SER:OG	2:H:190:THR:HB	2.07	0.54
2:A:147:SER:OG	2:A:190:THR:HB	2.07	0.54
1:I:255:VAL:HG11	2:A:100:ALA:O	2.08	0.54
2:A:2:ARG:HB3	2:A:133:GLN:NE2	2.23	0.54
2:E:147:SER:OG	2:E:190:THR:HB	2.07	0.54
2:F:210:TYR:O	2:F:213:CYS:SG	2.48	0.54
2:H:2:ARG:HB3	2:H:133:GLN:NE2	2.23	0.54
2:F:100:ALA:O	1:L:255:VAL:HG11	2.07	0.54
1:K:346:PRO:CG	2:B:394:LYS:HG3	2.37	0.54
2:E:2:ARG:HB3	2:E:133:GLN:NE2	2.23	0.54
2:E:394:LYS:HG3	1:C:346:PRO:CG	2.37	0.54
2:G:2:ARG:HB3	2:G:133:GLN:NE2	2.23	0.54
1:I:346:PRO:CG	2:A:394:LYS:HG3	2.37	0.54
2:A:63:PRO:HD3	2:A:86:LEU:HD12	1.90	0.54
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.23	0.54
2:F:2:ARG:HB3	2:F:133:GLN:NE2	2.23	0.54
2:H:63:PRO:HD3	2:H:86:LEU:HD12	1.89	0.54
2:F:147:SER:OG	2:F:190:THR:HB	2.07	0.54
2:G:147:SER:OG	2:G:190:THR:HB	2.07	0.54
1:I:203:ASP:OD2	1:I:302:ALA:HB2	2.08	0.54
2:A:173:PRO:HB3	2:A:183:GLU:OE1	2.07	0.54
2:F:283:HIS:CB	2:B:88:HIS:HB3	2.38	0.54
2:E:173:PRO:HB3	2:E:183:GLU:OE1	2.07	0.54
1:D:203:ASP:OD2	1:D:302:ALA:HB2	2.08	0.54
2:E:100:ALA:O	1:C:255:VAL:HG11	2.08	0.54
1:K:203:ASP:OD2	1:K:302:ALA:HB2	2.08	0.54
1:C:203:ASP:OD2	1:C:302:ALA:HB2	2.08	0.54
2:E:63:PRO:HD3	2:E:86:LEU:HD12	1.90	0.54
1:L:176:SER:OG	2:G:349:THR:HB	2.08	0.54
1:D:110:ALA:O	1:D:113:VAL:HG12	2.08	0.53
2:H:88:HIS:HB3	2:G:283:HIS:CB	2.38	0.53
1:J:203:ASP:OD2	1:J:302:ALA:HB2	2.08	0.53
1:K:110:ALA:O	1:K:113:VAL:HG12	2.08	0.53
1:L:203:ASP:OD2	1:L:302:ALA:HB2	2.08	0.53
1:I:110:ALA:O	1:I:113:VAL:HG12	2.08	0.53
1:C:110:ALA:O	1:C:113:VAL:HG12	2.08	0.53
1:I:286:VAL:HB	1:I:287:PRO:HD3	1.89	0.53
2:H:173:PRO:HB3	2:H:183:GLU:OE1	2.07	0.53
2:B:173:PRO:HB3	2:B:183:GLU:OE1	2.07	0.53
1:D:12:CYS:SG	1:D:13:GLY:N	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:332:ILE:HG23	2:F:351:PHE:CD2	2.44	0.53
2:H:209:ILE:HG21	2:H:227:LEU:HG	1.91	0.53
1:K:12:CYS:SG	1:K:13:GLY:N	2.81	0.53
1:C:286:VAL:HB	1:C:287:PRO:HD3	1.90	0.53
2:G:332:ILE:HG23	2:G:351:PHE:CD2	2.44	0.53
1:K:286:VAL:HB	1:K:287:PRO:HD3	1.89	0.53
2:A:332:ILE:HG23	2:A:351:PHE:CD2	2.44	0.53
1:D:286:VAL:HB	1:D:287:PRO:HD3	1.89	0.53
1:I:176:SER:OG	2:E:349:THR:HB	2.08	0.53
1:J:110:ALA:O	1:J:113:VAL:HG12	2.08	0.53
2:E:332:ILE:HG23	2:E:351:PHE:CD2	2.44	0.52
2:E:32:PRO:O	2:E:86:LEU:HD23	2.09	0.52
1:K:176:SER:OG	2:H:349:THR:HB	2.08	0.52
1:K:344:TRP:CD1	1:K:345:ILE:HG13	2.44	0.52
1:L:286:VAL:HB	1:L:287:PRO:HD3	1.89	0.52
1:C:12:CYS:SG	1:C:13:GLY:N	2.81	0.52
1:J:12:CYS:SG	1:J:13:GLY:N	2.81	0.52
1:J:286:VAL:HB	1:J:287:PRO:HD3	1.89	0.52
1:L:110:ALA:O	1:L:113:VAL:HG12	2.08	0.52
1:L:12:CYS:SG	1:L:13:GLY:N	2.81	0.52
2:B:209:ILE:HG21	2:B:227:LEU:HG	1.92	0.52
1:C:344:TRP:CD1	1:C:345:ILE:HG13	2.45	0.52
1:D:344:TRP:CD1	1:D:345:ILE:HG13	2.45	0.52
2:H:32:PRO:O	2:H:86:LEU:HD23	2.09	0.52
2:H:332:ILE:HG23	2:H:351:PHE:CD2	2.44	0.52
1:I:69:GLU:HG3	1:I:96:GLY:HA3	1.91	0.52
1:L:344:TRP:CD1	1:L:345:ILE:HG13	2.45	0.52
2:A:32:PRO:O	2:A:86:LEU:HD23	2.09	0.52
2:B:332:ILE:HG23	2:B:351:PHE:CD2	2.44	0.52
2:F:32:PRO:O	2:F:86:LEU:HD23	2.09	0.52
2:G:32:PRO:O	2:G:86:LEU:HD23	2.09	0.52
1:I:12:CYS:SG	1:I:13:GLY:N	2.81	0.52
1:I:344:TRP:CD1	1:I:345:ILE:HG13	2.45	0.52
1:J:344:TRP:CD1	1:J:345:ILE:HG13	2.45	0.52
2:B:32:PRO:O	2:B:86:LEU:HD23	2.09	0.52
1:K:255:VAL:HG11	2:B:100:ALA:O	2.10	0.52
1:K:69:GLU:HG3	1:K:96:GLY:HA3	1.91	0.52
1:L:69:GLU:HG3	1:L:96:GLY:HA3	1.91	0.52
1:C:69:GLU:HG3	1:C:96:GLY:HA3	1.91	0.52
1:D:69:GLU:HG3	1:D:96:GLY:HA3	1.91	0.52
2:F:199:ASP:OD1	2:F:256:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:ASP:OD1	2:A:256:GLN:NE2	2.43	0.52
2:B:199:ASP:OD1	2:B:256:GLN:NE2	2.43	0.52
1:K:346:PRO:HG3	2:B:394:LYS:CG	2.40	0.52
1:J:69:GLU:HG3	1:J:96:GLY:HA3	1.91	0.52
2:F:209:ILE:HG21	2:F:227:LEU:HG	1.92	0.51
2:E:199:ASP:OD1	2:E:256:GLN:NE2	2.43	0.51
2:G:209:ILE:HG21	2:G:227:LEU:HG	1.92	0.51
2:G:199:ASP:OD1	2:G:256:GLN:NE2	2.43	0.51
2:E:394:LYS:CG	1:C:346:PRO:HG3	2.40	0.51
2:E:209:ILE:HG21	2:E:227:LEU:HG	1.91	0.51
2:H:199:ASP:OD1	2:H:256:GLN:NE2	2.43	0.51
2:A:209:ILE:HG21	2:A:227:LEU:HG	1.92	0.51
2:F:394:LYS:CG	1:L:346:PRO:HG3	2.39	0.51
2:G:129:CYS:SG	2:G:132:LEU:HB3	2.51	0.51
2:H:394:LYS:HG3	1:D:346:PRO:CG	2.40	0.51
2:E:5:ILE:HD11	2:E:135:PHE:CE1	2.46	0.51
2:F:129:CYS:SG	2:F:132:LEU:HB3	2.51	0.51
2:G:5:ILE:HD11	2:G:135:PHE:CE1	2.46	0.51
2:H:129:CYS:SG	2:H:132:LEU:HB3	2.51	0.51
1:J:346:PRO:CG	2:G:394:LYS:HG3	2.40	0.51
2:B:129:CYS:SG	2:B:132:LEU:HB3	2.51	0.51
1:I:177:ASP:O	2:E:352:LYS:CD	2.58	0.51
1:I:46:ARG:O	1:I:49:VAL:HG12	2.11	0.51
1:C:46:ARG:O	1:C:49:VAL:HG12	2.11	0.51
1:D:46:ARG:O	1:D:49:VAL:HG12	2.11	0.51
2:F:5:ILE:HD11	2:F:135:PHE:CE1	2.46	0.51
2:H:5:ILE:HD11	2:H:135:PHE:CE1	2.46	0.51
1:K:46:ARG:O	1:K:49:VAL:HG12	2.11	0.51
2:A:129:CYS:SG	2:A:132:LEU:HB3	2.51	0.50
1:I:346:PRO:HG3	2:A:394:LYS:CG	2.41	0.50
2:A:5:ILE:HD11	2:A:135:PHE:CE1	2.46	0.50
2:E:129:CYS:SG	2:E:132:LEU:HB3	2.51	0.50
2:E:175:PRO:HG2	2:E:390:ARG:HD3	1.93	0.50
2:A:175:PRO:HG2	2:A:390:ARG:HD3	1.93	0.50
2:B:5:ILE:HD11	2:B:135:PHE:CE1	2.47	0.50
1:L:46:ARG:O	1:L:49:VAL:HG12	2.11	0.50
2:B:93:ILE:HD12	2:B:93:ILE:N	2.27	0.50
2:F:93:ILE:N	2:F:93:ILE:HD12	2.27	0.50
2:G:93:ILE:HD12	2:G:93:ILE:N	2.27	0.50
1:J:141:GLY:O	1:J:145:SER:OG	2.07	0.50
1:J:46:ARG:O	1:J:49:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:GLY:O	1:L:145:SER:OG	2.07	0.50
2:B:175:PRO:HG2	2:B:390:ARG:HD3	1.93	0.50
2:H:175:PRO:HG2	2:H:390:ARG:HD3	1.93	0.50
2:H:93:ILE:N	2:H:93:ILE:HD12	2.27	0.50
2:H:100:ALA:O	1:D:255:VAL:HG11	2.12	0.50
2:E:93:ILE:HD12	2:E:93:ILE:N	2.26	0.50
1:J:255:VAL:HG11	2:G:100:ALA:O	2.12	0.50
2:F:175:PRO:HG2	2:F:390:ARG:HD3	1.93	0.49
2:G:271:THR:HG22	2:G:377:MET:HB3	1.93	0.49
2:A:93:ILE:HD12	2:A:93:ILE:N	2.26	0.49
1:D:138:SER:HA	1:D:169:VAL:HG22	1.95	0.49
2:G:175:PRO:HG2	2:G:390:ARG:HD3	1.93	0.49
1:J:138:SER:HA	1:J:169:VAL:HG22	1.95	0.49
1:K:177:ASP:O	2:H:352:LYS:CD	2.58	0.49
1:C:138:SER:HA	1:C:169:VAL:HG22	1.95	0.49
2:E:271:THR:HG22	2:E:377:MET:HB3	1.93	0.49
2:A:183:GLU:N	2:A:184:PRO:CD	2.75	0.49
1:D:3:GLU:HB3	1:D:62:ARG:NH1	2.27	0.49
2:F:183:GLU:N	2:F:184:PRO:CD	2.75	0.49
2:F:271:THR:HG22	2:F:377:MET:HB3	1.93	0.49
2:G:183:GLU:N	2:G:184:PRO:CD	2.75	0.49
1:K:3:GLU:HB3	1:K:62:ARG:NH1	2.27	0.49
1:L:138:SER:HA	1:L:169:VAL:HG22	1.95	0.49
2:A:271:THR:HG22	2:A:377:MET:HB3	1.93	0.49
2:E:183:GLU:N	2:E:184:PRO:CD	2.76	0.49
1:K:138:SER:HA	1:K:169:VAL:HG22	1.95	0.49
1:C:317:PHE:CB	1:C:321:MET:CE	2.91	0.49
1:D:317:PHE:CB	1:D:321:MET:CE	2.91	0.49
1:I:138:SER:HA	1:I:169:VAL:HG22	1.95	0.49
1:I:317:PHE:CB	1:I:321:MET:CE	2.91	0.49
1:K:317:PHE:CB	1:K:321:MET:CE	2.91	0.49
1:L:177:ASP:O	2:G:352:LYS:CD	2.58	0.49
2:A:315:CYS:HB2	2:A:351:PHE:HD1	1.78	0.49
2:H:394:LYS:CG	1:D:346:PRO:HG3	2.43	0.49
2:E:315:CYS:HB2	2:E:351:PHE:HD1	1.78	0.49
2:H:271:THR:HG22	2:H:377:MET:HB3	1.93	0.49
1:L:3:GLU:HB3	1:L:62:ARG:NH1	2.27	0.49
2:H:183:GLU:N	2:H:184:PRO:CD	2.75	0.49
2:B:183:GLU:N	2:B:184:PRO:CD	2.75	0.49
2:B:271:THR:HG22	2:B:377:MET:HB3	1.93	0.49
2:E:238:ILE:CD1	2:E:378:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:315:CYS:HB2	2:F:351:PHE:HD1	1.78	0.49
1:J:317:PHE:CB	1:J:321:MET:CE	2.91	0.49
1:J:3:GLU:HB3	1:J:62:ARG:NH1	2.27	0.49
2:B:234:ILE:O	2:B:238:ILE:HG12	2.14	0.48
2:B:315:CYS:HB2	2:B:351:PHE:HD1	1.78	0.48
1:C:3:GLU:HB3	1:C:62:ARG:NH1	2.28	0.48
2:G:315:CYS:HB2	2:G:351:PHE:HD1	1.78	0.48
1:I:3:GLU:HB3	1:I:62:ARG:NH1	2.28	0.48
1:J:173:PRO:HD3	1:J:380:ARG:CZ	2.43	0.48
1:L:173:PRO:HD3	1:L:380:ARG:CZ	2.43	0.48
1:L:317:PHE:CB	1:L:321:MET:CE	2.91	0.48
2:A:238:ILE:CD1	2:A:378:LEU:HD21	2.43	0.48
2:H:315:CYS:HB2	2:H:351:PHE:HD1	1.78	0.48
1:L:69:GLU:OE2	2:G:251:ASP:OD2	2.30	0.48
2:F:238:ILE:CD1	2:F:378:LEU:HD21	2.43	0.48
2:G:238:ILE:CD1	2:G:378:LEU:HD21	2.43	0.48
2:H:238:ILE:CD1	2:H:378:LEU:HD21	2.42	0.48
1:J:344:TRP:HH2	1:J:425:TYR:HB3	1.79	0.48
1:L:344:TRP:HH2	1:L:425:TYR:HB3	1.78	0.48
2:B:238:ILE:CD1	2:B:378:LEU:HD21	2.42	0.48
2:H:234:ILE:O	2:H:238:ILE:HG12	2.14	0.48
1:K:69:GLU:OE2	2:H:251:ASP:OD2	2.30	0.48
1:I:32:PRO:HB3	1:I:81:PHE:CD1	2.49	0.48
1:J:32:PRO:HB3	1:J:81:PHE:CD1	2.49	0.48
1:C:32:PRO:HB3	1:C:81:PHE:CD1	2.49	0.48
1:D:344:TRP:HH2	1:D:425:TYR:HB3	1.78	0.48
1:I:323:MET:SD	2:A:224:TYR:CE2	3.06	0.48
1:I:173:PRO:HD3	1:I:380:ARG:CZ	2.43	0.48
1:K:173:PRO:HD3	1:K:380:ARG:CZ	2.43	0.48
1:L:32:PRO:HB3	1:L:81:PHE:CD1	2.49	0.48
1:C:173:PRO:HD3	1:C:380:ARG:CZ	2.43	0.48
1:D:173:PRO:HD3	1:D:380:ARG:CZ	2.43	0.48
2:B:238:ILE:HD11	2:B:378:LEU:HD21	1.96	0.48
2:H:238:ILE:HD11	2:H:378:LEU:HD21	1.96	0.48
1:J:173:PRO:HD3	1:J:380:ARG:NH2	2.29	0.48
1:K:344:TRP:HH2	1:K:425:TYR:HB3	1.79	0.48
1:L:173:PRO:HD3	1:L:380:ARG:NH2	2.29	0.48
2:E:224:TYR:CE2	1:C:323:MET:SD	3.07	0.48
2:E:238:ILE:HD11	2:E:378:LEU:HD21	1.96	0.48
2:B:305:CYS:O	2:B:306:ASP:HB2	2.13	0.48
2:A:238:ILE:HD11	2:A:378:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:234:ILE:O	2:A:238:ILE:HG12	2.14	0.48
2:H:305:CYS:O	2:H:306:ASP:HB2	2.14	0.48
1:J:37:VAL:O	1:J:37:VAL:HG12	2.14	0.48
1:L:37:VAL:HG12	1:L:37:VAL:O	2.14	0.48
1:D:32:PRO:HB3	1:D:81:PHE:CD1	2.49	0.47
2:E:234:ILE:O	2:E:238:ILE:HG12	2.14	0.47
2:F:234:ILE:O	2:F:238:ILE:HG12	2.14	0.47
2:G:234:ILE:O	2:G:238:ILE:HG12	2.14	0.47
2:A:305:CYS:O	2:A:306:ASP:HB2	2.13	0.47
1:D:37:VAL:O	1:D:37:VAL:HG12	2.14	0.47
2:G:238:ILE:HD11	2:G:378:LEU:HD21	1.96	0.47
1:K:32:PRO:HB3	1:K:81:PHE:CD1	2.49	0.47
2:E:305:CYS:O	2:E:306:ASP:HB2	2.14	0.47
2:F:238:ILE:HD11	2:F:378:LEU:HD21	1.96	0.47
2:F:305:CYS:O	2:F:306:ASP:HB2	2.13	0.47
2:G:145:THR:HB	5:G:501:GTP:O1B	2.14	0.47
1:I:344:TRP:HH2	1:I:425:TYR:HB3	1.79	0.47
1:I:69:GLU:OE2	2:E:251:ASP:OD2	2.31	0.47
1:K:37:VAL:O	1:K:37:VAL:HG12	2.14	0.47
2:E:103:TYR:CE2	2:E:148:GLY:HA2	2.49	0.47
2:G:305:CYS:O	2:G:306:ASP:HB2	2.13	0.47
2:A:103:TYR:CE2	2:A:148:GLY:HA2	2.49	0.47
1:C:344:TRP:HH2	1:C:425:TYR:HB3	1.79	0.47
1:I:173:PRO:HD3	1:I:380:ARG:NH2	2.30	0.47
1:C:173:PRO:HD3	1:C:380:ARG:NH2	2.30	0.47
2:B:103:TYR:CE2	2:B:148:GLY:HA2	2.49	0.47
1:D:173:PRO:HD3	1:D:380:ARG:NH2	2.29	0.47
1:K:173:PRO:HD3	1:K:380:ARG:NH2	2.29	0.47
2:F:103:TYR:CE2	2:F:148:GLY:HA2	2.49	0.47
2:G:103:TYR:CE2	2:G:148:GLY:HA2	2.49	0.47
2:H:103:TYR:CE2	2:H:148:GLY:HA2	2.49	0.47
2:B:67:PHE:HB2	2:B:92:LEU:HD23	1.96	0.47
2:G:67:PHE:HB2	2:G:92:LEU:HD23	1.96	0.47
2:H:67:PHE:HB2	2:H:92:LEU:HD23	1.96	0.47
2:F:67:PHE:HB2	2:F:92:LEU:HD23	1.97	0.47
1:I:330:MET:HG3	1:I:349:VAL:HG11	1.96	0.47
2:F:224:TYR:CE2	1:L:323:MET:SD	3.08	0.47
1:K:330:MET:HG3	1:K:349:VAL:HG11	1.96	0.47
1:L:330:MET:HG3	1:L:349:VAL:HG11	1.96	0.47
2:A:3:GLU:HB2	2:A:129:CYS:SG	2.55	0.46
2:A:67:PHE:HB2	2:A:92:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:MET:HG3	1:C:349:VAL:HG11	1.96	0.46
2:E:3:GLU:HB2	2:E:129:CYS:SG	2.55	0.46
2:E:67:PHE:HB2	2:E:92:LEU:HD23	1.96	0.46
1:J:346:PRO:HG3	2:G:394:LYS:CG	2.44	0.46
1:I:37:VAL:O	1:I:37:VAL:HG12	2.14	0.46
1:C:37:VAL:O	1:C:37:VAL:HG12	2.14	0.46
2:H:3:GLU:HB2	2:H:129:CYS:SG	2.55	0.46
2:B:3:GLU:HB2	2:B:129:CYS:SG	2.55	0.46
1:D:330:MET:HG3	1:D:349:VAL:HG11	1.96	0.46
1:J:330:MET:HG3	1:J:349:VAL:HG11	1.96	0.46
2:F:241:SER:HG	2:F:250:VAL:H	1.64	0.46
2:G:241:SER:HG	2:G:250:VAL:H	1.64	0.46
2:G:3:GLU:HB2	2:G:129:CYS:SG	2.55	0.46
2:A:242:LEU:HD11	2:A:252:LEU:CD1	2.42	0.46
2:F:3:GLU:HB2	2:F:129:CYS:SG	2.55	0.46
2:H:242:LEU:HD11	2:H:252:LEU:CD1	2.42	0.46
2:B:242:LEU:HD11	2:B:252:LEU:CD1	2.43	0.46
2:E:242:LEU:HD11	2:E:252:LEU:CD1	2.42	0.46
1:C:257:MET:HB3	1:C:266:PHE:CE1	2.52	0.45
2:G:242:LEU:HD11	2:G:252:LEU:CD1	2.42	0.45
1:J:257:MET:HB3	1:J:266:PHE:CE1	2.51	0.45
1:L:257:MET:HB3	1:L:266:PHE:CE1	2.51	0.45
1:C:44:LEU:HD12	1:C:47:ILE:HD12	1.98	0.45
1:I:44:LEU:HD12	1:I:47:ILE:HD12	1.98	0.45
2:F:242:LEU:HD11	2:F:252:LEU:CD1	2.43	0.45
2:H:145:THR:HB	5:H:501:GTP:O1B	2.17	0.45
1:I:257:MET:HB3	1:I:266:PHE:CE1	2.52	0.45
1:K:350:LYS:HD2	2:B:179:THR:O	2.17	0.45
1:J:323:MET:SD	2:G:224:TYR:CE2	3.10	0.45
1:I:49:VAL:HG13	1:I:50:TYR:N	2.32	0.45
2:A:145:THR:HB	5:A:501:GTP:O1B	2.17	0.45
1:L:44:LEU:HD12	1:L:47:ILE:HD12	1.97	0.45
1:C:49:VAL:HG13	1:C:50:TYR:N	2.32	0.45
2:H:224:TYR:CE2	1:D:323:MET:SD	3.10	0.45
2:E:145:THR:HB	5:E:501:GTP:O1B	2.17	0.45
1:I:175:VAL:HG12	2:E:329:ASN:OD1	2.17	0.45
1:J:44:LEU:HD12	1:J:47:ILE:HD12	1.98	0.45
2:B:269:LEU:N	2:B:269:LEU:HD12	2.32	0.44
2:F:269:LEU:HD12	2:F:269:LEU:N	2.32	0.44
1:K:267:MET:HE2	1:K:299:MET:HE3	1.99	0.44
1:K:44:LEU:HD12	1:K:47:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:MET:HB3	1:D:266:PHE:CE1	2.52	0.44
2:H:269:LEU:HD12	2:H:269:LEU:N	2.32	0.44
1:K:257:MET:HB3	1:K:266:PHE:CE1	2.52	0.44
2:A:15:GLN:O	2:A:18:ASN:HB2	2.18	0.44
1:K:323:MET:SD	2:B:224:TYR:CE2	3.11	0.44
2:E:15:GLN:O	2:E:18:ASN:HB2	2.18	0.44
1:K:49:VAL:HG13	1:K:50:TYR:N	2.33	0.44
2:A:269:LEU:N	2:A:269:LEU:HD12	2.32	0.44
1:D:44:LEU:HD12	1:D:47:ILE:HD12	1.98	0.44
1:D:49:VAL:HG13	1:D:50:TYR:N	2.33	0.44
2:G:269:LEU:HD12	2:G:269:LEU:N	2.33	0.44
1:L:175:VAL:HG12	2:G:329:ASN:OD1	2.18	0.44
2:B:15:GLN:O	2:B:18:ASN:HB2	2.18	0.44
2:E:172:TYR:OH	2:E:387:ALA:HB1	2.18	0.44
2:F:54:SER:CB	2:F:128:GLN:OE1	2.66	0.44
2:F:145:THR:HB	5:F:501:GTP:O1B	2.17	0.44
2:G:54:SER:CB	2:G:128:GLN:OE1	2.66	0.44
2:H:15:GLN:O	2:H:18:ASN:HB2	2.18	0.44
1:K:175:VAL:HG12	2:H:329:ASN:OD1	2.17	0.44
1:C:317:PHE:CB	1:C:321:MET:HE1	2.41	0.44
2:E:269:LEU:N	2:E:269:LEU:HD12	2.32	0.44
2:A:54:SER:CB	2:A:128:GLN:OE1	2.66	0.43
2:A:172:TYR:OH	2:A:387:ALA:HB1	2.18	0.43
1:I:317:PHE:CB	1:I:321:MET:HE1	2.41	0.43
1:C:267:MET:HE2	1:C:299:MET:HE3	2.00	0.43
1:C:3:GLU:OE2	1:C:127:CYS:HB2	2.18	0.43
2:E:54:SER:CB	2:E:128:GLN:OE1	2.66	0.43
2:F:15:GLN:O	2:F:18:ASN:HB2	2.18	0.43
2:H:54:SER:CB	2:H:128:GLN:OE1	2.66	0.43
1:I:3:GLU:OE2	1:I:127:CYS:HB2	2.18	0.43
1:J:49:VAL:HG13	1:J:50:TYR:N	2.33	0.43
1:K:3:GLU:OE2	1:K:127:CYS:HB2	2.18	0.43
1:L:49:VAL:HG13	1:L:50:TYR:N	2.33	0.43
2:A:181:VAL:HG11	2:A:404:PHE:CZ	2.53	0.43
2:B:54:SER:CB	2:B:128:GLN:OE1	2.66	0.43
1:C:80:ALA:O	1:C:81:PHE:CB	2.67	0.43
1:D:3:GLU:OE2	1:D:127:CYS:HB2	2.18	0.43
2:F:181:VAL:HG11	2:F:404:PHE:CZ	2.54	0.43
1:I:80:ALA:O	1:I:81:PHE:CB	2.67	0.43
2:B:145:THR:HB	5:B:501:GTP:O1B	2.19	0.43
2:G:15:GLN:O	2:G:18:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:ALA:O	1:K:81:PHE:CB	2.67	0.43
2:A:180:ALA:HB3	2:A:183:GLU:HG3	2.00	0.43
1:D:80:ALA:O	1:D:81:PHE:CB	2.67	0.43
2:E:180:ALA:HB3	2:E:183:GLU:HG3	2.00	0.43
2:G:181:VAL:HG11	2:G:404:PHE:CZ	2.54	0.43
2:B:115:ILE:HD11	2:B:156:ARG:HG3	1.99	0.43
2:B:180:ALA:HB3	2:B:183:GLU:HG3	2.00	0.43
2:E:181:VAL:HG11	2:E:404:PHE:CZ	2.53	0.43
2:H:115:ILE:HD11	2:H:156:ARG:HG3	1.99	0.43
2:H:180:ALA:HB3	2:H:183:GLU:HG3	2.00	0.43
2:H:332:ILE:HG23	2:H:351:PHE:HD2	1.82	0.43
2:H:172:TYR:OH	2:H:387:ALA:HB1	2.18	0.43
2:B:181:VAL:HG11	2:B:404:PHE:CZ	2.53	0.43
2:B:182:VAL:O	2:B:182:VAL:HG22	2.19	0.43
2:B:172:TYR:OH	2:B:387:ALA:HB1	2.18	0.43
2:B:332:ILE:HG23	2:B:351:PHE:HD2	1.82	0.43
2:H:181:VAL:HG11	2:H:404:PHE:CZ	2.53	0.43
2:F:172:TYR:OH	2:F:387:ALA:HB1	2.18	0.43
2:G:172:TYR:OH	2:G:387:ALA:HB1	2.18	0.43
2:H:182:VAL:O	2:H:182:VAL:HG22	2.19	0.43
1:J:80:ALA:O	1:J:81:PHE:CB	2.67	0.43
1:L:80:ALA:O	1:L:81:PHE:CB	2.67	0.43
2:A:184:PRO:HG3	2:A:394:LYS:CE	2.49	0.43
1:D:267:MET:HE2	1:D:299:MET:HE3	2.01	0.43
2:G:115:ILE:HD11	2:G:156:ARG:HG3	1.99	0.43
2:G:332:ILE:HG23	2:G:351:PHE:HD2	1.82	0.43
2:H:283:HIS:HB2	2:E:88:HIS:HB3	2.00	0.43
2:F:179:THR:O	1:L:350:LYS:HD2	2.19	0.43
1:L:3:GLU:OE2	1:L:127:CYS:HB2	2.18	0.43
2:A:115:ILE:HD11	2:A:156:ARG:HG3	1.99	0.42
2:E:184:PRO:HG3	2:E:394:LYS:CE	2.49	0.42
2:F:115:ILE:HD11	2:F:156:ARG:HG3	1.99	0.42
2:F:332:ILE:HG23	2:F:351:PHE:HD2	1.82	0.42
2:H:184:PRO:HG3	2:H:394:LYS:CE	2.49	0.42
1:I:267:MET:HE2	1:I:299:MET:HE3	2.01	0.42
1:J:3:GLU:OE2	1:J:127:CYS:HB2	2.18	0.42
2:B:3:GLU:HG2	2:B:51:THR:HA	2.02	0.42
2:E:210:TYR:CE1	1:C:324:LYS:HB2	2.54	0.42
2:F:180:ALA:HB3	2:F:183:GLU:HG3	2.00	0.42
2:G:180:ALA:HB3	2:G:183:GLU:HG3	2.00	0.42
2:H:88:HIS:HB3	2:G:283:HIS:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:GLU:HG2	2:H:51:THR:HA	2.02	0.42
2:B:184:PRO:HG3	2:B:394:LYS:CE	2.49	0.42
2:E:3:GLU:HG2	2:E:51:THR:HA	2.01	0.42
2:F:182:VAL:O	2:F:182:VAL:HG22	2.19	0.42
2:G:182:VAL:HG22	2:G:182:VAL:O	2.19	0.42
2:F:184:PRO:HG3	2:F:394:LYS:CE	2.49	0.42
2:G:184:PRO:HG3	2:G:394:LYS:CE	2.49	0.42
2:G:3:GLU:HG2	2:G:51:THR:HA	2.02	0.42
2:A:3:GLU:HG2	2:A:51:THR:HA	2.02	0.42
2:E:115:ILE:HD11	2:E:156:ARG:HG3	2.00	0.42
2:H:283:HIS:HB3	2:E:88:HIS:HB3	2.00	0.42
2:F:3:GLU:HG2	2:F:51:THR:HA	2.02	0.42
2:H:295:CYS:HB3	2:H:377:MET:HE2	2.01	0.42
2:F:283:HIS:HB3	2:B:88:HIS:HB3	2.00	0.42
2:H:177:VAL:O	2:H:177:VAL:HG12	2.19	0.42
1:I:324:LYS:HB2	2:A:210:TYR:CE1	2.55	0.42
2:A:88:HIS:HB3	2:B:283:HIS:HB3	2.00	0.42
2:B:177:VAL:HG12	2:B:177:VAL:O	2.20	0.42
2:B:295:CYS:HB3	2:B:377:MET:HE2	2.02	0.42
2:H:179:THR:O	1:D:350:LYS:HD2	2.20	0.42
1:J:267:MET:HE1	1:J:299:MET:HE2	2.02	0.42
2:A:177:VAL:HG12	2:A:177:VAL:O	2.19	0.42
2:A:182:VAL:O	2:A:182:VAL:HG22	2.19	0.42
2:A:269:LEU:HD23	2:A:303:VAL:HB	2.01	0.42
2:B:269:LEU:HD23	2:B:303:VAL:HB	2.01	0.42
2:F:295:CYS:HB3	2:F:377:MET:HE2	2.02	0.42
2:G:295:CYS:HB3	2:G:377:MET:HE2	2.02	0.42
2:E:179:THR:O	1:C:350:LYS:HD2	2.20	0.42
1:D:317:PHE:CB	1:D:321:MET:HE1	2.43	0.42
1:D:344:TRP:NE1	1:D:345:ILE:HG13	2.35	0.42
2:E:269:LEU:HD23	2:E:303:VAL:HB	2.01	0.42
2:H:265:ILE:HG23	2:H:432:TYR:CE2	2.55	0.42
1:K:344:TRP:NE1	1:K:345:ILE:HG13	2.35	0.42
1:L:344:TRP:NE1	1:L:345:ILE:HG13	2.35	0.42
1:D:52:ASN:HB2	1:D:60:VAL:HG23	2.02	0.41
2:E:177:VAL:O	2:E:177:VAL:HG12	2.20	0.41
2:E:182:VAL:O	2:E:182:VAL:HG22	2.19	0.41
2:H:269:LEU:HD23	2:H:303:VAL:HB	2.01	0.41
1:K:317:PHE:CB	1:K:321:MET:HE1	2.43	0.41
1:C:344:TRP:NE1	1:C:345:ILE:HG13	2.35	0.41
2:G:269:LEU:HD23	2:G:303:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:322:SER:HB2	2:B:221:ARG:HB2	2.01	0.41
2:A:332:ILE:HG23	2:A:351:PHE:HD2	1.82	0.41
2:B:265:ILE:HG23	2:B:432:TYR:CE2	2.55	0.41
1:C:52:ASN:HB2	1:C:60:VAL:HG23	2.02	0.41
1:J:313:VAL:HG13	1:J:349:VAL:HA	2.02	0.41
1:J:52:ASN:HB2	1:J:60:VAL:HG23	2.02	0.41
1:L:313:VAL:HG13	1:L:349:VAL:HA	2.02	0.41
2:A:88:HIS:HB3	2:B:283:HIS:HB2	2.02	0.41
1:C:257:MET:HB3	1:C:266:PHE:HE1	1.85	0.41
2:E:265:ILE:HG23	2:E:432:TYR:CE2	2.55	0.41
2:E:332:ILE:HG23	2:E:351:PHE:HD2	1.82	0.41
1:I:52:ASN:HB2	1:I:60:VAL:HG23	2.02	0.41
1:J:344:TRP:NE1	1:J:345:ILE:HG13	2.35	0.41
1:K:52:ASN:HB2	1:K:60:VAL:HG23	2.02	0.41
1:I:323:MET:CE	2:A:179:THR:HG21	2.51	0.41
2:A:265:ILE:HG23	2:A:432:TYR:CE2	2.55	0.41
2:F:269:LEU:HD23	2:F:303:VAL:HB	2.01	0.41
1:I:344:TRP:NE1	1:I:345:ILE:HG13	2.35	0.41
1:J:323:MET:CE	2:G:179:THR:HG21	2.50	0.41
1:L:52:ASN:HB2	1:L:60:VAL:HG23	2.02	0.41
1:D:313:VAL:HG13	1:D:349:VAL:HA	2.02	0.41
1:J:257:MET:HB3	1:J:266:PHE:HE1	1.85	0.41
1:J:317:PHE:CB	1:J:321:MET:HE1	2.43	0.41
1:L:257:MET:HB3	1:L:266:PHE:HE1	1.85	0.41
1:L:317:PHE:CB	1:L:321:MET:HE1	2.43	0.41
2:G:265:ILE:HG23	2:G:432:TYR:CE2	2.55	0.41
1:I:257:MET:HB3	1:I:266:PHE:HE1	1.85	0.41
1:K:313:VAL:HG13	1:K:349:VAL:HA	2.02	0.41
2:F:265:ILE:HG23	2:F:432:TYR:CE2	2.55	0.41
1:L:267:MET:HE1	1:L:299:MET:HE2	2.03	0.41
2:H:32:PRO:O	2:H:86:LEU:CD2	2.69	0.41
2:F:210:TYR:CE1	1:L:324:LYS:HB2	2.56	0.41
2:A:217:LEU:CD2	2:A:219:ILE:HD12	2.51	0.41
2:B:32:PRO:O	2:B:86:LEU:CD2	2.69	0.41
2:E:32:PRO:O	2:E:86:LEU:CD2	2.69	0.41
2:F:177:VAL:HG12	2:F:177:VAL:O	2.20	0.41
2:F:32:PRO:O	2:F:86:LEU:CD2	2.69	0.41
2:G:177:VAL:O	2:G:177:VAL:HG12	2.20	0.41
2:G:32:PRO:O	2:G:86:LEU:CD2	2.69	0.41
1:J:143:THR:O	1:J:147:MET:HG3	2.21	0.41
1:K:257:MET:HB3	1:K:266:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:143:THR:O	1:L:147:MET:HG3	2.21	0.41
1:C:313:VAL:HG13	1:C:349:VAL:HA	2.02	0.40
1:D:257:MET:HB3	1:D:266:PHE:HE1	1.85	0.40
2:E:217:LEU:CD2	2:E:219:ILE:HD12	2.52	0.40
1:I:350:LYS:HD2	2:A:179:THR:O	2.21	0.40
2:A:32:PRO:O	2:A:86:LEU:CD2	2.69	0.40
1:I:313:VAL:HG13	1:I:349:VAL:HA	2.02	0.40
1:D:143:THR:O	1:D:147:MET:HG3	2.21	0.40
2:F:283:HIS:HB2	2:B:88:HIS:HB3	2.03	0.40
1:J:350:LYS:HD2	2:G:179:THR:O	2.21	0.40
1:K:143:THR:O	1:K:147:MET:HG3	2.21	0.40
2:G:217:LEU:CD2	2:G:219:ILE:HD12	2.51	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	C	424/426 (100%)	408 (96%)	15 (4%)	1 (0%)	52	86
1	D	424/426 (100%)	408 (96%)	15 (4%)	1 (0%)	52	86
1	I	424/426 (100%)	408 (96%)	15 (4%)	1 (0%)	52	86
1	J	424/426 (100%)	408 (96%)	15 (4%)	1 (0%)	52	86
1	K	424/426 (100%)	408 (96%)	15 (4%)	1 (0%)	52	86
1	L	424/426 (100%)	408 (96%)	15 (4%)	1 (0%)	52	86
2	A	424/437 (97%)	404 (95%)	20 (5%)	0	100	100
2	B	424/437 (97%)	404 (95%)	20 (5%)	0	100	100
2	E	424/437 (97%)	404 (95%)	20 (5%)	0	100	100
2	F	424/437 (97%)	404 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	424/437 (97%)	404 (95%)	20 (5%)	0	100 100
2	H	424/437 (97%)	404 (95%)	20 (5%)	0	100 100
All	All	5088/5178 (98%)	4872 (96%)	210 (4%)	6 (0%)	59 90

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	339	SER
1	I	339	SER
1	J	339	SER
1	C	339	SER
1	D	339	SER
1	L	339	SER

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	C	365/367 (100%)	362 (99%)	3 (1%)	86 93
1	D	365/367 (100%)	362 (99%)	3 (1%)	86 93
1	I	365/367 (100%)	362 (99%)	3 (1%)	86 93
1	J	365/367 (100%)	362 (99%)	3 (1%)	86 93
1	K	365/367 (100%)	362 (99%)	3 (1%)	86 93
1	L	365/367 (100%)	362 (99%)	3 (1%)	86 93
2	A	357/367 (97%)	351 (98%)	6 (2%)	68 88
2	B	357/367 (97%)	351 (98%)	6 (2%)	68 88
2	E	357/367 (97%)	351 (98%)	6 (2%)	68 88
2	F	357/367 (97%)	351 (98%)	6 (2%)	68 88
2	G	357/367 (97%)	351 (98%)	6 (2%)	68 88
2	H	357/367 (97%)	351 (98%)	6 (2%)	68 88
All	All	4332/4404 (98%)	4278 (99%)	54 (1%)	79 90

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	77	ARG
1	K	159	TYR
1	K	222	TYR
2	H	86	LEU
2	H	132	LEU
2	H	192	HIS
2	H	195	LEU
2	H	224	TYR
2	H	433	GLU
1	I	77	ARG
1	I	159	TYR
1	I	222	TYR
2	E	86	LEU
2	E	132	LEU
2	E	192	HIS
2	E	195	LEU
2	E	224	TYR
2	E	433	GLU
1	J	77	ARG
1	J	159	TYR
1	J	222	TYR
1	C	77	ARG
1	C	159	TYR
1	C	222	TYR
1	D	77	ARG
1	D	159	TYR
1	D	222	TYR
2	F	86	LEU
2	F	132	LEU
2	F	192	HIS
2	F	195	LEU
2	F	224	TYR
2	F	433	GLU
2	A	86	LEU
2	A	132	LEU
2	A	192	HIS
2	A	195	LEU
2	A	224	TYR
2	A	433	GLU
2	B	86	LEU
2	B	132	LEU
2	B	192	HIS

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Mol	Chain	Res	Type
2	B	195	LEU
2	B	224	TYR
2	B	433	GLU
1	L	77	ARG
1	L	159	TYR
1	L	222	TYR
2	G	86	LEU
2	G	132	LEU
2	G	192	HIS
2	G	195	LEU
2	G	224	TYR
2	G	433	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	256	ASN
1	K	347	ASN
1	K	396	HIS
2	H	31	GLN
2	H	228	ASN
1	I	256	ASN
1	I	347	ASN
1	I	396	HIS
2	E	31	GLN
2	E	228	ASN
1	J	256	ASN
1	J	347	ASN
1	J	396	HIS
1	C	256	ASN
1	C	347	ASN
1	C	396	HIS
1	D	256	ASN
1	D	347	ASN
1	D	396	HIS
2	F	31	GLN
2	F	228	ASN
2	A	31	GLN
2	A	228	ASN
2	B	31	GLN
2	B	228	ASN
1	L	256	ASN

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Mol	Chain	Res	Type
1	L	347	ASN
1	L	396	HIS
2	G	31	GLN
2	G	228	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
5	GTP	A	501	4	26,34,34	1.38	3 (11%)	29,54,54	1.91	6 (20%)
5	GTP	B	501	4	26,34,34	1.39	3 (11%)	29,54,54	1.88	6 (20%)
3	G2P	C	501	4	29,34,34	2.82	8 (27%)	31,54,54	1.29	5 (16%)
3	G2P	D	501	4	29,34,34	2.78	9 (31%)	31,54,54	1.29	5 (16%)
5	GTP	E	501	4	26,34,34	1.37	3 (11%)	29,54,54	1.93	6 (20%)
5	GTP	F	501	4	26,34,34	1.36	3 (11%)	29,54,54	1.81	6 (20%)
5	GTP	G	501	4	26,34,34	1.36	3 (11%)	29,54,54	1.84	6 (20%)
5	GTP	H	501	4	26,34,34	1.36	3 (11%)	29,54,54	1.86	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	G2P	I	501	4	29,34,34	2.84	9 (31%)	31,54,54	1.32	4 (12%)
3	G2P	J	501	4	29,34,34	2.77	8 (27%)	31,54,54	1.26	4 (12%)
3	G2P	K	501	4	29,34,34	2.80	9 (31%)	31,54,54	1.30	4 (12%)
3	G2P	L	501	4	29,34,34	2.80	9 (31%)	31,54,54	1.28	4 (12%)

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
5	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	GTP	B	501	4	-	0/18/38/38	0/3/3/3
3	G2P	C	501	4	-	0/18/38/38	0/3/3/3
3	G2P	D	501	4	-	0/18/38/38	0/3/3/3
5	GTP	E	501	4	-	0/18/38/38	0/3/3/3
5	GTP	F	501	4	-	0/18/38/38	0/3/3/3
5	GTP	G	501	4	-	0/18/38/38	0/3/3/3
5	GTP	H	501	4	-	0/18/38/38	0/3/3/3
3	G2P	I	501	4	-	0/18/38/38	0/3/3/3
3	G2P	J	501	4	-	0/18/38/38	0/3/3/3
3	G2P	K	501	4	-	0/18/38/38	0/3/3/3
3	G2P	L	501	4	-	0/18/38/38	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	501	G2P	C4-N9	-10.61	1.33	1.47
3	C	501	G2P	C4-N9	-10.48	1.33	1.47
3	K	501	G2P	C4-N9	-10.40	1.33	1.47
3	D	501	G2P	C4-N9	-10.36	1.33	1.47
3	L	501	G2P	C4-N9	-10.32	1.34	1.47
3	J	501	G2P	C4-N9	-10.28	1.34	1.47
3	I	501	G2P	C8-N9	-3.82	1.35	1.47
3	K	501	G2P	C8-N9	-3.81	1.35	1.47
3	L	501	G2P	C8-N9	-3.79	1.35	1.47
3	C	501	G2P	C8-N9	-3.76	1.35	1.47
3	J	501	G2P	C8-N9	-3.75	1.35	1.47
3	D	501	G2P	C8-N9	-3.73	1.35	1.47
3	I	501	G2P	PB-O1B	-3.36	1.48	1.56
3	J	501	G2P	PB-O1B	-3.35	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	501	G2P	PB-O1B	-3.34	1.48	1.56
3	C	501	G2P	PB-O1B	-3.33	1.48	1.56
3	L	501	G2P	PA-O1A	-3.33	1.48	1.56
3	L	501	G2P	PB-O1B	-3.33	1.48	1.56
3	I	501	G2P	PA-O1A	-3.33	1.48	1.56
3	J	501	G2P	PA-O1A	-3.32	1.48	1.56
3	D	501	G2P	PA-O1A	-3.32	1.48	1.56
3	D	501	G2P	PB-O1B	-3.31	1.48	1.56
3	C	501	G2P	PA-O1A	-3.30	1.48	1.56
3	K	501	G2P	PA-O1A	-3.28	1.48	1.56
3	D	501	G2P	PB-O3B	2.00	1.60	1.58
3	I	501	G2P	PB-O3B	2.11	1.60	1.58
3	K	501	G2P	PB-O3B	2.20	1.60	1.58
3	L	501	G2P	PB-O3B	2.26	1.61	1.58
5	G	501	GTP	O4'-C1'	2.27	1.44	1.41
5	F	501	GTP	O4'-C1'	2.37	1.44	1.41
5	H	501	GTP	O4'-C1'	2.39	1.44	1.41
5	A	501	GTP	O4'-C1'	2.46	1.44	1.41
5	B	501	GTP	O4'-C1'	2.48	1.44	1.41
5	E	501	GTP	O4'-C1'	2.50	1.44	1.41
5	E	501	GTP	C5-C4	3.39	1.48	1.40
5	F	501	GTP	C5-C4	3.42	1.48	1.40
5	G	501	GTP	C5-C4	3.42	1.48	1.40
5	B	501	GTP	C5-C4	3.43	1.48	1.40
5	A	501	GTP	C5-C4	3.46	1.48	1.40
5	H	501	GTP	C5-C4	3.47	1.48	1.40
3	I	501	G2P	PB-O2B	3.64	1.61	1.51
3	J	501	G2P	PB-O2B	3.69	1.61	1.51
3	L	501	G2P	PB-O2B	3.69	1.61	1.51
3	C	501	G2P	PB-O2B	3.69	1.61	1.51
3	K	501	G2P	PB-O2B	3.70	1.61	1.51
3	D	501	G2P	PB-O2B	3.72	1.61	1.51
3	D	501	G2P	PA-O5'	3.80	1.61	1.57
3	K	501	G2P	PA-O2A	3.86	1.61	1.51
3	K	501	G2P	PA-O5'	3.88	1.61	1.57
3	D	501	G2P	PA-O2A	3.88	1.61	1.51
3	J	501	G2P	PA-O2A	3.89	1.61	1.51
3	I	501	G2P	PA-O2A	3.90	1.61	1.51
3	L	501	G2P	PA-O2A	3.91	1.61	1.51
3	C	501	G2P	PA-O2A	3.91	1.61	1.51
3	C	501	G2P	PA-O5'	4.01	1.61	1.57
3	J	501	G2P	PA-O5'	4.04	1.61	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	G2P	PA-O5'	4.17	1.61	1.57
3	I	501	G2P	PA-O5'	4.20	1.61	1.57
3	J	501	G2P	C1'-N9	4.24	1.50	1.42
3	L	501	G2P	C1'-N9	4.27	1.50	1.42
3	D	501	G2P	C1'-N9	4.39	1.50	1.42
3	K	501	G2P	C1'-N9	4.49	1.50	1.42
3	I	501	G2P	C1'-N9	4.53	1.50	1.42
3	C	501	G2P	C1'-N9	4.58	1.50	1.42
5	E	501	GTP	C6-C5	4.74	1.50	1.41
5	H	501	GTP	C6-C5	4.75	1.50	1.41
5	F	501	GTP	C6-C5	4.81	1.51	1.41
5	G	501	GTP	C6-C5	4.82	1.51	1.41
5	A	501	GTP	C6-C5	4.82	1.51	1.41
5	B	501	GTP	C6-C5	4.87	1.51	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	501	GTP	C5-C6-N1	-4.59	117.52	123.52
5	B	501	GTP	C5-C6-N1	-4.52	117.61	123.52
5	A	501	GTP	C5-C6-N1	-4.46	117.69	123.52
5	H	501	GTP	C5-C6-N1	-4.29	117.91	123.52
5	G	501	GTP	C5-C6-N1	-4.26	117.95	123.52
5	F	501	GTP	C5-C6-N1	-4.25	117.96	123.52
3	I	501	G2P	O6-C6-N1	-3.67	117.98	122.80
3	K	501	G2P	O6-C6-N1	-3.56	118.12	122.80
3	L	501	G2P	O6-C6-N1	-3.51	118.19	122.80
3	C	501	G2P	O6-C6-N1	-3.40	118.33	122.80
5	G	501	GTP	N3-C2-N1	-3.38	122.97	127.56
5	A	501	GTP	N3-C2-N1	-3.37	122.97	127.56
5	H	501	GTP	N3-C2-N1	-3.37	122.98	127.56
5	E	501	GTP	N3-C2-N1	-3.36	122.98	127.56
3	D	501	G2P	O6-C6-N1	-3.36	118.39	122.80
5	B	501	GTP	N3-C2-N1	-3.33	123.02	127.56
3	J	501	G2P	O6-C6-N1	-3.25	118.54	122.80
5	F	501	GTP	N3-C2-N1	-3.20	123.21	127.56
5	H	501	GTP	C6-C5-C4	-2.76	117.70	120.86
5	G	501	GTP	C6-C5-C4	-2.74	117.73	120.86
5	F	501	GTP	C6-C5-C4	-2.70	117.78	120.86
5	A	501	GTP	C6-C5-C4	-2.63	117.85	120.86
5	B	501	GTP	C6-C5-C4	-2.58	117.91	120.86
5	E	501	GTP	C6-C5-C4	-2.44	118.07	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	501	G2P	C8-N9-C4	2.03	107.10	104.78
3	D	501	G2P	O1A-PA-O5'	2.05	111.88	106.69
3	C	501	G2P	C8-N9-C4	2.10	107.17	104.78
3	C	501	G2P	O1A-PA-O5'	2.13	112.08	106.69
3	J	501	G2P	O6-C6-C5	2.19	123.88	119.69
3	K	501	G2P	C8-N9-C4	2.19	107.28	104.78
3	D	501	G2P	C8-N9-C4	2.33	107.44	104.78
3	J	501	G2P	C3'-C2'-C1'	2.35	106.16	101.44
3	L	501	G2P	C8-N9-C4	2.36	107.48	104.78
3	L	501	G2P	C3'-C2'-C1'	2.37	106.21	101.44
3	D	501	G2P	O6-C6-C5	2.38	124.25	119.69
3	L	501	G2P	O6-C6-C5	2.44	124.36	119.69
5	B	501	GTP	O3G-PG-O2G	2.47	116.49	107.44
3	C	501	G2P	O6-C6-C5	2.47	124.42	119.69
5	H	501	GTP	O3G-PG-O2G	2.48	116.55	107.44
3	D	501	G2P	C3'-C2'-C1'	2.48	106.43	101.44
3	I	501	G2P	C3'-C2'-C1'	2.49	106.45	101.44
5	F	501	GTP	O3G-PG-O2G	2.50	116.62	107.44
5	G	501	GTP	O3G-PG-O2G	2.53	116.73	107.44
3	J	501	G2P	C8-N9-C4	2.54	107.68	104.78
3	K	501	G2P	C3'-C2'-C1'	2.54	106.55	101.44
5	A	501	GTP	O3G-PG-O2G	2.56	116.86	107.44
5	E	501	GTP	O3G-PG-O2G	2.58	116.90	107.44
3	K	501	G2P	O6-C6-C5	2.60	124.66	119.69
3	C	501	G2P	C3'-C2'-C1'	2.63	106.72	101.44
3	I	501	G2P	O6-C6-C5	2.76	124.96	119.69
5	G	501	GTP	C4'-O4'-C1'	2.96	112.78	109.64
5	F	501	GTP	C4'-O4'-C1'	3.07	112.90	109.64
5	H	501	GTP	C4'-O4'-C1'	3.20	113.03	109.64
5	B	501	GTP	C4'-O4'-C1'	3.40	113.25	109.64
5	A	501	GTP	C4'-O4'-C1'	3.52	113.38	109.64
5	E	501	GTP	C4'-O4'-C1'	3.89	113.76	109.64
5	F	501	GTP	C6-N1-C2	5.13	121.89	115.88
5	G	501	GTP	C6-N1-C2	5.27	122.05	115.88
5	H	501	GTP	C6-N1-C2	5.31	122.11	115.88
5	B	501	GTP	C6-N1-C2	5.33	122.13	115.88
5	A	501	GTP	C6-N1-C2	5.40	122.21	115.88
5	E	501	GTP	C6-N1-C2	5.42	122.23	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
5	B	501	GTP	1	0
5	E	501	GTP	1	0
5	F	501	GTP	1	0
5	G	501	GTP	1	0
5	H	501	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.