



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 05:26 AM GMT

PDB ID : 1I33  
Title : LEISHMANIA MEXICANA GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE IN COMPLEX WITH INHIBITORS  
Authors : Suresh, S.; Bressi, J.C.; Kennedy, K.J.; Verlinde, C.L.M.J.; Gelb, M.H.; Hol, W.G.J.  
Deposited on : 2001-02-12  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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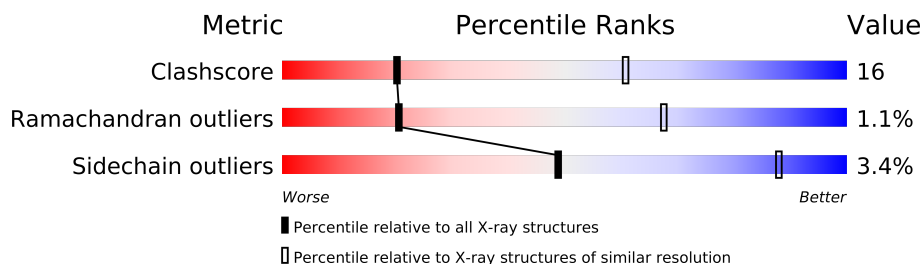
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	
1	B	360	
1	C	360	
1	D	360	
1	E	360	
1	F	360	

## 2 Entry composition i

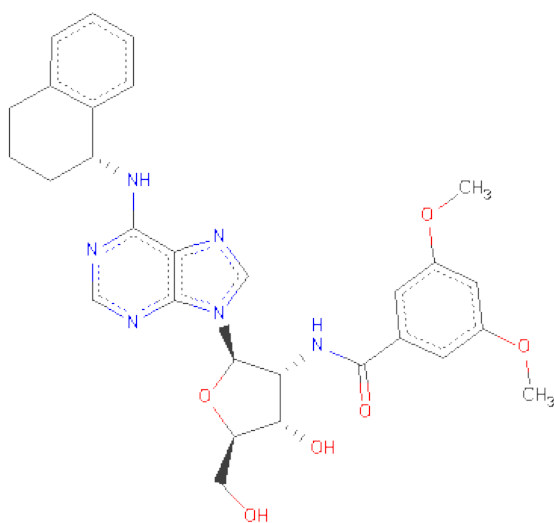
There are 2 unique types of molecules in this entry. The entry contains 16536 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	B	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	C	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	D	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	E	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	F	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			

- Molecule 2 is N-1,2,3,4-TETRAHYDRONAPHTH-1-YL-2'-[3,5-DIMETHOXYBENZAMID O]-2'-DEOXY-ADENOSINE (three-letter code: TND) (formula: C<sub>29</sub>H<sub>32</sub>N<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 41	C 29	N 6	O 6	0	0
2	B	1	Total 41	C 29	N 6	O 6	0	0
2	C	1	Total 41	C 29	N 6	O 6	0	0
2	D	1	Total 41	C 29	N 6	O 6	0	0
2	E	1	Total 41	C 29	N 6	O 6	0	0
2	F	1	Total 41	C 29	N 6	O 6	0	0

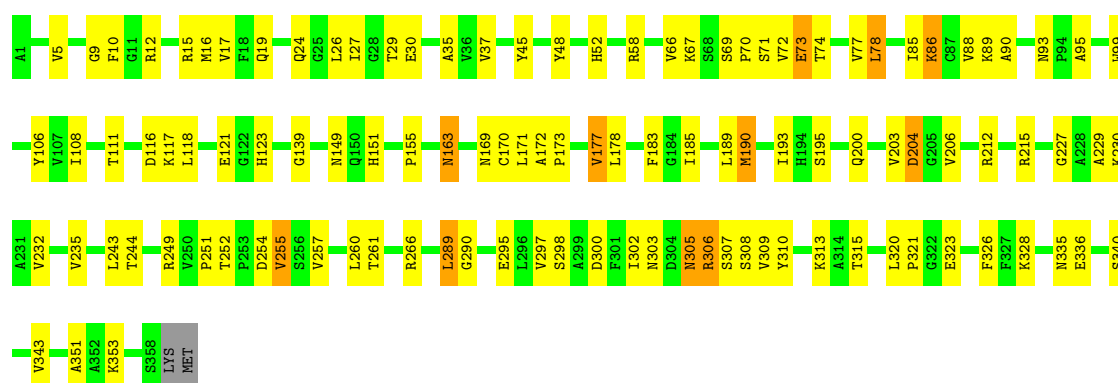
### 3 Residue-property plots

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

Note EDS was not executed.

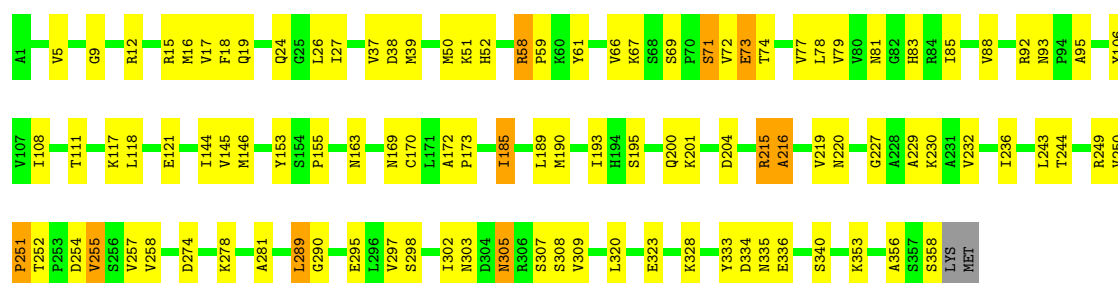
#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

Chain A: 



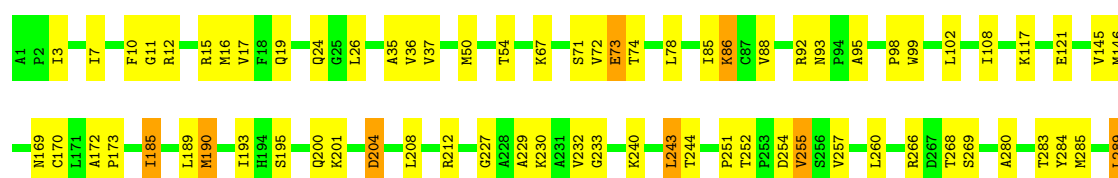
#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

Chain B: 



#### • Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

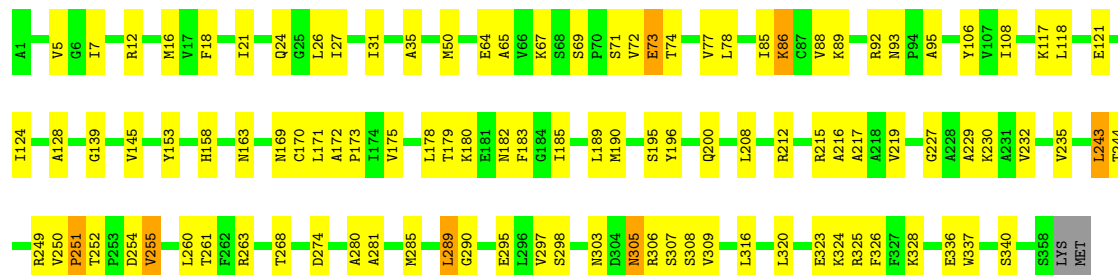
Chain C: 





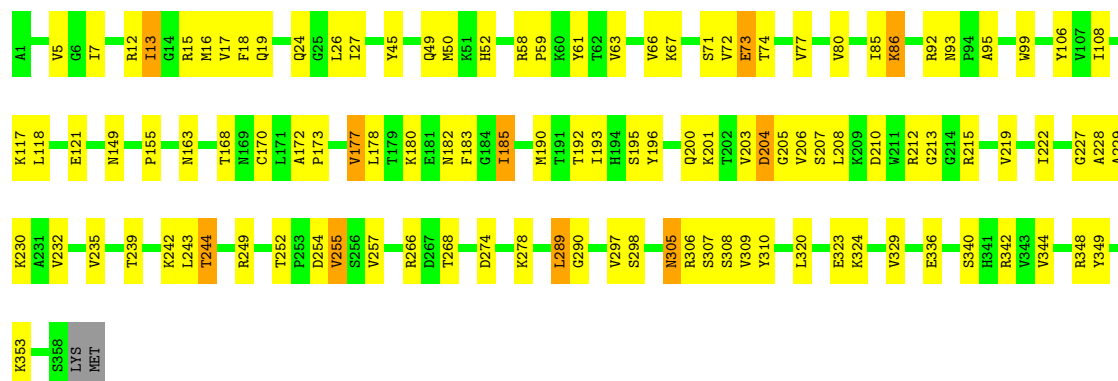
• Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

Chain D:



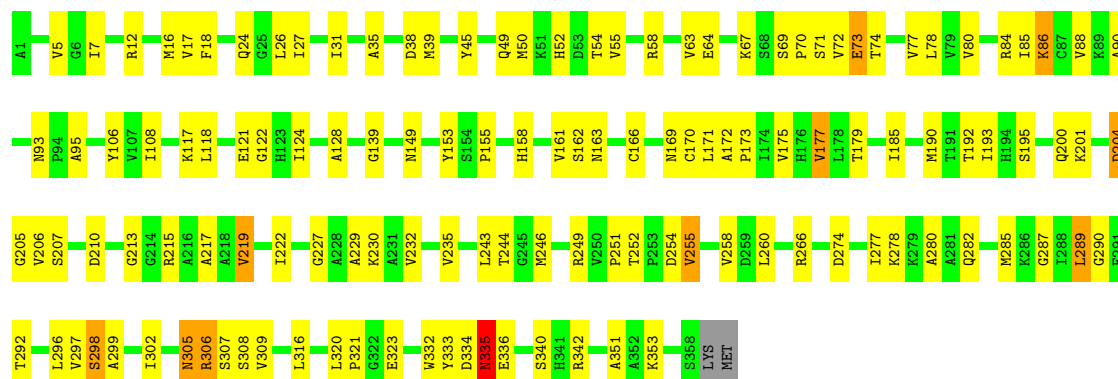
• Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

Chain E:



• Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

Chain F:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.52Å 393.56Å 70.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.211 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/2767	0.57	0/3752
1	B	0.41	0/2767	0.60	0/3752
1	C	0.43	0/2767	0.59	0/3752
1	D	0.40	0/2767	0.58	0/3752
1	E	0.39	0/2767	0.57	0/3752
1	F	0.37	0/2767	0.54	0/3752
All	All	0.40	0/16602	0.58	0/22512

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2715	0	2736	92	0
1	B	2715	0	2736	87	0
1	C	2715	0	2736	72	0
1	D	2715	0	2736	90	0
1	E	2715	0	2736	98	0
1	F	2715	0	2736	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	41	0	32	0	0
2	B	41	0	32	3	0
2	C	41	0	32	4	0
2	D	41	0	32	2	0
2	E	41	0	32	4	0
2	F	41	0	32	2	0
All	All	16536	0	16608	525	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (525) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:73:GLU:HG2	1:C:74:THR:HG23	1.44	0.98
1:E:73:GLU:HG2	1:E:74:THR:HG23	1.46	0.96
1:E:206:VAL:HG13	1:F:45:TYR:HE2	1.33	0.91
1:E:93:ASN:ND2	1:E:95:ALA:HB3	1.86	0.90
1:A:73:GLU:HG2	1:A:74:THR:HG23	1.54	0.89
1:B:73:GLU:HG2	1:B:74:THR:HG23	1.56	0.87
1:D:93:ASN:HD21	1:D:95:ALA:HB3	1.37	0.87
1:D:77:VAL:HG22	1:D:86:LYS:HE3	1.57	0.87
1:B:232:VAL:HG11	1:B:243:LEU:HD23	1.58	0.86
1:D:73:GLU:HG2	1:D:74:THR:HG23	1.55	0.86
1:E:93:ASN:HD21	1:E:95:ALA:HB3	1.41	0.84
1:B:229:ALA:O	1:B:232:VAL:HG12	1.78	0.84
1:F:73:GLU:HG2	1:F:74:THR:HG23	1.60	0.82
1:B:93:ASN:ND2	1:B:95:ALA:HB3	1.94	0.81
1:D:232:VAL:HG11	1:D:243:LEU:HD23	1.63	0.81
1:C:229:ALA:O	1:C:232:VAL:HG12	1.81	0.81
1:A:93:ASN:ND2	1:A:95:ALA:HB3	1.97	0.80
1:B:93:ASN:HD21	1:B:95:ALA:HB3	1.46	0.79
1:A:251:PRO:HB2	1:D:251:PRO:HB2	1.65	0.79
1:B:195:SER:HB3	1:B:252:THR:O	1.83	0.78
1:F:172:ALA:HB3	1:F:173:PRO:HD3	1.63	0.78
1:A:171:LEU:HD11	1:A:260:LEU:HD22	1.67	0.77
1:D:229:ALA:O	1:D:232:VAL:HG12	1.84	0.76
1:B:251:PRO:HB2	1:C:251:PRO:HB2	1.64	0.76
1:A:328:LYS:HB2	1:D:189:LEU:HD23	1.66	0.76
1:A:172:ALA:HB3	1:A:173:PRO:HD3	1.68	0.75
1:F:229:ALA:O	1:F:232:VAL:HG12	1.87	0.75
1:D:93:ASN:ND2	1:D:95:ALA:HB3	2.01	0.75
1:E:5:VAL:HG12	1:E:106:TYR:HB2	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:172:ALA:HB3	1:D:173:PRO:HD3	1.71	0.73
1:C:195:SER:HB3	1:C:252:THR:O	1.88	0.73
1:A:229:ALA:O	1:A:232:VAL:HG12	1.89	0.73
1:F:93:ASN:HD21	1:F:95:ALA:HB3	1.52	0.73
1:C:185:ILE:HD11	1:C:243:LEU:HD11	1.72	0.72
1:B:189:LEU:HD23	1:C:328:LYS:HB2	1.71	0.72
1:E:229:ALA:O	1:E:232:VAL:HG12	1.90	0.72
1:E:344:VAL:O	1:E:348:ARG:HG3	1.89	0.72
1:F:171:LEU:HD11	1:F:260:LEU:HD22	1.72	0.71
1:E:52:HIS:HB3	1:F:215:ARG:NH2	2.06	0.71
1:B:328:LYS:HB2	1:C:189:LEU:HD23	1.73	0.71
1:F:170:CYS:HA	1:F:308:SER:HB2	1.73	0.71
1:A:185:ILE:HD11	1:A:243:LEU:HD11	1.74	0.69
1:F:16:MET:HB3	1:F:340:SER:OG	1.92	0.69
1:F:77:VAL:HG22	1:F:86:LYS:HE3	1.73	0.69
1:F:232:VAL:HG11	1:F:243:LEU:HD23	1.75	0.69
1:F:93:ASN:ND2	1:F:95:ALA:HB3	2.07	0.68
1:C:172:ALA:HB3	1:C:173:PRO:HD3	1.76	0.68
1:F:185:ILE:HD11	1:F:243:LEU:HD11	1.76	0.68
1:A:24:GLN:CB	1:A:26:LEU:HD13	2.23	0.67
1:A:189:LEU:HD23	1:D:328:LYS:HB2	1.75	0.67
1:D:195:SER:HB3	1:D:252:THR:O	1.95	0.67
1:E:207:SER:N	1:F:45:TYR:OH	2.28	0.67
1:D:175:VAL:O	1:D:179:THR:HG23	1.96	0.66
1:C:227:GLY:HA3	1:C:230:LYS:HE2	1.78	0.66
1:E:289:LEU:HD23	1:E:308:SER:O	1.95	0.66
1:F:201:LYS:HG2	1:F:205:GLY:HA3	1.78	0.66
1:B:227:GLY:HA3	1:B:230:LYS:HE2	1.77	0.66
1:D:24:GLN:HB3	1:D:26:LEU:HD13	1.77	0.64
1:A:232:VAL:HG11	1:A:243:LEU:HD23	1.80	0.64
1:E:320:LEU:HB2	1:E:323:GLU:HB2	1.78	0.64
1:E:307:SER:OG	1:E:342:ARG:HD2	1.98	0.64
1:E:195:SER:HB3	1:E:252:THR:O	1.98	0.64
1:D:5:VAL:HG12	1:D:106:TYR:HB2	1.80	0.64
1:B:73:GLU:H	1:B:73:GLU:CD	2.02	0.64
1:C:169:ASN:O	1:C:307:SER:HB3	1.97	0.63
1:C:289:LEU:HD23	1:C:308:SER:O	1.98	0.63
1:C:302:ILE:O	1:C:303:ASN:HB2	1.98	0.63
1:F:35:ALA:HB2	1:F:86:LYS:HB2	1.79	0.63
1:D:117:LYS:HB3	1:D:139:GLY:HA3	1.81	0.63
1:A:290:GLY:HA3	1:A:306:ARG:NH1	2.14	0.63
1:C:232:VAL:HG11	1:C:243:LEU:HD23	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:ASP:OD1	1:B:215:ARG:HD2	1.99	0.62
1:A:171:LEU:CD1	1:A:260:LEU:HD22	2.29	0.62
1:D:16:MET:HB3	1:D:340:SER:OG	2.00	0.62
1:D:171:LEU:HD11	1:D:260:LEU:HD22	1.83	0.61
1:C:92:ARG:HG2	2:C:363:TND:C5	2.30	0.61
1:F:287:GLY:O	1:F:306:ARG:HG3	2.01	0.61
1:C:35:ALA:HB2	1:C:86:LYS:HB2	1.81	0.61
1:D:86:LYS:HE2	1:D:86:LYS:HA	1.83	0.60
1:D:185:ILE:HD11	1:D:243:LEU:HD11	1.83	0.60
1:F:67:LYS:HB3	1:F:72:VAL:CG2	2.31	0.60
1:C:170:CYS:HA	1:C:308:SER:HB2	1.82	0.60
1:F:69:SER:C	1:F:71:SER:H	2.03	0.60
1:B:193:ILE:HB	1:B:257:VAL:HG12	1.81	0.60
1:B:15:ARG:O	1:B:19:GLN:HG3	2.01	0.60
1:F:258:VAL:HG23	1:F:333:TYR:HE1	1.67	0.60
1:A:99:TRP:NE1	1:A:123:HIS:ND1	2.46	0.60
1:B:215:ARG:NH2	1:C:300:ASP:OD1	2.33	0.59
1:B:232:VAL:HG11	1:B:243:LEU:CD2	2.30	0.59
1:F:24:GLN:CB	1:F:26:LEU:HD13	2.32	0.59
1:B:169:ASN:O	1:B:307:SER:HB3	2.02	0.59
1:B:170:CYS:HA	1:B:308:SER:HB2	1.84	0.59
1:C:93:ASN:ND2	1:C:95:ALA:HB3	2.16	0.59
1:C:117:LYS:O	1:C:121:GLU:HG3	2.01	0.59
1:B:320:LEU:HB2	1:B:323:GLU:HB2	1.85	0.59
1:B:24:GLN:CB	1:B:26:LEU:HD13	2.33	0.59
1:D:117:LYS:O	1:D:121:GLU:HG3	2.03	0.59
1:E:201:LYS:N	1:E:201:LYS:HD2	2.18	0.59
1:A:117:LYS:HB3	1:A:139:GLY:HA3	1.84	0.59
1:A:12:ARG:HD3	1:B:204:ASP:O	2.03	0.59
1:D:227:GLY:HA3	1:D:230:LYS:HE2	1.85	0.58
1:A:93:ASN:HD21	1:A:95:ALA:HB3	1.68	0.58
1:B:185:ILE:HD11	1:B:243:LEU:HD11	1.85	0.58
1:D:320:LEU:HB2	1:D:323:GLU:HB2	1.85	0.58
1:F:169:ASN:O	1:F:307:SER:HB3	2.02	0.58
1:D:69:SER:C	1:D:71:SER:H	2.07	0.58
1:C:254:ASP:O	1:C:255:VAL:HB	2.04	0.58
1:F:117:LYS:O	1:F:121:GLU:HG3	2.03	0.58
1:F:193:ILE:HD12	1:F:193:ILE:N	2.19	0.58
1:A:27:ILE:O	1:A:27:ILE:HG23	2.03	0.58
1:A:254:ASP:OD1	1:A:336:GLU:HG3	2.04	0.58
1:A:155:PRO:HG3	1:A:353:LYS:HG2	1.86	0.58
1:C:67:LYS:HB3	1:C:72:VAL:CG2	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:ILE:HB	1:A:257:VAL:HG12	1.86	0.57
1:A:195:SER:HB3	1:A:252:THR:O	2.03	0.57
1:E:67:LYS:HB3	1:E:72:VAL:HG22	1.85	0.57
1:B:67:LYS:HD3	1:B:72:VAL:HG23	1.87	0.57
1:E:232:VAL:HG11	1:E:243:LEU:HD23	1.86	0.57
1:D:24:GLN:CB	1:D:26:LEU:HD13	2.34	0.57
1:D:12:ARG:HH21	1:D:336:GLU:CD	2.08	0.57
1:A:24:GLN:HB2	1:A:26:LEU:HD13	1.85	0.56
1:B:227:GLY:O	1:B:230:LYS:HG2	2.06	0.56
1:D:67:LYS:HB3	1:D:72:VAL:CG2	2.34	0.56
1:E:63:VAL:HG22	1:E:80:VAL:HG22	1.88	0.56
1:A:300:ASP:OD1	1:D:215:ARG:NH2	2.39	0.56
1:A:266:ARG:HH11	1:A:266:ARG:HG3	1.70	0.56
1:D:67:LYS:HB3	1:D:72:VAL:HG22	1.88	0.56
1:A:66:VAL:HG23	1:A:77:VAL:HB	1.86	0.56
1:F:227:GLY:HA3	1:F:230:LYS:HE2	1.88	0.56
1:C:227:GLY:CA	1:C:230:LYS:HE2	2.36	0.56
2:F:366:TND:H1	2:F:366:TND:N7A	2.20	0.56
1:A:215:ARG:NH2	1:B:52:HIS:HB3	2.22	0.55
1:A:24:GLN:HB3	1:A:26:LEU:HD13	1.87	0.55
1:A:17:VAL:HG11	1:A:108:ILE:HD13	1.88	0.55
1:A:106:TYR:OH	1:A:351:ALA:HA	2.07	0.55
1:F:86:LYS:HA	1:F:86:LYS:HE2	1.89	0.55
1:E:16:MET:HB3	1:E:340:SER:OG	2.06	0.55
1:F:232:VAL:HG11	1:F:243:LEU:CD2	2.36	0.55
1:A:12:ARG:HH21	1:A:336:GLU:CD	2.10	0.55
1:A:69:SER:C	1:A:71:SER:H	2.10	0.55
1:E:349:TYR:OH	1:E:353:LYS:HE3	2.07	0.54
1:E:172:ALA:HB3	1:E:173:PRO:HD3	1.89	0.54
1:B:37:VAL:HG22	1:B:88:VAL:HB	1.89	0.54
1:F:258:VAL:HG23	1:F:333:TYR:CE1	2.43	0.54
1:B:16:MET:HB3	1:B:340:SER:OG	2.06	0.54
1:D:86:LYS:HE2	1:D:86:LYS:CA	2.38	0.54
1:A:155:PRO:CG	1:A:353:LYS:HG2	2.37	0.54
1:E:45:TYR:HE2	1:F:206:VAL:HG13	1.73	0.54
2:C:363:TND:H3B	1:D:208:LEU:HD12	1.89	0.54
1:A:10:PHE:CE2	1:A:15:ARG:HG2	2.43	0.54
1:D:7:ILE:CD1	1:D:108:ILE:HD12	2.38	0.54
1:F:24:GLN:HB2	1:F:26:LEU:HD13	1.90	0.54
1:F:69:SER:O	1:F:71:SER:N	2.41	0.53
1:C:24:GLN:CB	1:C:26:LEU:HD13	2.37	0.53
1:D:281:ALA:HB2	1:D:289:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:161:VAL:HG12	1:F:162:SER:N	2.24	0.53
1:F:227:GLY:CA	1:F:230:LYS:HE2	2.38	0.53
1:E:92:ARG:HG2	2:E:365:TND:C5	2.39	0.53
1:E:24:GLN:CB	1:E:26:LEU:HD13	2.38	0.53
1:B:117:LYS:O	1:B:121:GLU:HG3	2.07	0.53
1:A:320:LEU:HB2	1:A:323:GLU:HB2	1.90	0.53
1:F:307:SER:OG	1:F:342:ARG:HD2	2.09	0.53
1:D:69:SER:O	1:D:71:SER:N	2.41	0.53
1:B:172:ALA:HB3	1:B:173:PRO:HD3	1.90	0.53
1:D:145:VAL:HG23	1:D:235:VAL:HG21	1.89	0.53
1:B:219:VAL:O	1:B:219:VAL:HG22	2.07	0.53
1:A:52:HIS:HB3	1:B:215:ARG:NH2	2.23	0.53
1:C:268:THR:O	1:C:324:LYS:HA	2.09	0.53
1:E:193:ILE:HD12	1:E:193:ILE:N	2.24	0.53
1:F:67:LYS:HB3	1:F:72:VAL:HG22	1.89	0.53
1:E:45:TYR:OH	1:F:207:SER:N	2.40	0.53
1:B:17:VAL:HG11	1:B:108:ILE:HD13	1.91	0.53
1:F:297:VAL:O	1:F:298:SER:C	2.46	0.53
1:E:206:VAL:HG13	1:F:45:TYR:CE2	2.25	0.53
1:A:261:THR:HG21	1:D:261:THR:HG21	1.90	0.53
1:A:170:CYS:HA	1:A:308:SER:HB2	1.91	0.53
1:A:16:MET:HB3	1:A:340:SER:OG	2.09	0.53
1:F:38:ASP:C	1:F:90:ALA:HB2	2.29	0.52
1:B:18:PHE:HE2	1:B:50:MET:HE1	1.74	0.52
1:B:305:ASN:HD22	1:B:305:ASN:C	2.11	0.52
1:F:86:LYS:CA	1:F:86:LYS:HE2	2.39	0.52
2:C:363:TND:H3B	1:D:208:LEU:CD1	2.39	0.52
1:E:15:ARG:O	1:E:19:GLN:HG3	2.09	0.52
1:C:7:ILE:CD1	1:C:108:ILE:HD12	2.40	0.52
1:A:254:ASP:O	1:A:255:VAL:HB	2.09	0.52
1:E:155:PRO:CG	1:E:353:LYS:HG2	2.39	0.52
1:E:254:ASP:O	1:E:255:VAL:HB	2.10	0.52
1:C:349:TYR:OH	1:C:353:LYS:HE3	2.08	0.52
1:B:69:SER:C	1:B:71:SER:H	2.12	0.52
1:F:90:ALA:HB1	2:F:366:TND:H8	1.92	0.52
1:A:163:ASN:OD1	1:A:343:VAL:HA	2.10	0.52
1:B:73:GLU:CD	1:B:73:GLU:N	2.63	0.52
1:B:229:ALA:HB1	1:B:244:THR:HA	1.90	0.52
1:B:24:GLN:HB2	1:B:26:LEU:HD13	1.92	0.52
1:D:69:SER:C	1:D:71:SER:N	2.62	0.52
1:C:67:LYS:HB3	1:C:72:VAL:HG22	1.92	0.52
1:D:18:PHE:HE2	1:D:50:MET:HE1	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:185:ILE:HG23	1:B:185:ILE:O	2.09	0.51
1:F:38:ASP:OD1	1:F:39:MET:N	2.42	0.51
1:E:239:THR:HA	1:E:242:LYS:HD2	1.92	0.51
1:C:290:GLY:O	1:C:309:VAL:HA	2.10	0.51
1:B:227:GLY:CA	1:B:230:LYS:HE2	2.40	0.51
1:B:69:SER:C	1:B:71:SER:N	2.63	0.51
1:B:67:LYS:HB3	1:B:72:VAL:CG2	2.40	0.51
1:B:69:SER:O	1:B:71:SER:N	2.43	0.51
1:C:190:MET:HB3	1:C:260:LEU:HD13	1.92	0.51
1:F:153:TYR:CE1	1:F:158:HIS:HB2	2.45	0.51
1:C:12:ARG:HH21	1:C:336:GLU:CD	2.14	0.51
1:B:5:VAL:HG12	1:B:106:TYR:HB2	1.92	0.51
1:C:193:ILE:HB	1:C:257:VAL:CG1	2.41	0.51
1:B:27:ILE:HG23	1:B:27:ILE:O	2.11	0.51
1:F:69:SER:C	1:F:71:SER:N	2.63	0.51
1:A:69:SER:O	1:A:71:SER:N	2.44	0.51
1:E:219:VAL:HG22	1:E:219:VAL:O	2.11	0.51
1:B:302:ILE:O	1:B:303:ASN:HB2	2.11	0.51
1:F:106:TYR:OH	1:F:351:ALA:HA	2.11	0.51
1:E:227:GLY:HA3	1:E:230:LYS:HE2	1.92	0.51
1:E:99:TRP:CE3	1:E:99:TRP:HA	2.46	0.51
1:C:227:GLY:O	1:C:230:LYS:HG2	2.11	0.50
1:B:200:GLN:OE1	1:B:249:ARG:NH1	2.44	0.50
1:F:18:PHE:CZ	1:F:80:VAL:HG21	2.46	0.50
2:C:363:TND:N7A	2:C:363:TND:H1	2.26	0.50
1:D:170:CYS:HA	1:D:308:SER:HB2	1.93	0.50
1:B:73:GLU:CD	1:B:74:THR:H	2.14	0.50
1:E:7:ILE:HD13	1:E:108:ILE:HB	1.93	0.50
1:E:193:ILE:HB	1:E:257:VAL:HG12	1.93	0.50
1:B:12:ARG:HH21	1:B:336:GLU:CD	2.14	0.50
1:F:320:LEU:HB2	1:F:323:GLU:HB2	1.93	0.50
1:F:254:ASP:O	1:F:255:VAL:HB	2.11	0.50
1:E:12:ARG:HD3	1:F:204:ASP:O	2.10	0.50
1:F:280:ALA:O	1:F:285:MET:HB2	2.12	0.50
1:C:268:THR:OG1	1:C:269:SER:N	2.43	0.50
1:A:310:TYR:HE1	1:A:315:THR:HG1	1.60	0.50
1:F:195:SER:HB3	1:F:252:THR:O	2.12	0.50
1:E:206:VAL:HG22	1:F:49:GLN:OE1	2.12	0.50
1:B:193:ILE:HD12	1:B:193:ILE:N	2.26	0.50
1:A:323:GLU:HG2	1:A:326:PHE:O	2.12	0.49
1:F:35:ALA:HB1	1:F:88:VAL:HG23	1.95	0.49
1:B:274:ASP:O	1:B:278:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:27:ILE:HG23	1:F:27:ILE:O	2.13	0.49
1:D:77:VAL:CG2	1:D:86:LYS:HE3	2.36	0.49
1:F:266:ARG:HG3	1:F:266:ARG:HH11	1.78	0.49
1:F:73:GLU:CD	1:F:73:GLU:H	2.15	0.49
1:E:92:ARG:HE	2:E:365:TND:H5	1.78	0.49
1:F:219:VAL:O	1:F:219:VAL:HG22	2.13	0.49
1:B:66:VAL:HG23	1:B:77:VAL:HB	1.94	0.49
1:E:168:THR:OG1	1:E:228:ALA:HA	2.13	0.49
1:D:185:ILE:O	1:D:185:ILE:HG23	2.12	0.49
1:F:124:ILE:HG23	1:F:128:ALA:O	2.13	0.49
1:E:208:LEU:HD23	1:F:45:TYR:HB2	1.95	0.48
1:D:35:ALA:HB2	1:D:86:LYS:HB2	1.95	0.48
1:E:201:LYS:HB3	1:E:203:VAL:O	2.13	0.48
1:A:295:GLU:HB3	1:D:212:ARG:HG3	1.96	0.48
1:D:169:ASN:O	1:D:307:SER:HB3	2.13	0.48
1:F:305:ASN:C	1:F:305:ASN:HD22	2.16	0.48
1:E:268:THR:O	1:E:324:LYS:HA	2.12	0.48
1:C:320:LEU:HB2	1:C:323:GLU:HB2	1.95	0.48
2:B:362:TND:H1	2:B:362:TND:N7A	2.29	0.48
1:C:93:ASN:HD21	1:C:95:ALA:HB3	1.78	0.48
1:F:210:ASP:OD2	1:F:213:GLY:HA3	2.14	0.48
1:D:85:ILE:HD12	1:D:85:ILE:N	2.29	0.48
1:F:118:LEU:N	1:F:118:LEU:HD12	2.28	0.48
1:E:243:LEU:O	1:E:244:THR:HB	2.14	0.48
1:E:204:ASP:O	1:F:12:ARG:HD3	2.12	0.48
1:D:24:GLN:HB3	1:D:26:LEU:CD1	2.43	0.48
1:D:5:VAL:HA	1:D:106:TYR:O	2.13	0.48
1:C:185:ILE:CD1	1:C:243:LEU:HD11	2.41	0.48
1:F:69:SER:O	1:F:72:VAL:HG22	2.14	0.48
1:A:193:ILE:HD12	1:A:193:ILE:N	2.27	0.48
1:E:212:ARG:O	1:E:215:ARG:HG2	2.14	0.48
1:D:153:TYR:CE1	1:D:158:HIS:HB2	2.49	0.48
1:D:67:LYS:HD3	1:D:72:VAL:O	2.13	0.48
1:B:216:ALA:HB1	1:B:219:VAL:HG12	1.95	0.48
1:E:196:TYR:HA	1:E:200:GLN:OE1	2.14	0.47
1:E:77:VAL:HG22	1:E:86:LYS:HE3	1.95	0.47
1:A:190:MET:O	1:A:190:MET:HG3	2.14	0.47
1:B:229:ALA:CB	1:B:244:THR:HA	2.44	0.47
1:B:145:VAL:O	1:B:146:MET:C	2.52	0.47
1:F:117:LYS:HB3	1:F:139:GLY:HA3	1.96	0.47
1:E:67:LYS:HB3	1:E:72:VAL:CG2	2.45	0.47
1:A:5:VAL:HA	1:A:106:TYR:O	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:ILE:CD1	1:B:153:TYR:HB2	2.45	0.47
1:A:212:ARG:HG2	1:D:295:GLU:HB3	1.96	0.47
1:B:229:ALA:HB1	1:B:244:THR:CA	2.45	0.47
1:D:227:GLY:O	1:D:230:LYS:HG2	2.15	0.47
1:C:10:PHE:CE1	1:C:36:VAL:HG11	2.50	0.47
1:A:305:ASN:HD22	1:A:305:ASN:C	2.17	0.47
1:B:61:TYR:HB3	1:B:81:ASN:HD21	1.79	0.47
1:F:175:VAL:O	1:F:179:THR:HG23	2.14	0.47
1:D:254:ASP:O	1:D:255:VAL:HB	2.15	0.47
1:B:92:ARG:HG2	2:B:362:TND:C5	2.45	0.47
1:B:258:VAL:HG23	1:B:333:TYR:HE1	1.79	0.47
2:E:365:TND:C4B	1:F:206:VAL:HG11	2.45	0.47
1:A:189:LEU:HA	1:A:244:THR:O	2.15	0.47
1:A:254:ASP:O	1:A:255:VAL:CB	2.63	0.47
1:A:69:SER:C	1:A:71:SER:N	2.67	0.47
1:A:289:LEU:HD23	1:A:308:SER:O	2.14	0.47
1:C:7:ILE:HD11	1:C:108:ILE:HD12	1.97	0.47
1:B:254:ASP:O	1:B:255:VAL:HB	2.13	0.47
1:C:233:GLY:O	1:C:240:LYS:HE2	2.15	0.47
1:B:155:PRO:CG	1:B:353:LYS:HG2	2.45	0.46
1:A:29:THR:OG1	1:A:30:GLU:N	2.47	0.46
1:A:45:TYR:O	1:A:48:TYR:HB3	2.14	0.46
1:F:200:GLN:HE21	1:F:222:ILE:HD12	1.80	0.46
1:F:204:ASP:OD1	1:F:215:ARG:HD2	2.16	0.46
1:B:67:LYS:HB3	1:B:72:VAL:HG22	1.97	0.46
1:A:297:VAL:O	1:A:298:SER:C	2.53	0.46
1:A:227:GLY:HA3	1:A:230:LYS:HE2	1.98	0.46
1:F:155:PRO:CG	1:F:353:LYS:HG2	2.45	0.46
1:A:24:GLN:HB3	1:A:26:LEU:CD1	2.45	0.46
1:D:92:ARG:HG2	2:D:364:TND:C5	2.45	0.46
1:E:118:LEU:HD12	1:E:118:LEU:N	2.31	0.46
1:E:85:ILE:HD12	1:E:85:ILE:N	2.31	0.46
1:C:200:GLN:C	1:C:201:LYS:HD2	2.35	0.46
1:B:220:ASN:OD1	1:C:299:ALA:HB2	2.15	0.46
1:C:73:GLU:CD	1:C:74:THR:H	2.17	0.46
1:F:5:VAL:HA	1:F:106:TYR:O	2.16	0.46
1:C:85:ILE:HD12	1:C:85:ILE:N	2.29	0.46
1:F:73:GLU:CD	1:F:74:THR:H	2.19	0.46
1:E:229:ALA:HB1	1:E:244:THR:HA	1.98	0.46
1:E:58:ARG:HG3	1:E:59:PRO:HD2	1.98	0.46
1:C:37:VAL:HG22	1:C:88:VAL:HB	1.98	0.46
1:A:9:GLY:HA3	1:A:111:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:173:PRO:O	1:F:177:VAL:HG13	2.15	0.45
1:F:289:LEU:HD23	1:F:308:SER:O	2.16	0.45
1:A:15:ARG:O	1:A:19:GLN:HG3	2.16	0.45
1:C:280:ALA:O	1:C:285:MET:HB2	2.17	0.45
1:D:285:MET:HB3	1:D:289:LEU:HB3	1.97	0.45
1:B:9:GLY:HA3	1:B:111:THR:HG22	1.98	0.45
1:B:236:ILE:HG22	1:B:236:ILE:O	2.16	0.45
1:F:289:LEU:HD22	1:F:290:GLY:N	2.31	0.45
1:E:201:LYS:HG2	1:E:205:GLY:HA3	1.99	0.45
2:E:365:TND:N7A	2:E:365:TND:H1	2.31	0.45
1:D:200:GLN:OE1	1:D:249:ARG:NH1	2.50	0.45
1:D:178:LEU:O	1:D:183:PHE:HB2	2.16	0.45
1:A:35:ALA:HB2	1:A:86:LYS:HB2	1.99	0.45
1:A:116:ASP:OD2	1:A:118:LEU:HB2	2.17	0.45
1:C:54:THR:HG21	1:D:219:VAL:CG1	2.47	0.45
1:C:229:ALA:CB	1:C:244:THR:HA	2.47	0.45
1:A:290:GLY:O	1:A:309:VAL:HA	2.17	0.45
1:B:144:ILE:HD11	1:B:153:TYR:HB2	1.98	0.45
1:A:178:LEU:O	1:A:183:PHE:HB2	2.17	0.45
1:C:204:ASP:O	1:D:12:ARG:HD3	2.17	0.45
1:B:18:PHE:CE2	1:B:50:MET:HE1	2.52	0.45
1:F:95:ALA:HA	1:F:122:GLY:O	2.16	0.45
1:A:117:LYS:O	1:A:121:GLU:HG3	2.17	0.45
1:E:155:PRO:HG2	1:E:353:LYS:HG2	1.98	0.45
1:E:215:ARG:NH1	1:F:54:THR:OG1	2.50	0.45
1:F:12:ARG:HH21	1:F:336:GLU:CD	2.20	0.45
1:D:124:ILE:HG23	1:D:128:ALA:O	2.17	0.45
1:E:149:ASN:CG	1:E:235:VAL:HG13	2.37	0.45
1:C:24:GLN:HB3	1:C:26:LEU:HD13	1.98	0.45
1:C:323:GLU:HG2	1:C:326:PHE:O	2.17	0.45
1:C:16:MET:HB3	1:C:340:SER:OG	2.16	0.45
1:E:117:LYS:O	1:E:121:GLU:HG3	2.17	0.45
1:A:37:VAL:CG1	1:A:90:ALA:HA	2.47	0.45
1:E:203:VAL:O	1:E:205:GLY:N	2.51	0.44
1:E:24:GLN:HB2	1:E:26:LEU:HD13	1.98	0.44
1:E:297:VAL:O	1:E:298:SER:C	2.55	0.44
1:F:84:ARG:C	1:F:85:ILE:HD12	2.38	0.44
1:E:45:TYR:CE2	1:F:206:VAL:HG13	2.51	0.44
1:A:88:VAL:HG12	1:A:89:LYS:N	2.32	0.44
1:A:149:ASN:OD1	1:A:235:VAL:HG13	2.16	0.44
1:E:274:ASP:OD1	1:E:278:LYS:HE3	2.17	0.44
1:E:349:TYR:CZ	1:E:353:LYS:HE2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:208:LEU:HD12	2:D:364:TND:H1M3	2.00	0.44
1:B:59:PRO:HB2	1:B:61:TYR:CZ	2.53	0.44
1:C:15:ARG:O	1:C:19:GLN:HG3	2.17	0.44
1:F:26:LEU:HD23	1:F:31:ILE:HD12	1.99	0.44
1:A:85:ILE:N	1:A:85:ILE:HD12	2.32	0.44
1:F:86:LYS:CE	1:F:86:LYS:HA	2.48	0.44
1:A:320:LEU:HA	1:A:321:PRO:HD2	1.76	0.44
1:D:303:ASN:HA	1:D:337:TRP:CD1	2.53	0.44
1:D:323:GLU:HG2	1:D:326:PHE:O	2.18	0.44
1:E:215:ARG:NH2	1:F:52:HIS:HB3	2.33	0.44
1:A:37:VAL:HG22	1:A:88:VAL:HB	2.00	0.44
1:B:201:LYS:HD2	1:B:201:LYS:N	2.33	0.44
1:F:334:ASP:O	1:F:335:ASN:C	2.55	0.44
1:F:77:VAL:HG13	1:F:85:ILE:O	2.18	0.44
1:D:18:PHE:CE2	1:D:50:MET:HE1	2.52	0.44
1:A:78:LEU:HA	1:A:78:LEU:HD12	1.85	0.44
1:D:67:LYS:HD3	1:D:72:VAL:HG23	2.00	0.43
1:C:193:ILE:HB	1:C:257:VAL:HG12	2.00	0.43
1:F:171:LEU:CD1	1:F:260:LEU:HD22	2.46	0.43
1:A:193:ILE:HB	1:A:257:VAL:CG1	2.48	0.43
1:E:200:GLN:OE1	1:E:249:ARG:NH1	2.51	0.43
1:E:66:VAL:HG23	1:E:77:VAL:HB	1.98	0.43
1:F:200:GLN:HB3	1:F:217:ALA:HB2	2.00	0.43
1:E:185:ILE:O	1:E:185:ILE:HG23	2.18	0.43
1:D:21:ILE:HG23	1:D:31:ILE:HD12	1.99	0.43
1:E:180:LYS:C	1:E:182:ASN:H	2.20	0.43
1:D:7:ILE:HD13	1:D:108:ILE:HB	2.00	0.43
1:E:310:TYR:CE1	1:E:329:VAL:HG13	2.53	0.43
1:B:51:LYS:O	1:B:58:ARG:HG3	2.18	0.43
1:E:49:GLN:OE1	1:F:206:VAL:HG22	2.17	0.43
1:E:222:ILE:HB	1:E:249:ARG:HB2	2.00	0.43
1:A:73:GLU:H	1:A:73:GLU:CD	2.21	0.43
1:B:290:GLY:O	1:B:309:VAL:HA	2.19	0.43
1:F:309:VAL:HG13	1:F:332:TRP:HB2	1.99	0.43
1:F:274:ASP:HB2	1:F:316:LEU:HD21	1.99	0.43
1:A:266:ARG:NH1	1:A:266:ARG:HG3	2.32	0.43
1:D:274:ASP:HB2	1:D:316:LEU:HD21	2.01	0.43
1:B:79:VAL:HA	1:B:83:HIS:O	2.18	0.43
1:A:206:VAL:HG11	2:B:362:TND:C4B	2.48	0.43
1:A:203:VAL:O	1:A:204:ASP:C	2.57	0.43
1:F:229:ALA:HB1	1:F:244:THR:HA	2.00	0.43
1:B:24:GLN:HB3	1:B:26:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:LYS:HE2	1:A:353:LYS:HB2	1.92	0.43
1:B:356:ALA:C	1:B:358:SER:H	2.22	0.43
1:D:280:ALA:O	1:D:285:MET:HB2	2.19	0.43
1:C:12:ARG:NH2	1:C:336:GLU:OE1	2.52	0.43
1:E:59:PRO:HB2	1:E:61:TYR:CZ	2.53	0.43
1:A:302:ILE:O	1:A:303:ASN:HB2	2.18	0.43
1:B:38:ASP:OD1	1:B:39:MET:N	2.52	0.43
1:D:180:LYS:C	1:D:182:ASN:H	2.22	0.43
1:A:173:PRO:O	1:A:177:VAL:HG13	2.19	0.43
1:D:195:SER:OG	1:D:255:VAL:O	2.37	0.43
1:F:55:VAL:HG11	1:F:254:ASP:CB	2.48	0.43
1:F:192:THR:HG22	1:F:246:MET:O	2.19	0.43
1:F:292:THR:HG21	1:F:296:LEU:HD12	2.00	0.43
1:E:208:LEU:HD23	1:F:45:TYR:CG	2.54	0.42
1:A:232:VAL:HG11	1:A:243:LEU:CD2	2.46	0.42
1:F:85:ILE:N	1:F:85:ILE:HD12	2.34	0.42
1:F:18:PHE:CE2	1:F:80:VAL:HG21	2.54	0.42
1:E:210:ASP:OD2	1:E:213:GLY:HA3	2.19	0.42
1:A:67:LYS:HB3	1:A:72:VAL:HG22	2.01	0.42
1:D:145:VAL:CG2	1:D:235:VAL:HG21	2.48	0.42
1:E:18:PHE:HD2	1:E:50:MET:HE3	1.82	0.42
1:D:118:LEU:N	1:D:118:LEU:HD12	2.34	0.42
1:F:274:ASP:O	1:F:278:LYS:HG3	2.19	0.42
1:C:98:PRO:HG2	1:C:102:LEU:CD1	2.48	0.42
1:F:299:ALA:O	1:F:302:ILE:HG13	2.20	0.42
1:F:73:GLU:CD	1:F:73:GLU:N	2.72	0.42
1:F:229:ALA:CB	1:F:244:THR:HA	2.49	0.42
1:D:86:LYS:CE	1:D:86:LYS:HA	2.48	0.42
1:C:193:ILE:N	1:C:193:ILE:HD12	2.35	0.42
1:F:5:VAL:HG12	1:F:106:TYR:HB2	2.01	0.42
1:E:204:ASP:OD2	1:F:54:THR:N	2.44	0.42
1:D:196:TYR:HA	1:D:200:GLN:OE1	2.20	0.42
1:A:67:LYS:HB3	1:A:72:VAL:CG2	2.49	0.42
1:C:99:TRP:HA	1:C:99:TRP:CE3	2.54	0.42
1:A:185:ILE:CD1	1:A:243:LEU:HD11	2.46	0.42
1:B:281:ALA:HB2	1:B:289:LEU:HD13	2.01	0.42
1:B:67:LYS:HD3	1:B:72:VAL:O	2.19	0.42
1:F:229:ALA:HB1	1:F:244:THR:CA	2.49	0.42
1:E:7:ILE:HD13	1:E:108:ILE:HD12	2.02	0.42
1:E:17:VAL:HG11	1:E:108:ILE:HD13	2.02	0.42
1:F:155:PRO:HG3	1:F:353:LYS:HG2	2.01	0.42
1:A:200:GLN:OE1	1:A:249:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:50:MET:HB3	1:C:50:MET:HE2	1.85	0.42
1:D:189:LEU:HA	1:D:244:THR:O	2.19	0.42
1:E:232:VAL:HG11	1:E:243:LEU:CD2	2.48	0.42
1:D:215:ARG:O	1:D:216:ALA:C	2.58	0.42
1:A:313:LYS:HA	1:A:313:LYS:HD3	1.87	0.42
1:E:27:ILE:O	1:E:27:ILE:HG23	2.20	0.42
1:D:263:ARG:HA	1:D:325:ARG:O	2.20	0.42
1:C:243:LEU:O	1:C:244:THR:HB	2.19	0.41
1:B:289:LEU:HD22	1:B:290:GLY:N	2.35	0.41
1:A:116:ASP:O	1:A:117:LYS:C	2.58	0.41
1:E:309:VAL:O	1:E:309:VAL:HG13	2.20	0.41
1:C:338:ALA:O	1:C:339:TYR:C	2.58	0.41
1:F:7:ILE:HD13	1:F:108:ILE:HB	2.01	0.41
1:D:73:GLU:CD	1:D:73:GLU:H	2.23	0.41
1:E:229:ALA:CB	1:E:244:THR:HA	2.51	0.41
1:B:250:VAL:HA	1:B:251:PRO:HD3	1.82	0.41
1:F:17:VAL:HG11	1:F:108:ILE:HD13	2.01	0.41
1:C:145:VAL:O	1:C:146:MET:C	2.59	0.41
1:D:189:LEU:HD12	1:D:244:THR:HG22	2.02	0.41
1:E:5:VAL:HA	1:E:106:TYR:O	2.20	0.41
1:E:99:TRP:HE3	1:E:99:TRP:HA	1.84	0.41
1:A:227:GLY:O	1:A:230:LYS:HG2	2.20	0.41
1:E:290:GLY:O	1:E:309:VAL:HA	2.20	0.41
1:B:85:ILE:HD12	1:B:85:ILE:N	2.35	0.41
1:E:349:TYR:CZ	1:E:353:LYS:CE	3.03	0.41
1:B:12:ARG:HA	1:B:12:ARG:HD2	1.92	0.41
1:E:149:ASN:OD1	1:E:235:VAL:HG13	2.19	0.41
1:C:3:ILE:HD13	1:C:351:ALA:CB	2.50	0.41
1:E:13:ILE:HG12	1:E:13:ILE:H	1.56	0.41
1:E:192:THR:HG23	1:E:192:THR:O	2.20	0.41
1:C:297:VAL:O	1:C:298:SER:C	2.59	0.41
1:A:169:ASN:O	1:A:307:SER:HB3	2.21	0.41
1:C:305:ASN:C	1:C:305:ASN:HD22	2.24	0.41
1:C:232:VAL:HG11	1:C:243:LEU:CD2	2.49	0.41
1:F:277:ILE:HG23	1:F:289:LEU:HD11	2.03	0.41
1:E:173:PRO:O	1:E:177:VAL:HG13	2.21	0.41
1:C:17:VAL:HG11	1:C:108:ILE:HD13	2.01	0.41
1:F:18:PHE:HE2	1:F:50:MET:HE1	1.86	0.41
1:F:124:ILE:HA	1:F:128:ALA:O	2.21	0.41
1:D:305:ASN:C	1:D:305:ASN:HD22	2.24	0.41
1:D:297:VAL:O	1:D:298:SER:C	2.57	0.41
1:E:170:CYS:HA	1:E:308:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:227:GLY:O	1:E:230:LYS:HG2	2.20	0.41
1:D:200:GLN:HB3	1:D:217:ALA:HB2	2.03	0.41
1:F:149:ASN:CG	1:F:235:VAL:HG13	2.41	0.41
1:B:118:LEU:N	1:B:118:LEU:HD12	2.35	0.41
1:D:64:GLU:HG2	1:D:65:ALA:N	2.34	0.41
1:F:24:GLN:HB3	1:F:26:LEU:HD13	2.02	0.41
1:B:289:LEU:HD23	1:B:308:SER:O	2.21	0.41
1:A:261:THR:HG22	1:D:326:PHE:HZ	1.86	0.41
1:F:320:LEU:HA	1:F:321:PRO:HD2	1.78	0.41
1:F:200:GLN:OE1	1:F:249:ARG:NH1	2.54	0.41
1:E:178:LEU:O	1:E:183:PHE:HB2	2.21	0.41
1:D:290:GLY:O	1:D:309:VAL:HA	2.21	0.41
1:E:178:LEU:HA	1:E:178:LEU:HD23	1.89	0.41
1:B:334:ASP:O	1:B:335:ASN:C	2.59	0.41
1:D:250:VAL:HA	1:D:251:PRO:HD3	1.85	0.40
1:C:24:GLN:HB2	1:C:26:LEU:HD13	2.03	0.40
1:F:335:ASN:OD1	1:F:335:ASN:N	2.53	0.40
1:B:295:GLU:HB3	1:C:212:ARG:HG2	2.02	0.40
1:D:27:ILE:O	1:D:27:ILE:HG23	2.21	0.40
1:E:266:ARG:HH11	1:E:266:ARG:HG3	1.86	0.40
1:E:170:CYS:O	1:E:173:PRO:HD2	2.21	0.40
1:D:88:VAL:HG12	1:D:89:LYS:N	2.36	0.40
1:B:297:VAL:O	1:B:298:SER:C	2.59	0.40
1:E:305:ASN:C	1:E:305:ASN:HD22	2.25	0.40
1:C:11:GLY:O	1:C:12:ARG:C	2.58	0.40
1:D:268:THR:O	1:D:324:LYS:HA	2.21	0.40
1:E:12:ARG:HH21	1:E:336:GLU:CD	2.25	0.40
1:A:149:ASN:HA	1:A:151:HIS:CE1	2.56	0.40
1:C:266:ARG:HH11	1:C:266:ARG:HG3	1.86	0.40
1:D:12:ARG:O	1:D:16:MET:HG2	2.21	0.40
1:D:124:ILE:HA	1:D:128:ALA:O	2.21	0.40
1:C:283:THR:OG1	1:C:284:TYR:N	2.54	0.40
1:F:63:VAL:HG12	1:F:64:GLU:N	2.36	0.40
1:F:282:GLN:HB2	1:F:282:GLN:HE21	1.63	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/360 (99%)	311 (87%)	41 (12%)	4 (1%)	21	67
1	B	356/360 (99%)	320 (90%)	32 (9%)	4 (1%)	21	67
1	C	356/360 (99%)	314 (88%)	39 (11%)	3 (1%)	27	76
1	D	356/360 (99%)	317 (89%)	37 (10%)	2 (1%)	33	81
1	E	356/360 (99%)	313 (88%)	39 (11%)	4 (1%)	21	67
1	F	356/360 (99%)	315 (88%)	34 (10%)	7 (2%)	11	48
All	All	2136/2160 (99%)	1890 (88%)	222 (10%)	24 (1%)	21	67

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	204	ASP
1	A	255	VAL
1	B	251	PRO
1	B	255	VAL
1	A	335	ASN
1	C	255	VAL
1	D	251	PRO
1	D	255	VAL
1	E	255	VAL
1	F	204	ASP
1	F	255	VAL
1	F	298	SER
1	A	204	ASP
1	B	216	ALA
1	C	204	ASP
1	E	185	ILE
1	E	244	THR
1	F	251	PRO
1	F	335	ASN
1	C	185	ILE
1	B	185	ILE

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Mol	Chain	Res	Type
1	F	70	PRO
1	F	219	VAL
1	A	70	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/296 (99%)	284 (97%)	10 (3%)	49	88
1	B	294/296 (99%)	285 (97%)	9 (3%)	52	89
1	C	294/296 (99%)	284 (97%)	10 (3%)	49	88
1	D	294/296 (99%)	285 (97%)	9 (3%)	52	89
1	E	294/296 (99%)	284 (97%)	10 (3%)	49	88
1	F	294/296 (99%)	282 (96%)	12 (4%)	41	83
All	All	1764/1776 (99%)	1704 (97%)	60 (3%)	49	88

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	73	GLU
1	A	78	LEU
1	A	86	LYS
1	A	163	ASN
1	A	177	VAL
1	A	190	MET
1	A	289	LEU
1	A	305	ASN
1	A	306	ARG
1	B	58	ARG
1	B	71	SER
1	B	73	GLU
1	B	78	LEU
1	B	163	ASN
1	B	190	MET

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Mol	Chain	Res	Type
1	B	215	ARG
1	B	289	LEU
1	B	305	ASN
1	C	71	SER
1	C	73	GLU
1	C	78	LEU
1	C	86	LYS
1	C	190	MET
1	C	243	LEU
1	C	289	LEU
1	C	305	ASN
1	C	306	ARG
1	C	335	ASN
1	D	73	GLU
1	D	78	LEU
1	D	86	LYS
1	D	163	ASN
1	D	190	MET
1	D	243	LEU
1	D	289	LEU
1	D	305	ASN
1	D	306	ARG
1	E	13	ILE
1	E	71	SER
1	E	73	GLU
1	E	86	LYS
1	E	163	ASN
1	E	177	VAL
1	E	190	MET
1	E	289	LEU
1	E	305	ASN
1	E	306	ARG
1	F	58	ARG
1	F	73	GLU
1	F	78	LEU
1	F	86	LYS
1	F	163	ASN
1	F	166	CYS
1	F	177	VAL
1	F	190	MET
1	F	289	LEU
1	F	305	ASN

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Mol	Chain	Res	Type
1	F	306	ARG
1	F	335	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	93	ASN
1	A	282	GLN
1	A	305	ASN
1	A	341	HIS
1	B	49	GLN
1	B	81	ASN
1	B	93	ASN
1	B	282	GLN
1	B	305	ASN
1	B	318	ASN
1	C	49	GLN
1	C	282	GLN
1	C	305	ASN
1	D	49	GLN
1	D	282	GLN
1	D	305	ASN
1	D	341	HIS
1	E	52	HIS
1	E	93	ASN
1	E	220	ASN
1	E	282	GLN
1	E	305	ASN
1	F	52	HIS
1	F	93	ASN
1	F	282	GLN
1	F	305	ASN
1	F	341	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	TND	A	361	-	46,46,46	2.69	15 (32%)	66,66,66	1.37	7 (10%)
2	TND	B	362	-	46,46,46	2.78	16 (34%)	66,66,66	1.19	6 (9%)
2	TND	C	363	-	46,46,46	2.69	16 (34%)	66,66,66	1.28	5 (7%)
2	TND	D	364	-	46,46,46	2.74	15 (32%)	66,66,66	1.29	5 (7%)
2	TND	E	365	-	46,46,46	2.80	16 (34%)	66,66,66	1.32	7 (10%)
2	TND	F	366	-	46,46,46	2.92	16 (34%)	66,66,66	1.34	4 (6%)

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	TND	A	361	-	-	1/22/48/48	0/2/6/6
2	TND	B	362	-	-	1/22/48/48	0/2/6/6
2	TND	C	363	-	-	1/22/48/48	0/2/6/6
2	TND	D	364	-	-	1/22/48/48	0/2/6/6
2	TND	E	365	-	-	1/22/48/48	0/2/6/6
2	TND	F	366	-	-	1/22/48/48	0/2/6/6

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	363	TND	C8-C9	8.63	1.52	1.39
2	F	366	TND	C8-C9	8.60	1.52	1.39
2	B	362	TND	C8-C9	8.54	1.51	1.39
2	D	364	TND	C8-C9	8.38	1.51	1.39
2	E	365	TND	C8-C9	8.35	1.51	1.39
2	A	361	TND	C8-C9	8.18	1.51	1.39
2	D	364	TND	C10-C9	7.77	1.53	1.39
2	F	366	TND	C10-C9	7.67	1.53	1.39
2	B	362	TND	C10-C9	7.35	1.52	1.39
2	E	365	TND	C10-C9	7.29	1.52	1.39
2	C	363	TND	C10-C9	7.25	1.52	1.39
2	B	362	TND	C5-C10	7.18	1.52	1.39
2	E	365	TND	C5-C10	6.87	1.52	1.39
2	F	366	TND	C5-C10	6.81	1.51	1.39
2	A	361	TND	C5-C10	6.48	1.51	1.39
2	A	361	TND	C10-C9	6.39	1.50	1.39
2	C	363	TND	C5-C10	6.38	1.51	1.39
2	D	364	TND	C5-C10	6.27	1.50	1.39
2	F	366	TND	C7-C8	5.36	1.51	1.39
2	F	366	TND	C6-C5	5.35	1.51	1.39
2	C	363	TND	C6-C5	5.31	1.51	1.39
2	B	362	TND	C6-C5	5.30	1.51	1.39
2	A	361	TND	C6-C5	5.17	1.51	1.39
2	E	365	TND	C7-C8	5.16	1.51	1.39
2	B	362	TND	C7-C8	5.12	1.50	1.39
2	D	364	TND	C7-C8	5.06	1.50	1.39
2	E	365	TND	C6-C5	5.03	1.50	1.39
2	A	361	TND	C7-C8	5.02	1.50	1.39
2	C	363	TND	C7-C8	4.99	1.50	1.39
2	D	364	TND	C6-C5	4.97	1.50	1.39
2	A	361	TND	C6-C7	4.49	1.50	1.37
2	F	366	TND	C6-C7	4.49	1.50	1.37
2	C	363	TND	C6-C7	4.39	1.50	1.37
2	B	362	TND	C6-C7	4.37	1.50	1.37
2	D	364	TND	C6-C7	4.34	1.50	1.37
2	E	365	TND	C6-C7	4.31	1.50	1.37
2	D	364	TND	C9-C1	4.20	1.56	1.52
2	F	366	TND	C1B-C6B	3.94	1.45	1.39
2	B	362	TND	C3B-C2B	3.92	1.46	1.38
2	F	366	TND	C3B-C2B	3.83	1.46	1.38
2	E	365	TND	C3B-C2B	3.71	1.46	1.38
2	F	366	TND	C5B-C4B	3.65	1.45	1.38
2	A	361	TND	C3B-C2B	3.61	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	364	TND	C3B-C2B	3.61	1.45	1.38
2	C	363	TND	C3B-C2B	3.59	1.45	1.38
2	F	366	TND	C5B-C6B	3.56	1.44	1.39
2	E	365	TND	C9-C1	3.52	1.55	1.52
2	E	365	TND	C1B-C6B	3.52	1.44	1.39
2	F	366	TND	C9-C1	3.47	1.55	1.52
2	A	361	TND	C1B-C6B	3.40	1.44	1.39
2	E	365	TND	C5B-C4B	3.33	1.45	1.38
2	D	364	TND	C1B-C6B	3.28	1.44	1.39
2	A	361	TND	C5B-C4B	3.25	1.45	1.38
2	F	366	TND	C3B-C4B	3.15	1.45	1.38
2	A	361	TND	C5B-C6B	3.08	1.44	1.39
2	E	365	TND	C3B-C4B	3.07	1.44	1.38
2	B	362	TND	C1B-C6B	3.06	1.44	1.39
2	C	363	TND	C1B-C6B	3.05	1.44	1.39
2	C	363	TND	C3B-C4B	3.03	1.44	1.38
2	E	365	TND	C1B-C2B	3.03	1.44	1.38
2	B	362	TND	C9-C1	2.99	1.54	1.52
2	F	366	TND	C1B-C2B	2.98	1.44	1.38
2	C	363	TND	C5B-C6B	2.93	1.43	1.39
2	C	363	TND	C5B-C4B	2.89	1.44	1.38
2	B	362	TND	C3B-C4B	2.84	1.44	1.38
2	D	364	TND	C3B-C4B	2.83	1.44	1.38
2	B	362	TND	C6A-N1A	2.80	1.39	1.34
2	B	362	TND	C5B-C6B	2.80	1.43	1.39
2	E	365	TND	C5B-C6B	2.79	1.43	1.39
2	A	361	TND	O4'-C1'	2.76	1.45	1.41
2	D	364	TND	C1B-C2B	2.74	1.44	1.38
2	A	361	TND	C3B-C4B	2.74	1.44	1.38
2	D	364	TND	C5B-C6B	2.71	1.43	1.39
2	D	364	TND	C5B-C4B	2.67	1.44	1.38
2	E	365	TND	C6A-N1A	2.59	1.38	1.34
2	B	362	TND	C5B-C4B	2.58	1.43	1.38
2	B	362	TND	C1B-C2B	2.58	1.43	1.38
2	A	361	TND	C9-C1	2.57	1.54	1.52
2	B	362	TND	C4-C10	2.52	1.56	1.51
2	A	361	TND	C1B-C2B	2.49	1.43	1.38
2	F	366	TND	C4-C10	2.48	1.55	1.51
2	E	365	TND	C4-C10	2.47	1.55	1.51
2	F	366	TND	C6A-N1A	2.35	1.38	1.34
2	C	363	TND	C1B-C2B	2.34	1.43	1.38
2	E	365	TND	O4'-C1'	2.34	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	363	TND	C4-C10	2.34	1.55	1.51
2	D	364	TND	C4-C10	2.32	1.55	1.51
2	A	361	TND	C6A-N1A	2.31	1.38	1.34
2	D	364	TND	C6A-N1A	2.28	1.38	1.34
2	C	363	TND	C9-C1	2.22	1.54	1.52
2	B	362	TND	O4'-C1'	2.19	1.44	1.41
2	C	363	TND	C6A-N1A	2.18	1.38	1.34
2	C	363	TND	O4'-C1'	2.11	1.44	1.41
2	F	366	TND	C2A-N3A	2.05	1.36	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	366	TND	C9-C1-N6A	6.01	115.47	109.97
2	D	364	TND	C2A-N1A-C6A	4.83	119.72	116.69
2	E	365	TND	C2A-N1A-C6A	4.56	119.55	116.69
2	E	365	TND	C9-C1-N6A	4.42	114.01	109.97
2	C	363	TND	C2A-N1A-C6A	4.36	119.43	116.69
2	A	361	TND	C2A-N1A-C6A	4.34	119.42	116.69
2	D	364	TND	C9-C1-N6A	4.31	113.91	109.97
2	B	362	TND	C2A-N1A-C6A	4.16	119.30	116.69
2	F	366	TND	C2A-N1A-C6A	4.13	119.28	116.69
2	C	363	TND	C9-C1-N6A	3.95	113.58	109.97
2	A	361	TND	C10-C9-C1	-3.76	117.84	121.87
2	A	361	TND	C9-C1-N6A	3.71	113.35	109.97
2	B	362	TND	C9-C1-N6A	3.03	112.74	109.97
2	D	364	TND	C5A-C6A-N6A	2.97	125.64	120.50
2	F	366	TND	C10-C9-C1	-2.86	118.80	121.87
2	E	365	TND	C5A-C6A-N6A	2.86	125.45	120.50
2	A	361	TND	C5A-C6A-N6A	2.77	125.29	120.50
2	C	363	TND	C3'-C2'-C1'	-2.71	101.47	104.26
2	C	363	TND	C10-C9-C1	-2.63	119.04	121.87
2	B	362	TND	C5A-C6A-N6A	2.60	125.01	120.50
2	C	363	TND	C5A-C6A-N6A	2.56	124.93	120.50
2	D	364	TND	O4'-C1'-N9A	2.53	110.79	108.44
2	A	361	TND	C2-C3-C4	2.44	116.42	110.92
2	E	365	TND	C10-C9-C1	-2.41	119.28	121.87
2	B	362	TND	C10-C9-C1	-2.40	119.30	121.87
2	A	361	TND	O4'-C1'-N9A	2.27	110.55	108.44
2	B	362	TND	C8A-N9A-C4A	-2.23	105.20	106.90
2	E	365	TND	C2'-C1'-N9A	2.22	118.16	114.80
2	E	365	TND	C3'-C2'-C1'	-2.22	101.98	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	364	TND	C8A-N9A-C4A	-2.17	105.25	106.90
2	B	362	TND	C3'-C2'-C1'	-2.14	102.06	104.26
2	F	366	TND	C5A-C6A-N6A	2.13	124.19	120.50
2	E	365	TND	C2'-N2'-C7B	2.04	125.56	122.19
2	A	361	TND	C8A-N9A-C4A	-2.03	105.35	106.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	365	TND	C5A-C6A-N6A-C1
2	B	362	TND	C5A-C6A-N6A-C1
2	A	361	TND	C5A-C6A-N6A-C1
2	C	363	TND	C5A-C6A-N6A-C1
2	D	364	TND	C5A-C6A-N6A-C1
2	F	366	TND	C5A-C6A-N6A-C1

There are no ring outliers.

## 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.