wwPDB EM Map/Model Validation Report (i)

May 2, 2016 – 06:52 PM EDT

PDB ID	:	3JD2
EMDB ID:	:	EMD-6635
Title	:	Glutamate dehydrogenase in complex with NADH, open conformation
Authors	:	Borgnia, M.J.; Banerjee, S.; Merk, A.; Matthies, D.; Bartesaghi, A.; Rao, P.; Pierson, J.; Earl, L.A.; Falconieri, V.; Subramaniam, S.; Milne, J.L.S.
Deposited on	:	2016-03-28
Resolution	:	3.30 Å(reported)
Based on PDB ID	:	3MW9

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

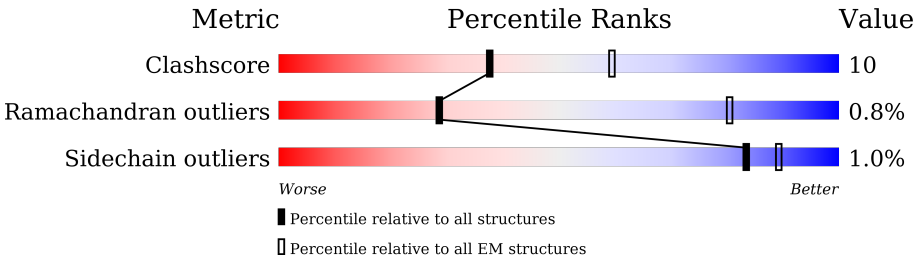
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	501	78% 20% ••
1	B	501	77% 21% ••
1	C	501	77% 21% ••
1	D	501	78% 20% ••
1	E	501	77% 21% ••
1	F	501	77% 21% ••

2 Entry composition

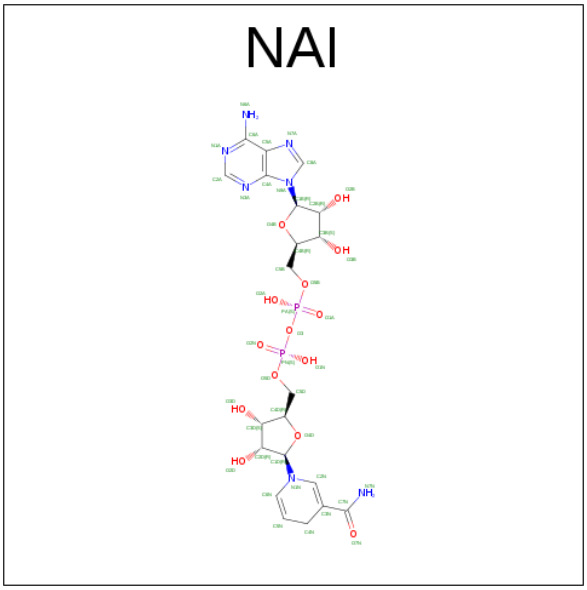
There are 2 unique types of molecules in this entry. The entry contains 23814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	496	Total	C	N	O	S	0	0
			3881	2454	679	729	19		
1	B	496	Total	C	N	O	S	0	0
			3881	2454	679	729	19		
1	C	496	Total	C	N	O	S	0	0
			3881	2454	679	729	19		
1	D	496	Total	C	N	O	S	0	0
			3881	2454	679	729	19		
1	E	496	Total	C	N	O	S	0	0
			3881	2454	679	729	19		
1	F	496	Total	C	N	O	S	0	0
			3881	2454	679	729	19		

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



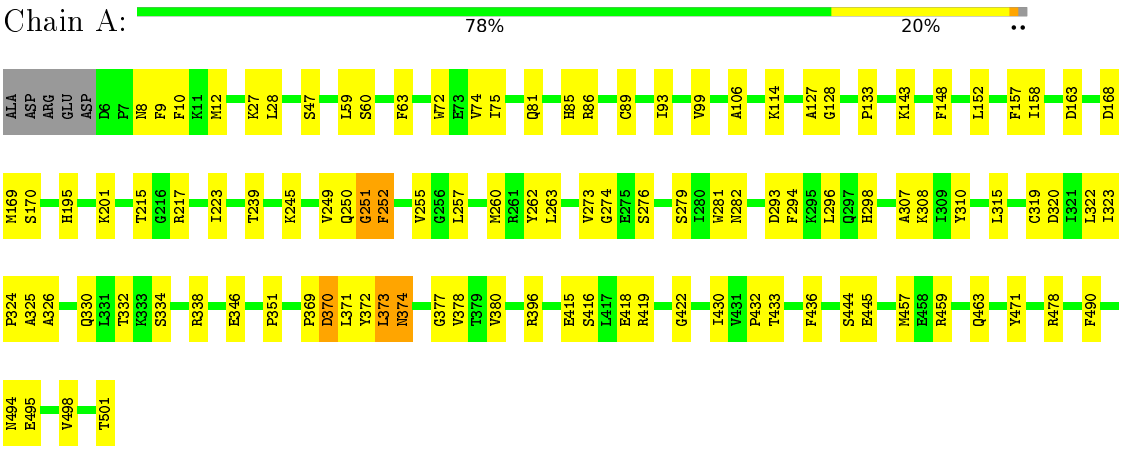
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	D	1	Total	C	N	O	P	0
	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

3 Residue-property plots (i)

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

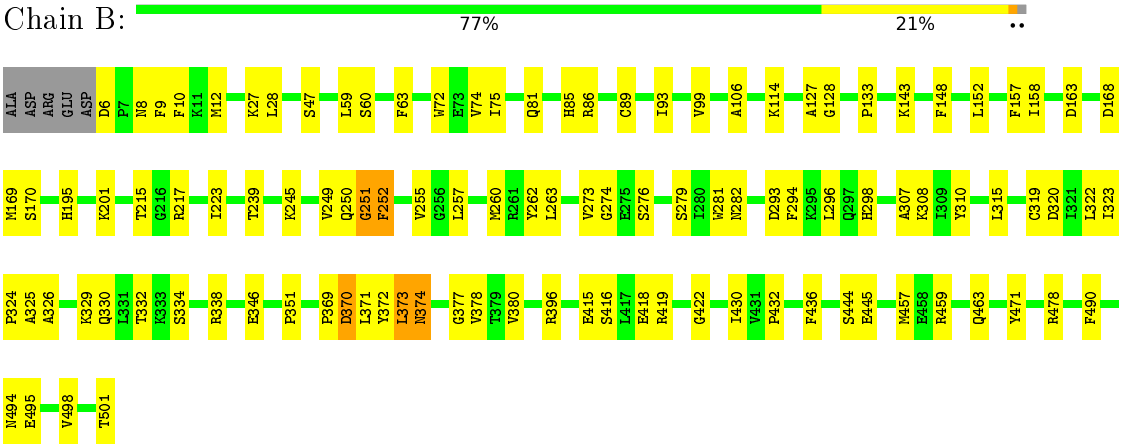
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain A:



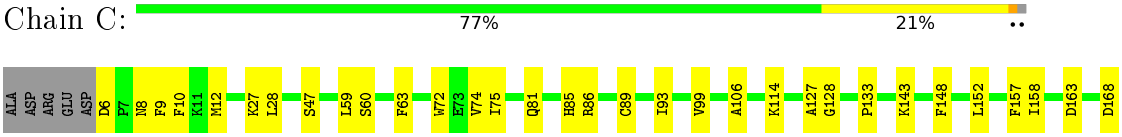
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain B:



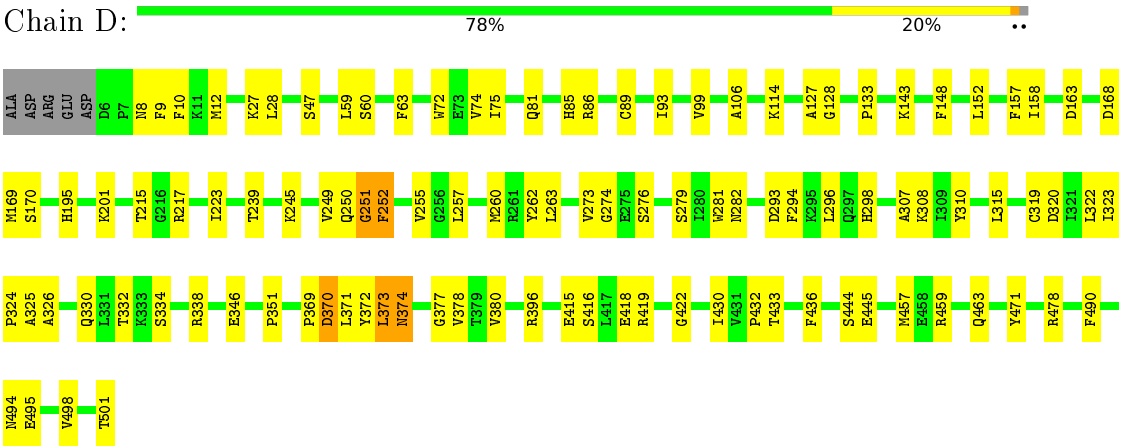
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:



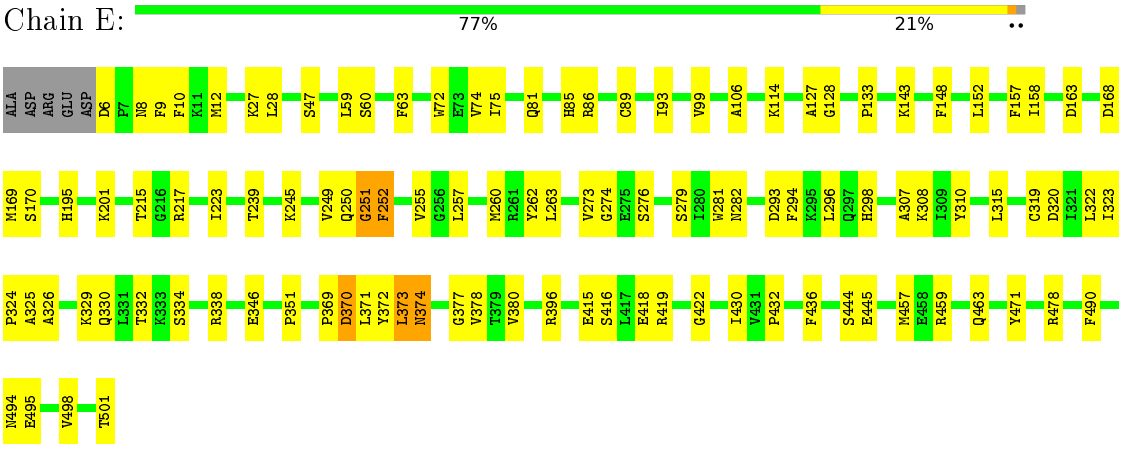
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D:



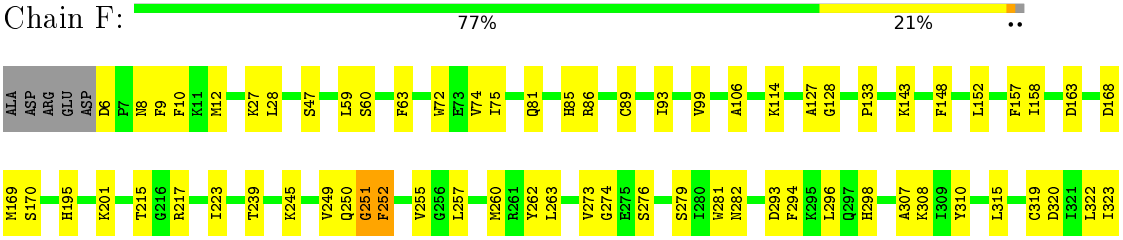
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

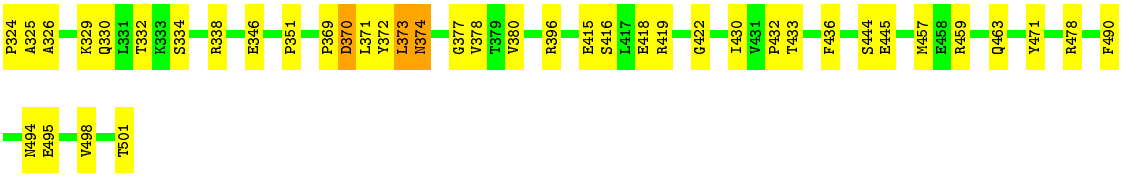
Chain E:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:




P324
A325
A326
K329
Q330
L331
T332
K333
S334
R338
E346
P351
P369
D370
L371
Y372
L373
N374
G377
V378
T379
V380
R396
E415
S416
L417
E418
R419
G422
T430
V431
P432
T433
F436
S444
E445
N457
E458
R459
Q463
Y471
R478
F490
N494
E495
V498
T501

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	34716	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.42	0/3964	0.49	1/5351 (0.0%)
1	B	0.42	0/3964	0.49	1/5351 (0.0%)
1	C	0.42	0/3964	0.49	1/5351 (0.0%)
1	D	0.42	0/3964	0.49	1/5351 (0.0%)
1	E	0.42	0/3964	0.49	1/5351 (0.0%)
1	F	0.42	0/3964	0.49	1/5351 (0.0%)
All	All	0.42	0/23784	0.49	6/32106 (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})
1	A	323	ILE	C-N-CD	5.08	139.06	128.40
1	D	323	ILE	C-N-CD	5.08	139.06	128.40
1	B	323	ILE	C-N-CD	5.06	139.03	128.40
1	E	323	ILE	C-N-CD	5.06	139.03	128.40
1	C	323	ILE	C-N-CD	5.06	139.02	128.40
1	F	323	ILE	C-N-CD	5.06	139.02	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3881	0	3848	84	0
1	B	3881	0	3848	83	0
1	C	3881	0	3848	82	0
1	D	3881	0	3848	84	0
1	E	3881	0	3848	83	0
1	F	3881	0	3848	82	0
2	A	88	0	54	12	0
2	B	88	0	54	11	0
2	C	88	0	54	11	0
2	D	88	0	54	12	0
2	E	88	0	54	11	0
2	F	88	0	54	11	0
All	All	23814	0	23412	464	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 10.

All (464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:GLN:HE22	2:A:602:NAI:C5N	1.73	1.00
1:D:463:GLN:HE22	2:D:602:NAI:C5N	1.73	1.00
1:C:463:GLN:HE22	2:C:601:NAI:C5N	1.74	1.00
1:F:463:GLN:HE22	2:F:601:NAI:C5N	1.74	1.00
1:B:463:GLN:HE22	2:B:602:NAI:C5N	1.73	0.99
1:E:463:GLN:HE22	2:E:602:NAI:C5N	1.73	0.99
1:B:463:GLN:NE2	2:B:602:NAI:C5N	2.26	0.98
1:E:463:GLN:NE2	2:E:602:NAI:C5N	2.26	0.98
1:F:463:GLN:NE2	2:F:601:NAI:C5N	2.26	0.98
1:C:463:GLN:NE2	2:C:601:NAI:C5N	2.26	0.98
1:D:463:GLN:NE2	2:D:602:NAI:C5N	2.26	0.98
1:A:463:GLN:NE2	2:A:602:NAI:C5N	2.26	0.98
1:C:143:LYS:HE2	1:F:501:THR:HG21	1.56	0.88
1:C:501:THR:HG21	1:F:143:LYS:HE2	1.56	0.87
1:B:143:LYS:HE2	1:D:501:THR:HG21	1.56	0.87
1:A:501:THR:HG21	1:E:143:LYS:HE2	1.56	0.87
1:C:463:GLN:HE22	2:C:601:NAI:H5N	1.41	0.85
1:F:463:GLN:HE22	2:F:601:NAI:H5N	1.41	0.85
1:B:501:THR:HG21	1:D:143:LYS:HE2	1.56	0.85
1:A:143:LYS:HE2	1:E:501:THR:HG21	1.56	0.85
1:B:463:GLN:HE22	2:B:602:NAI:H5N	1.41	0.84
1:E:463:GLN:HE22	2:E:602:NAI:H5N	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:GLN:HE22	2:A:602:NAI:H5N	1.41	0.83
1:D:463:GLN:HE22	2:D:602:NAI:H5N	1.41	0.83
1:D:252:PHE:HD1	1:D:273:VAL:HG11	1.44	0.82
1:A:252:PHE:HD1	1:A:273:VAL:HG11	1.44	0.82
1:C:252:PHE:HD1	1:C:273:VAL:HG11	1.45	0.82
1:F:252:PHE:HD1	1:F:273:VAL:HG11	1.45	0.82
1:B:252:PHE:HD1	1:B:273:VAL:HG11	1.44	0.81
1:E:252:PHE:HD1	1:E:273:VAL:HG11	1.44	0.81
1:B:99:VAL:HG11	1:B:128:GLY:HA3	1.69	0.74
1:E:99:VAL:HG11	1:E:128:GLY:HA3	1.69	0.74
1:D:99:VAL:HG11	1:D:128:GLY:HA3	1.69	0.74
1:A:99:VAL:HG11	1:A:128:GLY:HA3	1.69	0.73
1:C:72:TRP:HB2	1:F:47:SER:HB2	1.70	0.73
1:C:47:SER:HB2	1:F:72:TRP:HB2	1.70	0.73
1:C:99:VAL:HG11	1:C:128:GLY:HA3	1.69	0.73
1:A:47:SER:HB2	1:E:72:TRP:HB2	1.70	0.73
1:F:99:VAL:HG11	1:F:128:GLY:HA3	1.69	0.73
1:B:72:TRP:HB2	1:D:47:SER:HB2	1.70	0.73
1:A:72:TRP:HB2	1:E:47:SER:HB2	1.70	0.72
1:B:59:LEU:HB2	1:B:157:PHE:HE2	1.55	0.72
1:B:47:SER:HB2	1:D:72:TRP:HB2	1.70	0.72
1:E:59:LEU:HB2	1:E:157:PHE:HE2	1.55	0.71
1:C:59:LEU:HB2	1:C:157:PHE:HE2	1.55	0.70
1:D:59:LEU:HB2	1:D:157:PHE:HE2	1.55	0.70
1:F:59:LEU:HB2	1:F:157:PHE:HE2	1.55	0.70
1:A:59:LEU:HB2	1:A:157:PHE:HE2	1.55	0.70
1:F:81:GLN:NE2	1:F:163:ASP:OD2	2.24	0.70
1:C:81:GLN:NE2	1:C:163:ASP:OD2	2.24	0.70
1:D:81:GLN:NE2	1:D:163:ASP:OD2	2.24	0.70
1:A:81:GLN:NE2	1:A:163:ASP:OD2	2.24	0.69
1:B:81:GLN:NE2	1:B:163:ASP:OD2	2.24	0.69
1:E:81:GLN:NE2	1:E:163:ASP:OD2	2.24	0.69
1:E:415:GLU:OE2	1:E:419:ARG:NH2	2.24	0.69
1:B:415:GLU:OE2	1:B:419:ARG:NH2	2.24	0.68
1:D:415:GLU:OE2	1:D:419:ARG:NH2	2.24	0.67
1:A:415:GLU:OE2	1:A:419:ARG:NH2	2.24	0.67
1:C:463:GLN:NE2	2:C:601:NAI:H5N	2.04	0.67
1:F:463:GLN:NE2	2:F:601:NAI:H5N	2.04	0.66
1:A:463:GLN:NE2	2:A:602:NAI:H5N	2.04	0.66
1:F:415:GLU:OE2	1:F:419:ARG:NH2	2.24	0.66
1:D:463:GLN:NE2	2:D:602:NAI:H5N	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLU:OE2	1:C:419:ARG:NH2	2.24	0.66
1:E:239:THR:O	1:E:245:LYS:NZ	2.22	0.65
1:B:239:THR:O	1:B:245:LYS:NZ	2.22	0.65
1:E:463:GLN:NE2	2:E:602:NAI:H5N	2.04	0.65
1:B:463:GLN:NE2	2:B:602:NAI:H5N	2.04	0.65
1:A:239:THR:O	1:A:245:LYS:NZ	2.22	0.64
1:D:239:THR:O	1:D:245:LYS:NZ	2.22	0.64
1:C:239:THR:O	1:C:245:LYS:NZ	2.22	0.64
1:F:239:THR:O	1:F:245:LYS:NZ	2.22	0.63
1:D:252:PHE:CZ	1:D:257:LEU:HD13	2.34	0.63
1:A:252:PHE:CZ	1:A:257:LEU:HD13	2.34	0.62
1:C:252:PHE:CZ	1:C:257:LEU:HD13	2.34	0.62
1:F:252:PHE:CZ	1:F:257:LEU:HD13	2.34	0.62
2:B:602:NAI:O2N	1:C:396:ARG:NH2	2.29	0.61
2:E:602:NAI:O2N	1:F:396:ARG:NH2	2.29	0.61
1:A:319:CYS:SG	1:A:320:ASP:N	2.74	0.61
1:D:319:CYS:SG	1:D:320:ASP:N	2.74	0.61
1:B:319:CYS:SG	1:B:320:ASP:N	2.74	0.61
1:E:319:CYS:SG	1:E:320:ASP:N	2.74	0.61
1:F:370:ASP:N	1:F:370:ASP:OD1	2.32	0.61
1:E:252:PHE:CZ	1:E:257:LEU:HD13	2.34	0.60
1:B:252:PHE:CZ	1:B:257:LEU:HD13	2.34	0.60
1:A:315:LEU:HD11	1:A:330:GLN:HG3	1.83	0.60
1:F:315:LEU:HD11	1:F:330:GLN:HG3	1.83	0.60
1:C:315:LEU:HD11	1:C:330:GLN:HG3	1.83	0.60
1:D:315:LEU:HD11	1:D:330:GLN:HG3	1.83	0.60
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.67	0.60
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.67	0.60
1:F:319:CYS:SG	1:F:320:ASP:N	2.74	0.60
1:B:315:LEU:HD11	1:B:330:GLN:HG3	1.83	0.60
1:C:319:CYS:SG	1:C:320:ASP:N	2.74	0.60
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.67	0.59
1:E:315:LEU:HD11	1:E:330:GLN:HG3	1.83	0.59
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.67	0.59
1:D:396:ARG:NH2	2:F:601:NAI:O2N	2.29	0.59
1:A:396:ARG:NH2	2:C:601:NAI:O2N	2.29	0.59
2:A:602:NAI:O2N	1:B:396:ARG:NH2	2.29	0.59
1:C:223:ILE:HD11	1:C:263:LEU:HD21	1.85	0.59
1:F:223:ILE:HD11	1:F:263:LEU:HD21	1.85	0.59
1:A:223:ILE:HD11	1:A:263:LEU:HD21	1.85	0.58
1:C:334:SER:O	1:C:338:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ILE:HD11	1:D:263:LEU:HD21	1.85	0.58
1:F:334:SER:O	1:F:338:ARG:NH2	2.36	0.58
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.66	0.58
1:A:372:TYR:CD2	1:A:373:LEU:HD23	2.38	0.58
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.66	0.58
1:D:10:PHE:HD1	1:D:106:ALA:HB2	1.69	0.58
1:D:372:TYR:CD2	1:D:373:LEU:HD23	2.38	0.58
1:A:10:PHE:HD1	1:A:106:ALA:HB2	1.69	0.58
2:D:602:NAI:O2N	1:E:396:ARG:NH2	2.29	0.58
1:E:10:PHE:HD1	1:E:106:ALA:HB2	1.69	0.58
1:F:372:TYR:CD2	1:F:373:LEU:HD23	2.38	0.58
1:A:370:ASP:OD1	1:A:370:ASP:N	2.32	0.58
1:B:215:THR:HG21	2:B:601:NAI:H42N	1.86	0.58
1:C:372:TYR:CD2	1:C:373:LEU:HD23	2.38	0.58
1:D:334:SER:O	1:D:338:ARG:NH2	2.36	0.58
1:E:215:THR:HG21	2:E:601:NAI:H42N	1.86	0.58
1:A:334:SER:O	1:A:338:ARG:NH2	2.36	0.58
1:B:10:PHE:HD1	1:B:106:ALA:HB2	1.69	0.58
1:D:370:ASP:OD1	1:D:370:ASP:N	2.32	0.58
1:B:223:ILE:HD11	1:B:263:LEU:HD21	1.85	0.57
1:C:10:PHE:HD1	1:C:106:ALA:HB2	1.69	0.57
1:F:10:PHE:HD1	1:F:106:ALA:HB2	1.69	0.57
1:A:215:THR:HG21	2:A:601:NAI:H42N	1.86	0.57
1:B:334:SER:O	1:B:338:ARG:NH2	2.36	0.57
1:D:215:THR:HG21	2:D:601:NAI:H42N	1.86	0.57
1:E:223:ILE:HD11	1:E:263:LEU:HD21	1.85	0.57
1:E:334:SER:O	1:E:338:ARG:NH2	2.36	0.57
1:B:372:TYR:CD2	1:B:373:LEU:HD23	2.38	0.57
1:C:215:THR:HG21	2:C:602:NAI:H42N	1.86	0.57
1:E:372:TYR:CD2	1:E:373:LEU:HD23	2.38	0.57
1:F:215:THR:HG21	2:F:602:NAI:H42N	1.86	0.57
1:C:294:PHE:O	1:C:298:HIS:ND1	2.38	0.57
1:F:294:PHE:O	1:F:298:HIS:ND1	2.38	0.57
1:B:114:LYS:HE3	1:B:378:VAL:HG21	1.87	0.57
1:E:114:LYS:HE3	1:E:378:VAL:HG21	1.87	0.57
1:B:294:PHE:O	1:B:298:HIS:ND1	2.38	0.56
1:E:294:PHE:O	1:E:298:HIS:ND1	2.38	0.56
1:A:332:THR:HG23	1:A:334:SER:H	1.71	0.56
1:C:255:VAL:HG23	2:C:602:NAI:O2N	2.05	0.56
1:A:294:PHE:O	1:A:298:HIS:ND1	2.38	0.56
1:D:294:PHE:O	1:D:298:HIS:ND1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:THR:HG23	1:D:334:SER:H	1.71	0.56
1:F:255:VAL:HG23	2:F:602:NAI:O2N	2.05	0.56
1:B:255:VAL:HG23	2:B:601:NAI:O2N	2.05	0.56
1:E:255:VAL:HG23	2:E:601:NAI:O2N	2.05	0.56
1:F:332:THR:HG23	1:F:334:SER:H	1.71	0.56
1:C:332:THR:HG23	1:C:334:SER:H	1.71	0.56
1:C:114:LYS:HE3	1:C:378:VAL:HG21	1.87	0.56
1:D:114:LYS:HE3	1:D:378:VAL:HG21	1.87	0.56
1:F:114:LYS:HE3	1:F:378:VAL:HG21	1.87	0.56
1:A:255:VAL:HG23	2:A:601:NAI:O2N	2.05	0.56
1:A:114:LYS:HE3	1:A:378:VAL:HG21	1.87	0.56
1:D:255:VAL:HG23	2:D:601:NAI:O2N	2.05	0.56
1:E:332:THR:HG23	1:E:334:SER:H	1.71	0.55
1:B:332:THR:HG23	1:B:334:SER:H	1.71	0.55
1:F:274:GLY:HA2	1:F:279:SER:HA	1.88	0.55
1:C:274:GLY:HA2	1:C:279:SER:HA	1.88	0.55
1:B:195:HIS:O	1:B:201:LYS:NZ	2.38	0.55
1:E:195:HIS:O	1:E:201:LYS:NZ	2.38	0.55
1:D:274:GLY:HA2	1:D:279:SER:HA	1.88	0.54
1:A:274:GLY:HA2	1:A:279:SER:HA	1.88	0.54
1:B:274:GLY:HA2	1:B:279:SER:HA	1.88	0.54
1:C:195:HIS:O	1:C:201:LYS:NZ	2.38	0.54
1:E:274:GLY:HA2	1:E:279:SER:HA	1.88	0.54
1:F:195:HIS:O	1:F:201:LYS:NZ	2.38	0.54
1:A:195:HIS:O	1:A:201:LYS:NZ	2.38	0.54
1:C:89:CYS:HB2	1:C:163:ASP:OD1	2.09	0.53
1:D:195:HIS:O	1:D:201:LYS:NZ	2.38	0.53
1:F:89:CYS:HB2	1:F:163:ASP:OD1	2.09	0.53
1:A:276:SER:HB3	2:A:601:NAI:C4A	2.39	0.53
1:E:89:CYS:HB2	1:E:163:ASP:OD1	2.09	0.53
1:A:89:CYS:HB2	1:A:163:ASP:OD1	2.09	0.53
1:B:89:CYS:HB2	1:B:163:ASP:OD1	2.09	0.53
1:D:276:SER:HB3	2:D:601:NAI:C4A	2.39	0.53
1:F:276:SER:HB3	2:F:602:NAI:C4A	2.39	0.53
1:C:276:SER:HB3	2:C:602:NAI:C4A	2.39	0.53
1:D:89:CYS:HB2	1:D:163:ASP:OD1	2.09	0.52
1:E:276:SER:HB3	2:E:601:NAI:C4A	2.39	0.52
1:B:276:SER:HB3	2:B:601:NAI:C4A	2.39	0.52
1:C:63:PHE:CZ	1:C:148:PHE:HD1	2.29	0.51
1:F:63:PHE:CZ	1:F:148:PHE:HD1	2.29	0.51
1:A:432:PRO:HB3	1:A:436:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:PRO:HB3	1:D:436:PHE:CD2	2.46	0.50
1:B:418:GLU:O	1:B:422:GLY:HA3	2.12	0.50
1:E:418:GLU:O	1:E:422:GLY:HA3	2.12	0.50
1:F:432:PRO:HB3	1:F:436:PHE:CD2	2.46	0.50
1:C:432:PRO:HB3	1:C:436:PHE:CD2	2.46	0.50
1:C:252:PHE:C	1:C:252:PHE:CD2	2.86	0.50
1:F:252:PHE:CD2	1:F:252:PHE:C	2.86	0.50
1:E:63:PHE:CZ	1:E:148:PHE:HD1	2.29	0.49
1:A:418:GLU:O	1:A:422:GLY:HA3	2.12	0.49
1:B:63:PHE:CZ	1:B:148:PHE:HD1	2.29	0.49
1:A:63:PHE:CZ	1:A:148:PHE:HD1	2.29	0.49
1:B:63:PHE:HB2	1:B:75:ILE:HB	1.95	0.49
1:C:374:ASN:OD1	2:C:602:NAI:C5N	2.61	0.49
1:D:418:GLU:O	1:D:422:GLY:HA3	2.12	0.49
1:E:63:PHE:HB2	1:E:75:ILE:HB	1.95	0.49
1:F:374:ASN:OD1	2:F:602:NAI:C5N	2.61	0.49
1:B:63:PHE:HZ	1:B:148:PHE:HD1	1.59	0.49
1:D:63:PHE:CZ	1:D:148:PHE:HD1	2.29	0.49
1:F:252:PHE:HZ	1:F:257:LEU:HD13	1.77	0.49
1:A:252:PHE:CD2	1:A:252:PHE:C	2.86	0.49
1:A:374:ASN:OD1	2:A:601:NAI:C5N	2.61	0.49
1:B:252:PHE:HZ	1:B:257:LEU:HD13	1.77	0.49
1:B:374:ASN:OD1	2:B:601:NAI:C5N	2.61	0.49
1:C:252:PHE:HZ	1:C:257:LEU:HD13	1.77	0.49
1:D:252:PHE:CD2	1:D:252:PHE:C	2.86	0.49
1:D:374:ASN:OD1	2:D:601:NAI:C5N	2.61	0.49
1:E:63:PHE:HZ	1:E:148:PHE:HD1	1.59	0.49
1:E:374:ASN:OD1	2:E:601:NAI:C5N	2.61	0.49
1:F:252:PHE:CD1	1:F:273:VAL:HG11	2.36	0.49
1:F:63:PHE:HB2	1:F:75:ILE:HB	1.95	0.49
1:B:432:PRO:HB3	1:B:436:PHE:CD2	2.46	0.49
1:C:63:PHE:HB2	1:C:75:ILE:HB	1.95	0.49
1:C:293:ASP:HA	1:C:296:LEU:HD12	1.95	0.49
1:C:418:GLU:O	1:C:422:GLY:HA3	2.12	0.49
1:E:252:PHE:HZ	1:E:257:LEU:HD13	1.77	0.49
1:E:432:PRO:HB3	1:E:436:PHE:CD2	2.46	0.49
1:F:293:ASP:HA	1:F:296:LEU:HD12	1.95	0.49
1:D:250:GLN:O	1:D:325:ALA:HB3	2.13	0.49
1:F:418:GLU:O	1:F:422:GLY:HA3	2.12	0.49
1:A:250:GLN:O	1:A:325:ALA:HB3	2.13	0.48
1:A:346:GLU:OE2	1:A:478:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG21	1:B:260:MET:HG2	1.95	0.48
1:B:315:LEU:HA	1:B:322:LEU:HD11	1.95	0.48
1:B:370:ASP:N	1:B:370:ASP:OD1	2.32	0.48
1:C:252:PHE:CD1	1:C:273:VAL:HG11	2.36	0.48
1:C:63:PHE:HZ	1:C:148:PHE:HD1	1.59	0.48
1:D:346:GLU:OE2	1:D:478:ARG:NH2	2.46	0.48
1:E:249:VAL:HG21	1:E:260:MET:HG2	1.95	0.48
1:E:315:LEU:HA	1:E:322:LEU:HD11	1.95	0.48
1:F:372:TYR:OH	1:F:457:MET:O	2.30	0.48
1:B:346:GLU:OE2	1:B:478:ARG:NH2	2.46	0.48
1:C:346:GLU:OE2	1:C:478:ARG:NH2	2.46	0.48
1:E:346:GLU:OE2	1:E:478:ARG:NH2	2.46	0.48
1:F:63:PHE:HZ	1:F:148:PHE:HD1	1.59	0.48
1:B:293:ASP:HA	1:B:296:LEU:HD12	1.96	0.48
1:C:372:TYR:OH	1:C:457:MET:O	2.30	0.48
1:E:293:ASP:HA	1:E:296:LEU:HD12	1.96	0.48
1:F:346:GLU:OE2	1:F:478:ARG:NH2	2.46	0.48
1:E:370:ASP:N	1:E:370:ASP:OD1	2.32	0.48
1:A:293:ASP:HA	1:A:296:LEU:HD12	1.95	0.48
1:B:252:PHE:CD2	1:B:252:PHE:C	2.86	0.48
1:C:315:LEU:HA	1:C:322:LEU:HD11	1.95	0.48
1:D:63:PHE:HZ	1:D:148:PHE:HD1	1.59	0.48
1:E:252:PHE:C	1:E:252:PHE:CD2	2.86	0.48
1:A:63:PHE:HB2	1:A:75:ILE:HB	1.95	0.48
1:D:252:PHE:CD1	1:D:273:VAL:HG11	2.36	0.48
1:D:293:ASP:HA	1:D:296:LEU:HD12	1.95	0.48
1:D:372:TYR:OH	1:D:457:MET:O	2.30	0.48
1:F:315:LEU:HA	1:F:322:LEU:HD11	1.95	0.48
1:A:372:TYR:OH	1:A:457:MET:O	2.30	0.48
1:A:63:PHE:HZ	1:A:148:PHE:HD1	1.59	0.48
1:A:430:ILE:HD13	1:B:416:SER:HB3	1.96	0.48
1:D:63:PHE:HB2	1:D:75:ILE:HB	1.95	0.48
1:E:250:GLN:O	1:E:325:ALA:HB3	2.13	0.48
1:D:430:ILE:HD13	1:E:416:SER:HB3	1.96	0.48
1:A:252:PHE:HZ	1:A:257:LEU:HD13	1.77	0.48
1:B:250:GLN:O	1:B:325:ALA:HB3	2.13	0.48
1:C:250:GLN:O	1:C:325:ALA:HB3	2.13	0.48
1:D:252:PHE:HZ	1:D:257:LEU:HD13	1.77	0.48
1:F:250:GLN:O	1:F:325:ALA:HB3	2.13	0.48
1:A:168:ASP:OD1	1:A:169:MET:N	2.45	0.48
1:A:252:PHE:CD1	1:A:273:VAL:HG11	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ASP:OD1	1:D:169:MET:N	2.45	0.47
1:A:72:TRP:CH2	1:E:498:VAL:HB	2.49	0.47
1:B:498:VAL:HB	1:D:72:TRP:CH2	2.49	0.47
1:B:372:TYR:OH	1:B:457:MET:O	2.30	0.47
1:E:430:ILE:HD13	1:F:416:SER:HB3	1.96	0.47
1:B:430:ILE:HD13	1:C:416:SER:HB3	1.96	0.47
1:C:72:TRP:CH2	1:F:498:VAL:HB	2.49	0.47
1:A:498:VAL:HB	1:E:72:TRP:CH2	2.49	0.47
1:C:498:VAL:HB	1:F:72:TRP:CH2	2.49	0.47
1:D:249:VAL:HG21	1:D:260:MET:HG2	1.95	0.47
1:B:72:TRP:CH2	1:D:498:VAL:HB	2.49	0.47
1:E:372:TYR:OH	1:E:457:MET:O	2.30	0.47
1:A:249:VAL:HG21	1:A:260:MET:HG2	1.95	0.47
1:A:315:LEU:HA	1:A:322:LEU:HD11	1.95	0.47
1:D:315:LEU:HA	1:D:322:LEU:HD11	1.95	0.47
1:A:63:PHE:O	1:A:74:VAL:HA	2.15	0.47
1:C:249:VAL:HG21	1:C:260:MET:HG2	1.95	0.47
1:D:63:PHE:O	1:D:74:VAL:HA	2.15	0.47
1:F:249:VAL:HG21	1:F:260:MET:HG2	1.95	0.47
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.97	0.47
1:A:416:SER:HB3	1:C:430:ILE:HD13	1.96	0.47
1:D:416:SER:HB3	1:F:430:ILE:HD13	1.96	0.47
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.97	0.47
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.97	0.46
1:C:63:PHE:O	1:C:74:VAL:HA	2.15	0.46
1:F:63:PHE:O	1:F:74:VAL:HA	2.15	0.46
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.97	0.46
1:B:282:ASN:HB2	1:B:307:ALA:HB1	1.98	0.46
1:E:85:HIS:CD2	1:E:86:ARG:HG3	2.51	0.46
1:A:251:GLY:HA2	2:A:601:NAI:H1B	1.98	0.46
1:A:85:HIS:CD2	1:A:86:ARG:HG3	2.50	0.46
1:B:168:ASP:OD1	1:B:169:MET:N	2.45	0.46
1:B:85:HIS:CD2	1:B:86:ARG:HG3	2.51	0.46
1:D:85:HIS:CD2	1:D:86:ARG:HG3	2.50	0.46
1:E:282:ASN:HB2	1:E:307:ALA:HB1	1.98	0.46
1:D:251:GLY:HA2	2:D:601:NAI:H1B	1.98	0.46
1:D:282:ASN:HB2	1:D:307:ALA:HB1	1.98	0.46
1:E:168:ASP:OD1	1:E:169:MET:N	2.45	0.46
1:B:377:GLY:HA2	1:B:380:VAL:HG22	1.98	0.46
1:A:282:ASN:HB2	1:A:307:ALA:HB1	1.98	0.46
1:C:85:HIS:CD2	1:C:86:ARG:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:GLY:HA2	1:E:380:VAL:HG22	1.98	0.46
1:B:63:PHE:O	1:B:74:VAL:HA	2.15	0.45
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.97	0.45
1:E:63:PHE:O	1:E:74:VAL:HA	2.15	0.45
1:F:85:HIS:CD2	1:F:86:ARG:HG3	2.51	0.45
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.97	0.45
1:C:251:GLY:HA2	2:C:602:NAI:H1B	1.98	0.45
1:C:8:ASN:OD1	1:C:9:PHE:N	2.49	0.45
1:F:251:GLY:HA2	2:F:602:NAI:H1B	1.98	0.45
1:C:168:ASP:OD1	1:C:169:MET:N	2.45	0.45
1:F:377:GLY:HA2	1:F:380:VAL:HG22	1.98	0.45
1:B:463:GLN:NE2	2:B:602:NAI:C4N	2.79	0.45
1:C:282:ASN:HB2	1:C:307:ALA:HB1	1.98	0.45
1:C:377:GLY:HA2	1:C:380:VAL:HG22	1.98	0.45
1:E:8:ASN:OD1	1:E:9:PHE:N	2.49	0.45
1:F:8:ASN:OD1	1:F:9:PHE:N	2.49	0.45
1:A:8:ASN:OD1	1:A:9:PHE:N	2.49	0.44
1:A:377:GLY:HA2	1:A:380:VAL:HG22	1.98	0.44
1:B:8:ASN:OD1	1:B:9:PHE:N	2.49	0.44
1:D:377:GLY:HA2	1:D:380:VAL:HG22	1.98	0.44
1:E:463:GLN:NE2	2:E:602:NAI:C4N	2.79	0.44
1:F:168:ASP:OD1	1:F:169:MET:N	2.45	0.44
1:F:282:ASN:HB2	1:F:307:ALA:HB1	1.98	0.44
1:D:8:ASN:OD1	1:D:9:PHE:N	2.49	0.44
1:E:252:PHE:CD1	1:E:273:VAL:HG11	2.36	0.44
1:B:251:GLY:HA2	2:B:601:NAI:H1B	1.98	0.44
1:E:251:GLY:HA2	2:E:601:NAI:H1B	1.98	0.44
1:B:252:PHE:CD1	1:B:273:VAL:HG11	2.36	0.44
1:A:217:ARG:HD3	1:A:262:TYR:CZ	2.54	0.43
1:C:63:PHE:CZ	1:C:148:PHE:HA	2.53	0.43
1:D:28:LEU:HD21	1:D:490:PHE:CD2	2.54	0.43
1:F:63:PHE:CZ	1:F:148:PHE:HA	2.53	0.43
1:F:281:TRP:CE3	1:F:308:LYS:HD3	2.53	0.43
1:A:28:LEU:HD21	1:A:490:PHE:CD2	2.54	0.43
1:B:494:ASN:HB3	1:B:495:GLU:OE1	2.19	0.43
1:C:217:ARG:HD3	1:C:262:TYR:CZ	2.54	0.43
1:C:281:TRP:CE3	1:C:308:LYS:HD3	2.53	0.43
1:D:217:ARG:HD3	1:D:262:TYR:CZ	2.54	0.43
1:E:28:LEU:HD21	1:E:490:PHE:CD2	2.54	0.43
1:E:281:TRP:CE3	1:E:308:LYS:HD3	2.53	0.43
1:E:63:PHE:CZ	1:E:148:PHE:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TRP:CE3	1:A:308:LYS:HD3	2.53	0.43
1:B:63:PHE:CZ	1:B:148:PHE:HA	2.53	0.43
1:B:217:ARG:HD3	1:B:262:TYR:CZ	2.54	0.43
1:B:281:TRP:CE3	1:B:308:LYS:HD3	2.53	0.43
1:B:28:LEU:HD21	1:B:490:PHE:CD2	2.54	0.43
1:E:217:ARG:HD3	1:E:262:TYR:CZ	2.54	0.43
1:E:494:ASN:HB3	1:E:495:GLU:OE1	2.19	0.43
1:F:217:ARG:HD3	1:F:262:TYR:CZ	2.54	0.43
1:C:28:LEU:HD21	1:C:490:PHE:CD2	2.54	0.43
1:C:370:ASP:OD1	1:C:370:ASP:N	2.32	0.43
1:D:281:TRP:CE3	1:D:308:LYS:HD3	2.53	0.43
1:F:28:LEU:HD21	1:F:490:PHE:CD2	2.54	0.43
1:A:463:GLN:NE2	2:A:602:NAI:C4N	2.79	0.43
1:A:494:ASN:HB3	1:A:495:GLU:OE1	2.19	0.43
1:D:494:ASN:HB3	1:D:495:GLU:OE1	2.19	0.43
1:D:463:GLN:NE2	2:D:602:NAI:C4N	2.79	0.42
1:A:346:GLU:HB3	1:A:351:PRO:HG2	2.01	0.42
1:D:346:GLU:HB3	1:D:351:PRO:HG2	2.01	0.42
1:F:133:PRO:HG2	1:F:170:SER:HB3	2.02	0.42
1:A:63:PHE:CZ	1:A:148:PHE:HA	2.54	0.42
1:C:133:PRO:HG2	1:C:170:SER:HB3	2.02	0.42
1:C:494:ASN:HB3	1:C:495:GLU:OE1	2.19	0.42
1:A:252:PHE:C	1:A:252:PHE:HD2	2.23	0.42
1:D:63:PHE:CZ	1:D:148:PHE:HA	2.54	0.42
1:F:494:ASN:HB3	1:F:495:GLU:OE1	2.19	0.42
1:C:463:GLN:NE2	2:C:601:NAI:C4N	2.79	0.42
1:A:279:SER:HB3	1:A:310:TYR:O	2.20	0.42
1:D:252:PHE:C	1:D:252:PHE:HD2	2.23	0.42
1:D:279:SER:HB3	1:D:310:TYR:O	2.20	0.42
1:A:444:SER:OG	1:A:445:GLU:N	2.53	0.42
1:B:459:ARG:HH22	1:C:396:ARG:NH2	2.18	0.42
1:D:444:SER:OG	1:D:445:GLU:N	2.53	0.42
1:E:459:ARG:HH22	1:F:396:ARG:NH2	2.18	0.41
1:F:463:GLN:NE2	2:F:601:NAI:C4N	2.79	0.41
1:B:133:PRO:HG2	1:B:170:SER:HB3	2.02	0.41
1:B:27:LYS:HG3	1:B:471:TYR:CE1	2.56	0.41
1:E:133:PRO:HG2	1:E:170:SER:HB3	2.02	0.41
1:E:27:LYS:HG3	1:E:471:TYR:CE1	2.56	0.41
1:F:346:GLU:HB3	1:F:351:PRO:HG2	2.01	0.41
1:A:369:PRO:HB3	1:A:478:ARG:HA	2.03	0.41
1:C:346:GLU:HB3	1:C:351:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:PRO:HB3	1:D:478:ARG:HA	2.03	0.41
1:E:372:TYR:CD2	1:E:373:LEU:CD2	3.03	0.41
1:F:152:LEU:HD23	1:F:158:ILE:HD11	2.03	0.41
1:F:217:ARG:HD3	1:F:262:TYR:CE1	2.55	0.41
1:B:372:TYR:CD2	1:B:373:LEU:CD2	3.03	0.41
1:C:152:LEU:HD23	1:C:158:ILE:HD11	2.03	0.41
1:C:217:ARG:HD3	1:C:262:TYR:CE1	2.55	0.41
1:E:444:SER:OG	1:E:445:GLU:N	2.53	0.41
1:A:459:ARG:HH22	1:B:396:ARG:NH2	2.18	0.41
1:B:152:LEU:HD23	1:B:158:ILE:HD11	2.03	0.41
1:B:217:ARG:HD3	1:B:262:TYR:CE1	2.55	0.41
1:B:369:PRO:HB3	1:B:478:ARG:HA	2.03	0.41
1:C:279:SER:HB3	1:C:310:TYR:O	2.20	0.41
1:E:152:LEU:HD23	1:E:158:ILE:HD11	2.03	0.41
1:E:369:PRO:HB3	1:E:478:ARG:HA	2.03	0.41
1:A:372:TYR:CD2	1:A:373:LEU:CD2	3.03	0.41
1:A:8:ASN:O	1:A:12:MET:HG3	2.21	0.41
1:B:444:SER:OG	1:B:445:GLU:N	2.53	0.41
1:D:152:LEU:HD23	1:D:158:ILE:HD11	2.03	0.41
1:D:459:ARG:HH22	1:E:396:ARG:NH2	2.18	0.41
1:D:8:ASN:O	1:D:12:MET:HG3	2.21	0.41
1:E:217:ARG:HD3	1:E:262:TYR:CE1	2.55	0.41
1:F:279:SER:HB3	1:F:310:TYR:O	2.20	0.41
1:A:133:PRO:HG2	1:A:170:SER:HB3	2.02	0.41
1:A:152:LEU:HD23	1:A:158:ILE:HD11	2.03	0.41
1:C:252:PHE:C	1:C:252:PHE:HD2	2.23	0.41
1:C:444:SER:OG	1:C:445:GLU:N	2.53	0.41
1:D:133:PRO:HG2	1:D:170:SER:HB3	2.02	0.41
1:D:372:TYR:CD2	1:D:373:LEU:CD2	3.03	0.41
1:E:252:PHE:C	1:E:252:PHE:HD2	2.23	0.41
1:E:279:SER:HB3	1:E:310:TYR:O	2.20	0.41
1:F:444:SER:OG	1:F:445:GLU:N	2.53	0.41
1:A:27:LYS:HG3	1:A:471:TYR:CE1	2.56	0.41
1:A:374:ASN:OD1	2:A:601:NAI:H5N	2.21	0.41
1:B:279:SER:HB3	1:B:310:TYR:O	2.20	0.41
1:D:27:LYS:HG3	1:D:471:TYR:CE1	2.56	0.41
1:A:433:THR:HG22	1:B:415:GLU:OE1	2.21	0.41
1:B:9:PHE:O	1:B:12:MET:N	2.54	0.41
1:C:372:TYR:CD2	1:C:373:LEU:CD2	3.03	0.41
1:D:374:ASN:OD1	2:D:601:NAI:H5N	2.21	0.41
1:D:59:LEU:HG	1:D:60:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:THR:HG22	1:E:415:GLU:OE1	2.21	0.41
1:E:9:PHE:O	1:E:12:MET:N	2.54	0.41
1:F:252:PHE:HD2	1:F:252:PHE:C	2.23	0.41
1:F:27:LYS:HG3	1:F:471:TYR:CE1	2.56	0.41
1:A:217:ARG:HD3	1:A:262:TYR:CE1	2.55	0.41
1:A:396:ARG:NH2	1:C:459:ARG:HH22	2.18	0.41
1:A:59:LEU:HG	1:A:60:SER:H	1.86	0.41
1:B:8:ASN:O	1:B:12:MET:HG3	2.21	0.41
1:C:27:LYS:HG3	1:C:471:TYR:CE1	2.56	0.41
1:C:6:ASP:OD1	1:C:329:LYS:HD2	2.22	0.41
1:D:217:ARG:HD3	1:D:262:TYR:CE1	2.55	0.41
1:F:8:ASN:O	1:F:12:MET:HG3	2.21	0.41
1:F:6:ASP:OD1	1:F:329:LYS:HD2	2.22	0.41
1:F:372:TYR:CD2	1:F:373:LEU:CD2	3.03	0.41
1:B:252:PHE:HD2	1:B:252:PHE:C	2.23	0.40
1:D:396:ARG:NH2	1:F:459:ARG:HH22	2.18	0.40
1:E:8:ASN:O	1:E:12:MET:HG3	2.21	0.40
1:F:59:LEU:HG	1:F:60:SER:H	1.86	0.40
1:C:8:ASN:O	1:C:12:MET:HG3	2.21	0.40
1:C:369:PRO:HB3	1:C:478:ARG:HA	2.03	0.40
1:E:346:GLU:HB3	1:E:351:PRO:HG2	2.01	0.40
1:F:369:PRO:HB3	1:F:478:ARG:HA	2.03	0.40
1:C:59:LEU:HG	1:C:60:SER:H	1.86	0.40
1:D:59:LEU:HG	1:D:60:SER:N	2.37	0.40
1:E:59:LEU:HG	1:E:60:SER:H	1.86	0.40
1:E:6:ASP:OD1	1:E:329:LYS:HD2	2.22	0.40
1:A:59:LEU:HG	1:A:60:SER:N	2.37	0.40
1:B:346:GLU:HB3	1:B:351:PRO:HG2	2.01	0.40
1:B:6:ASP:OD1	1:B:329:LYS:HD2	2.22	0.40
1:A:415:GLU:OE1	1:C:433:THR:HG22	2.21	0.40
1:D:415:GLU:OE1	1:F:433:THR:HG22	2.21	0.40
1:B:59:LEU:HG	1:B:60:SER:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/501 (99%)	462 (94%)	28 (6%)	4 (1%)	24	62
1	B	494/501 (99%)	462 (94%)	28 (6%)	4 (1%)	24	62
1	C	494/501 (99%)	463 (94%)	27 (6%)	4 (1%)	24	62
1	D	494/501 (99%)	462 (94%)	28 (6%)	4 (1%)	24	62
1	E	494/501 (99%)	462 (94%)	28 (6%)	4 (1%)	24	62
1	F	494/501 (99%)	463 (94%)	27 (6%)	4 (1%)	24	62
All	All	2964/3006 (99%)	2774 (94%)	166 (6%)	24 (1%)	29	62

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	GLY
1	A	326	ALA
1	B	251	GLY
1	B	326	ALA
1	C	251	GLY
1	C	326	ALA
1	D	251	GLY
1	D	326	ALA
1	E	251	GLY
1	E	326	ALA
1	F	251	GLY
1	F	326	ALA
1	A	374	ASN
1	B	374	ASN
1	C	374	ASN
1	D	374	ASN
1	E	374	ASN
1	F	374	ASN
1	A	324	PRO
1	B	324	PRO
1	C	324	PRO
1	D	324	PRO
1	E	324	PRO
1	F	324	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	416/420 (99%)	412 (99%)	4 (1%)	82 91
1	B	416/420 (99%)	412 (99%)	4 (1%)	82 91
1	C	416/420 (99%)	412 (99%)	4 (1%)	82 91
1	D	416/420 (99%)	412 (99%)	4 (1%)	82 91
1	E	416/420 (99%)	412 (99%)	4 (1%)	82 91
1	F	416/420 (99%)	412 (99%)	4 (1%)	82 91
All	All	2496/2520 (99%)	2472 (99%)	24 (1%)	83 91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	PHE
1	A	370	ASP
1	A	371	LEU
1	A	373	LEU
1	B	252	PHE
1	B	370	ASP
1	B	371	LEU
1	B	373	LEU
1	C	252	PHE
1	C	370	ASP
1	C	371	LEU
1	C	373	LEU
1	D	252	PHE
1	D	370	ASP
1	D	371	LEU
1	D	373	LEU
1	E	252	PHE
1	E	370	ASP
1	E	371	LEU
1	E	373	LEU
1	F	252	PHE
1	F	370	ASP

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Mol	Chain	Res	Type
1	F	371	LEU
1	F	373	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	258	HIS
1	A	463	GLN
1	B	225	ASN
1	B	258	HIS
1	B	463	GLN
1	C	225	ASN
1	C	258	HIS
1	C	463	GLN
1	D	225	ASN
1	D	258	HIS
1	D	463	GLN
1	E	225	ASN
1	E	258	HIS
1	E	463	GLN
1	F	225	ASN
1	F	258	HIS
1	F	463	GLN

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 (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAI	A	601	-	41,48,48	1.64	8 (19%)	46,73,73	2.05	10 (21%)
2	NAI	A	602	-	41,48,48	1.61	9 (21%)	46,73,73	2.07	12 (26%)
2	NAI	B	601	-	41,48,48	1.64	9 (21%)	46,73,73	2.04	10 (21%)
2	NAI	B	602	-	41,48,48	1.62	9 (21%)	46,73,73	2.06	12 (26%)
2	NAI	C	601	-	41,48,48	1.62	9 (21%)	46,73,73	2.07	12 (26%)
2	NAI	C	602	-	41,48,48	1.64	9 (21%)	46,73,73	2.05	10 (21%)
2	NAI	D	601	-	41,48,48	1.64	8 (19%)	46,73,73	2.05	10 (21%)
2	NAI	D	602	-	41,48,48	1.61	9 (21%)	46,73,73	2.07	12 (26%)
2	NAI	E	601	-	41,48,48	1.64	9 (21%)	46,73,73	2.04	10 (21%)
2	NAI	E	602	-	41,48,48	1.62	9 (21%)	46,73,73	2.06	12 (26%)
2	NAI	F	601	-	41,48,48	1.62	9 (21%)	46,73,73	2.07	12 (26%)
2	NAI	F	602	-	41,48,48	1.64	9 (21%)	46,73,73	2.05	10 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	601	-	-	0/25/72/72	0/5/5/5
2	NAI	A	602	-	-	0/25/72/72	0/5/5/5
2	NAI	B	601	-	-	0/25/72/72	0/5/5/5
2	NAI	B	602	-	-	0/25/72/72	0/5/5/5
2	NAI	C	601	-	-	0/25/72/72	0/5/5/5
2	NAI	C	602	-	-	0/25/72/72	0/5/5/5
2	NAI	D	601	-	-	0/25/72/72	0/5/5/5
2	NAI	D	602	-	-	0/25/72/72	0/5/5/5
2	NAI	E	601	-	-	0/25/72/72	0/5/5/5
2	NAI	E	602	-	-	0/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	F	601	-	-	0/25/72/72	0/5/5/5
2	NAI	F	602	-	-	0/25/72/72	0/5/5/5

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NAI	PN-O2N	-2.65	1.41	1.51
2	B	601	NAI	PN-O2N	-2.65	1.41	1.51
2	A	601	NAI	PN-O2N	-2.64	1.41	1.51
2	D	601	NAI	PN-O2N	-2.64	1.41	1.51
2	F	602	NAI	PN-O2N	-2.64	1.41	1.51
2	C	602	NAI	PN-O2N	-2.64	1.41	1.51
2	F	602	NAI	O3D-C3D	-2.42	1.37	1.43
2	C	602	NAI	O3D-C3D	-2.42	1.37	1.43
2	B	602	NAI	PN-O2N	-2.40	1.42	1.51
2	E	602	NAI	PN-O2N	-2.40	1.42	1.51
2	C	601	NAI	PN-O2N	-2.39	1.42	1.51
2	F	601	NAI	PN-O2N	-2.39	1.42	1.51
2	D	602	NAI	PN-O2N	-2.39	1.42	1.51
2	A	602	NAI	PN-O2N	-2.39	1.42	1.51
2	A	601	NAI	O3D-C3D	-2.38	1.37	1.43
2	E	601	NAI	O3D-C3D	-2.38	1.37	1.43
2	D	601	NAI	O3D-C3D	-2.38	1.37	1.43
2	B	601	NAI	O3D-C3D	-2.38	1.37	1.43
2	B	602	NAI	PA-O2A	-2.16	1.45	1.55
2	C	601	NAI	PA-O2A	-2.16	1.45	1.55
2	F	601	NAI	PA-O2A	-2.16	1.45	1.55
2	E	602	NAI	PA-O2A	-2.16	1.45	1.55
2	D	602	NAI	PA-O2A	-2.15	1.45	1.55
2	A	602	NAI	PA-O2A	-2.15	1.45	1.55
2	D	602	NAI	O3D-C3D	-2.13	1.37	1.43
2	A	602	NAI	O3D-C3D	-2.13	1.37	1.43
2	B	602	NAI	O3D-C3D	-2.11	1.38	1.43
2	E	602	NAI	O3D-C3D	-2.11	1.38	1.43
2	E	601	NAI	C3D-C4D	-2.11	1.47	1.53
2	B	601	NAI	C3D-C4D	-2.11	1.47	1.53
2	A	601	NAI	C3D-C4D	-2.11	1.47	1.53
2	D	601	NAI	C3D-C4D	-2.11	1.47	1.53
2	F	602	NAI	C3D-C4D	-2.11	1.47	1.53
2	C	602	NAI	C3D-C4D	-2.11	1.47	1.53
2	E	601	NAI	PA-O1A	-2.10	1.43	1.51
2	B	601	NAI	PA-O1A	-2.10	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAI	O3D-C3D	-2.10	1.38	1.43
2	F	601	NAI	O3D-C3D	-2.10	1.38	1.43
2	F	602	NAI	PA-O1A	-2.10	1.43	1.51
2	C	602	NAI	PA-O1A	-2.10	1.43	1.51
2	A	601	NAI	PA-O1A	-2.10	1.43	1.51
2	D	601	NAI	PA-O1A	-2.10	1.43	1.51
2	B	602	NAI	C3D-C4D	-2.06	1.47	1.53
2	E	602	NAI	C3D-C4D	-2.06	1.47	1.53
2	C	601	NAI	C3D-C4D	-2.05	1.47	1.53
2	F	601	NAI	C3D-C4D	-2.05	1.47	1.53
2	D	602	NAI	C3D-C4D	-2.05	1.47	1.53
2	A	602	NAI	C3D-C4D	-2.05	1.47	1.53
2	E	601	NAI	C4N-C5N	-2.04	1.44	1.49
2	B	601	NAI	C4N-C5N	-2.04	1.44	1.49
2	F	602	NAI	C4N-C5N	-2.03	1.44	1.49
2	C	602	NAI	C4N-C5N	-2.03	1.44	1.49
2	A	601	NAI	C4N-C5N	-2.03	1.44	1.49
2	D	601	NAI	C4N-C5N	-2.03	1.44	1.49
2	A	601	NAI	C5B-C4B	-2.03	1.45	1.51
2	D	601	NAI	C5B-C4B	-2.03	1.45	1.51
2	F	602	NAI	C5B-C4B	-2.02	1.45	1.51
2	C	602	NAI	C5B-C4B	-2.02	1.45	1.51
2	E	601	NAI	C5B-C4B	-2.02	1.45	1.51
2	B	601	NAI	C5B-C4B	-2.02	1.45	1.51
2	E	601	NAI	C2A-N1A	2.02	1.37	1.33
2	B	601	NAI	C2A-N1A	2.02	1.37	1.33
2	F	602	NAI	C6N-C5N	2.02	1.36	1.33
2	C	602	NAI	C6N-C5N	2.02	1.36	1.33
2	C	601	NAI	C3B-C4B	2.22	1.58	1.53
2	F	601	NAI	C3B-C4B	2.22	1.58	1.53
2	D	602	NAI	C3B-C4B	2.23	1.59	1.53
2	A	602	NAI	C3B-C4B	2.23	1.59	1.53
2	B	602	NAI	C3B-C4B	2.23	1.59	1.53
2	E	602	NAI	C3B-C4B	2.23	1.59	1.53
2	D	602	NAI	C2B-C1B	2.46	1.57	1.53
2	A	602	NAI	C2B-C1B	2.46	1.57	1.53
2	B	602	NAI	C2B-C1B	2.46	1.57	1.53
2	E	602	NAI	C2B-C1B	2.46	1.57	1.53
2	C	601	NAI	C2B-C1B	2.47	1.57	1.53
2	F	601	NAI	C2B-C1B	2.47	1.57	1.53
2	D	602	NAI	O4B-C1B	3.23	1.45	1.41
2	A	602	NAI	O4B-C1B	3.23	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAI	O4B-C1B	3.26	1.45	1.41
2	E	602	NAI	O4B-C1B	3.26	1.45	1.41
2	C	601	NAI	O4B-C1B	3.28	1.45	1.41
2	F	601	NAI	O4B-C1B	3.28	1.45	1.41
2	B	602	NAI	C4A-N3A	3.93	1.41	1.35
2	E	602	NAI	C4A-N3A	3.93	1.41	1.35
2	C	601	NAI	C4A-N3A	3.94	1.41	1.35
2	F	601	NAI	C4A-N3A	3.94	1.41	1.35
2	D	602	NAI	C4A-N3A	3.96	1.41	1.35
2	A	602	NAI	C4A-N3A	3.96	1.41	1.35
2	D	602	NAI	C6N-C5N	4.08	1.40	1.33
2	A	602	NAI	C6N-C5N	4.08	1.40	1.33
2	C	601	NAI	C6N-C5N	4.10	1.40	1.33
2	F	601	NAI	C6N-C5N	4.10	1.40	1.33
2	B	602	NAI	C6N-C5N	4.15	1.40	1.33
2	E	602	NAI	C6N-C5N	4.15	1.40	1.33
2	F	602	NAI	O4B-C1B	4.16	1.47	1.41
2	C	602	NAI	O4B-C1B	4.16	1.47	1.41
2	A	601	NAI	O4B-C1B	4.19	1.47	1.41
2	D	601	NAI	O4B-C1B	4.19	1.47	1.41
2	E	601	NAI	O4B-C1B	4.20	1.47	1.41
2	B	601	NAI	O4B-C1B	4.20	1.47	1.41
2	F	602	NAI	C4A-N3A	5.36	1.43	1.35
2	C	602	NAI	C4A-N3A	5.36	1.43	1.35
2	E	601	NAI	C4A-N3A	5.37	1.43	1.35
2	B	601	NAI	C4A-N3A	5.37	1.43	1.35
2	A	601	NAI	C4A-N3A	5.37	1.43	1.35
2	D	601	NAI	C4A-N3A	5.37	1.43	1.35

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	NAI	C3N-C2N-N1N	-7.13	112.77	123.24
2	D	601	NAI	C3N-C2N-N1N	-7.13	112.77	123.24
2	F	602	NAI	C3N-C2N-N1N	-7.11	112.79	123.24
2	C	602	NAI	C3N-C2N-N1N	-7.11	112.79	123.24
2	E	601	NAI	C3N-C2N-N1N	-7.10	112.80	123.24
2	B	601	NAI	C3N-C2N-N1N	-7.10	112.80	123.24
2	D	602	NAI	N3A-C2A-N1A	-6.37	123.87	128.87
2	A	602	NAI	N3A-C2A-N1A	-6.37	123.87	128.87
2	C	601	NAI	N3A-C2A-N1A	-6.35	123.88	128.87
2	F	601	NAI	N3A-C2A-N1A	-6.35	123.88	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	NAI	N3A-C2A-N1A	-6.32	123.91	128.87
2	E	602	NAI	N3A-C2A-N1A	-6.32	123.91	128.87
2	C	601	NAI	C3N-C2N-N1N	-5.67	114.91	123.24
2	F	601	NAI	C3N-C2N-N1N	-5.67	114.91	123.24
2	D	602	NAI	C3N-C2N-N1N	-5.67	114.91	123.24
2	A	602	NAI	C3N-C2N-N1N	-5.67	114.91	123.24
2	B	602	NAI	C3N-C2N-N1N	-5.65	114.93	123.24
2	E	602	NAI	C3N-C2N-N1N	-5.65	114.93	123.24
2	A	601	NAI	N3A-C2A-N1A	-5.43	124.61	128.87
2	D	601	NAI	N3A-C2A-N1A	-5.43	124.61	128.87
2	F	602	NAI	N3A-C2A-N1A	-5.41	124.62	128.87
2	C	602	NAI	N3A-C2A-N1A	-5.41	124.62	128.87
2	E	601	NAI	N3A-C2A-N1A	-5.39	124.64	128.87
2	B	601	NAI	N3A-C2A-N1A	-5.39	124.64	128.87
2	C	601	NAI	C1D-N1N-C2N	-3.48	114.81	120.85
2	F	601	NAI	C1D-N1N-C2N	-3.48	114.81	120.85
2	D	602	NAI	C1D-N1N-C2N	-3.48	114.81	120.85
2	A	602	NAI	C1D-N1N-C2N	-3.48	114.81	120.85
2	B	602	NAI	C1D-N1N-C2N	-3.47	114.81	120.85
2	E	602	NAI	C1D-N1N-C2N	-3.47	114.81	120.85
2	A	601	NAI	C1D-N1N-C6N	-3.30	113.42	120.80
2	D	601	NAI	C1D-N1N-C6N	-3.30	113.42	120.80
2	E	601	NAI	C1D-N1N-C6N	-3.29	113.44	120.80
2	B	601	NAI	C1D-N1N-C6N	-3.29	113.44	120.80
2	F	602	NAI	C1D-N1N-C6N	-3.28	113.47	120.80
2	C	602	NAI	C1D-N1N-C6N	-3.28	113.47	120.80
2	E	601	NAI	C1B-N9A-C4A	-3.17	123.26	126.81
2	B	601	NAI	C1B-N9A-C4A	-3.17	123.26	126.81
2	F	602	NAI	C1B-N9A-C4A	-3.17	123.27	126.81
2	C	602	NAI	C1B-N9A-C4A	-3.17	123.27	126.81
2	A	601	NAI	C1B-N9A-C4A	-3.16	123.28	126.81
2	D	601	NAI	C1B-N9A-C4A	-3.16	123.28	126.81
2	B	602	NAI	C3D-C2D-C1D	-3.10	95.21	101.44
2	E	602	NAI	C3D-C2D-C1D	-3.10	95.21	101.44
2	D	602	NAI	C3D-C2D-C1D	-3.09	95.22	101.44
2	A	602	NAI	C3D-C2D-C1D	-3.09	95.22	101.44
2	C	601	NAI	C3D-C2D-C1D	-3.08	95.25	101.44
2	F	601	NAI	C3D-C2D-C1D	-3.08	95.25	101.44
2	F	602	NAI	C3D-C2D-C1D	-3.05	95.31	101.44
2	C	602	NAI	C3D-C2D-C1D	-3.05	95.31	101.44
2	A	601	NAI	C3D-C2D-C1D	-3.05	95.31	101.44
2	D	601	NAI	C3D-C2D-C1D	-3.05	95.31	101.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	NAI	C3D-C2D-C1D	-3.04	95.32	101.44
2	B	601	NAI	C3D-C2D-C1D	-3.04	95.32	101.44
2	B	602	NAI	C4D-O4D-C1D	-2.99	102.93	109.52
2	E	602	NAI	C4D-O4D-C1D	-2.99	102.93	109.52
2	D	602	NAI	C4D-O4D-C1D	-2.98	102.96	109.52
2	A	602	NAI	C4D-O4D-C1D	-2.98	102.96	109.52
2	C	601	NAI	C4D-O4D-C1D	-2.98	102.96	109.52
2	F	601	NAI	C4D-O4D-C1D	-2.98	102.96	109.52
2	C	601	NAI	O4B-C1B-N9A	-2.89	102.64	108.11
2	F	601	NAI	O4B-C1B-N9A	-2.89	102.64	108.11
2	D	602	NAI	O4B-C1B-N9A	-2.89	102.65	108.11
2	A	602	NAI	O4B-C1B-N9A	-2.89	102.65	108.11
2	B	602	NAI	O4B-C1B-N9A	-2.86	102.70	108.11
2	E	602	NAI	O4B-C1B-N9A	-2.86	102.70	108.11
2	A	601	NAI	C4B-O4B-C1B	-2.75	106.73	109.64
2	D	601	NAI	C4B-O4B-C1B	-2.75	106.73	109.64
2	E	601	NAI	C4B-O4B-C1B	-2.72	106.76	109.64
2	B	601	NAI	C4B-O4B-C1B	-2.72	106.76	109.64
2	F	602	NAI	C4B-O4B-C1B	-2.71	106.77	109.64
2	C	602	NAI	C4B-O4B-C1B	-2.71	106.77	109.64
2	C	601	NAI	C1B-N9A-C4A	-2.47	124.05	126.81
2	F	601	NAI	C1B-N9A-C4A	-2.47	124.05	126.81
2	B	602	NAI	C1B-N9A-C4A	-2.42	124.10	126.81
2	E	602	NAI	C1B-N9A-C4A	-2.42	124.10	126.81
2	D	602	NAI	C1B-N9A-C4A	-2.41	124.12	126.81
2	A	602	NAI	C1B-N9A-C4A	-2.41	124.12	126.81
2	F	602	NAI	N6A-C6A-N1A	2.06	121.98	118.52
2	C	602	NAI	N6A-C6A-N1A	2.06	121.98	118.52
2	A	601	NAI	N6A-C6A-N1A	2.07	121.99	118.52
2	D	601	NAI	N6A-C6A-N1A	2.07	121.99	118.52
2	E	601	NAI	N6A-C6A-N1A	2.07	121.99	118.52
2	B	601	NAI	N6A-C6A-N1A	2.07	121.99	118.52
2	C	601	NAI	C2B-C3B-C4B	2.34	107.43	102.64
2	F	601	NAI	C2B-C3B-C4B	2.34	107.43	102.64
2	D	602	NAI	C2B-C3B-C4B	2.35	107.44	102.64
2	A	602	NAI	C2B-C3B-C4B	2.35	107.44	102.64
2	B	602	NAI	C2B-C3B-C4B	2.37	107.48	102.64
2	E	602	NAI	C2B-C3B-C4B	2.37	107.48	102.64
2	B	602	NAI	O2A-PA-O5B	2.38	119.58	108.24
2	E	602	NAI	O2A-PA-O5B	2.38	119.58	108.24
2	D	602	NAI	O2A-PA-O5B	2.38	119.59	108.24
2	A	602	NAI	O2A-PA-O5B	2.38	119.59	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NAI	O2A-PA-O5B	2.38	119.60	108.24
2	F	601	NAI	O2A-PA-O5B	2.38	119.60	108.24
2	F	602	NAI	O2A-PA-O5B	2.67	120.98	108.24
2	C	602	NAI	O2A-PA-O5B	2.67	120.98	108.24
2	A	601	NAI	O2A-PA-O5B	2.68	121.00	108.24
2	D	601	NAI	O2A-PA-O5B	2.68	121.00	108.24
2	E	601	NAI	O2A-PA-O5B	2.68	121.02	108.24
2	B	601	NAI	O2A-PA-O5B	2.68	121.02	108.24
2	C	601	NAI	C6N-N1N-C2N	3.34	127.13	118.52
2	F	601	NAI	C6N-N1N-C2N	3.34	127.13	118.52
2	B	602	NAI	C6N-N1N-C2N	3.35	127.13	118.52
2	E	602	NAI	C6N-N1N-C2N	3.35	127.13	118.52
2	D	602	NAI	C6N-N1N-C2N	3.35	127.15	118.52
2	A	602	NAI	C6N-N1N-C2N	3.35	127.15	118.52
2	E	601	NAI	C6N-N1N-C2N	3.58	127.75	118.52
2	B	601	NAI	C6N-N1N-C2N	3.58	127.75	118.52
2	A	601	NAI	C6N-N1N-C2N	3.59	127.76	118.52
2	D	601	NAI	C6N-N1N-C2N	3.59	127.76	118.52
2	F	602	NAI	C6N-N1N-C2N	3.59	127.76	118.52
2	C	602	NAI	C6N-N1N-C2N	3.59	127.76	118.52
2	E	601	NAI	C2A-N1A-C6A	3.89	125.70	118.77
2	B	601	NAI	C2A-N1A-C6A	3.89	125.70	118.77
2	F	602	NAI	C2A-N1A-C6A	3.89	125.70	118.77
2	C	602	NAI	C2A-N1A-C6A	3.89	125.70	118.77
2	A	601	NAI	C2A-N1A-C6A	3.91	125.75	118.77
2	D	601	NAI	C2A-N1A-C6A	3.91	125.75	118.77
2	B	602	NAI	O4D-C1D-N1N	3.94	115.61	108.09
2	E	602	NAI	O4D-C1D-N1N	3.94	115.61	108.09
2	C	601	NAI	O4D-C1D-N1N	3.96	115.65	108.09
2	F	601	NAI	O4D-C1D-N1N	3.96	115.65	108.09
2	D	602	NAI	O4D-C1D-N1N	3.96	115.65	108.09
2	A	602	NAI	O4D-C1D-N1N	3.96	115.65	108.09
2	B	602	NAI	C2A-N1A-C6A	4.21	126.29	118.77
2	E	602	NAI	C2A-N1A-C6A	4.21	126.29	118.77
2	C	601	NAI	C2A-N1A-C6A	4.21	126.29	118.77
2	F	601	NAI	C2A-N1A-C6A	4.21	126.29	118.77
2	D	602	NAI	C2A-N1A-C6A	4.24	126.33	118.77
2	A	602	NAI	C2A-N1A-C6A	4.24	126.33	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAI	6	0
2	A	602	NAI	6	0
2	B	601	NAI	5	0
2	B	602	NAI	6	0
2	C	601	NAI	6	0
2	C	602	NAI	5	0
2	D	601	NAI	6	0
2	D	602	NAI	6	0
2	E	601	NAI	5	0
2	E	602	NAI	6	0
2	F	601	NAI	6	0
2	F	602	NAI	5	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.