



wwPDB EM Map/Model Validation Report ⓘ

May 2, 2016 – 06:57 PM EDT

PDB ID : 3JD1
EMDB ID: : EMD-6634
Title : Glutamate dehydrogenase in complex with NADH, closed conformation
Authors : Borgnia, M.J.; Banerjee, S.; Merk, A.; Matthies, D.; Bartesaghi, A.; Rao, P.;
Pierson, J.; Earl, L.A.; Falconieri, V.; Subramaniam, S.; Milne, J.L.S.
Deposited on : 2016-03-28
Resolution : 3.30 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

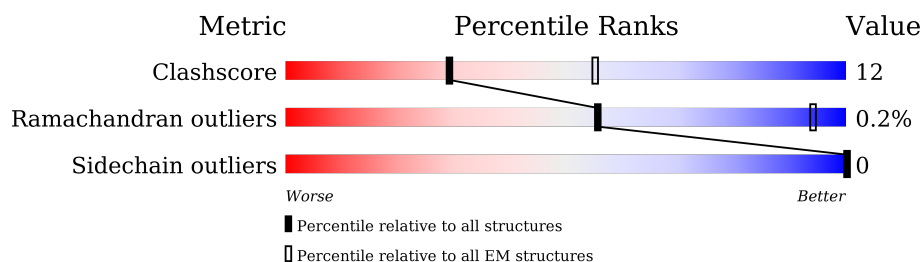
1 Overall quality at a glance

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	501	76% 22% .
1	B	501	76% 23% .
1	C	501	74% 24% .
1	D	501	75% 23% .
1	E	501	76% 22% .
1	F	501	74% 24% .

2 Entry composition [i](#)

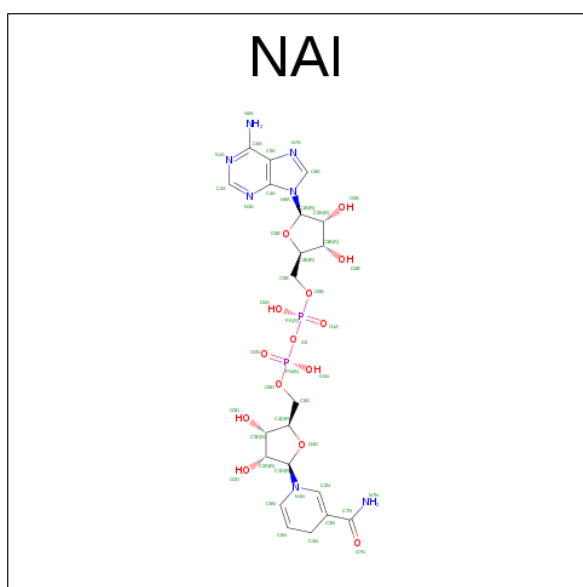
There are 2 unique types of molecules in this entry. The entry contains 23814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₂₁H₂₉N₇O₁₄P₂).

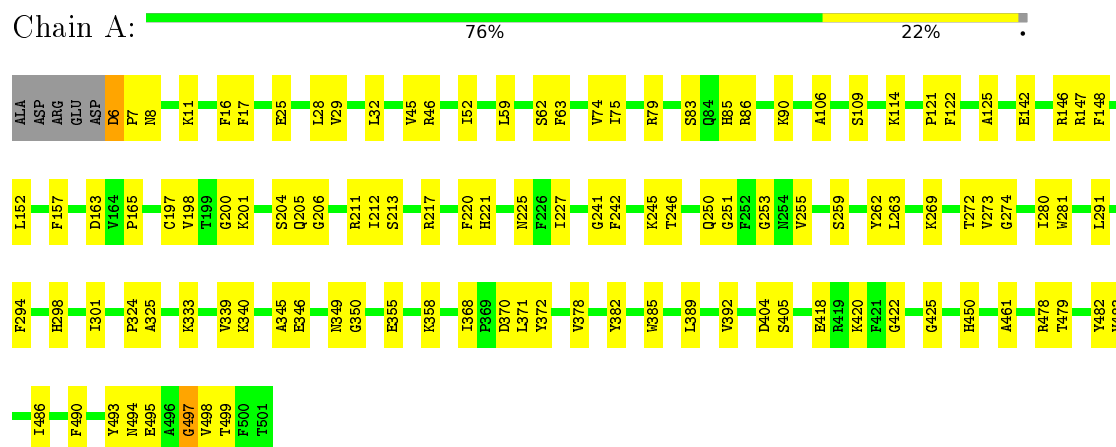


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	D	1	Total	C	N	O	P	0
	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

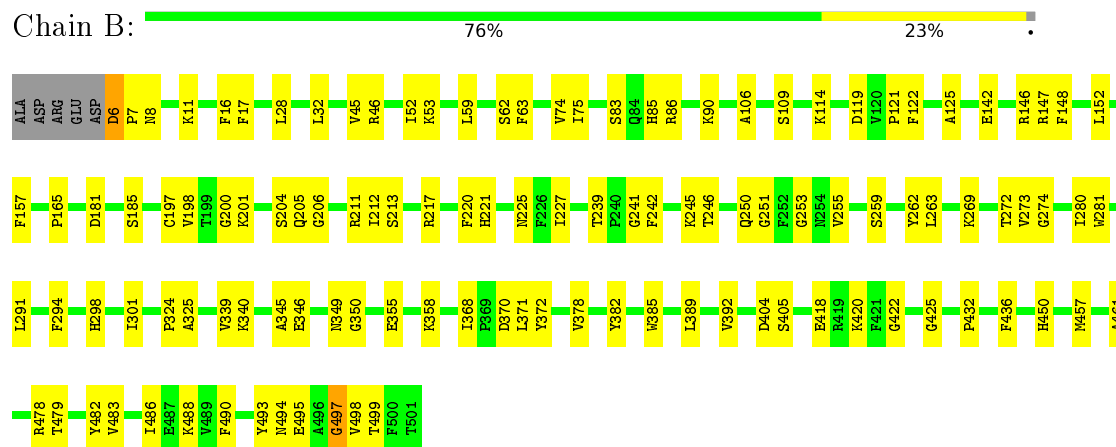
3 Residue-property plots [i](#)

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.

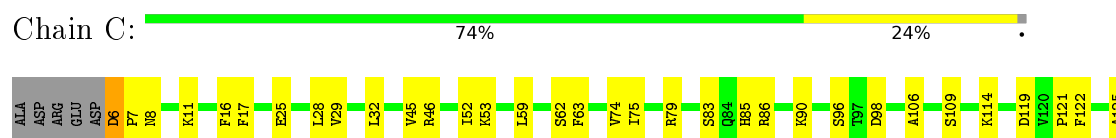
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



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T272	T273	G274	I280	W281	L291	F294	H298	T301	P324	A325	K333	Y339	K340	A345	E346	N349	G350	T355	K356	I368	P369	D370	L371	Y372	Y378	Y382	H385	L389	Y392	D404	S405	E415	E418	R419	K420	F421	G422
G425	P432	F436	H450	A461	R478	T479	Y482	V483	I486	E487	K488	Y489	F490	Y493	N494	E495	A496	G497	V498	T499	F500	T501															

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	34926	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 ($e^-/\text{\AA}^2$)	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	0.63	0/3964	0.52	1/5351 (0.0%)
1	B	0.63	0/3964	0.52	1/5351 (0.0%)
1	C	0.63	0/3964	0.52	1/5351 (0.0%)
1	D	0.63	0/3964	0.52	1/5351 (0.0%)
1	E	0.63	0/3964	0.52	1/5351 (0.0%)
1	F	0.63	0/3964	0.52	1/5351 (0.0%)
All	All	0.63	0/23784	0.52	6/32106 (0.0%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ASP	C-N-CD	5.24	139.40	128.40
1	D	6	ASP	C-N-CD	5.24	139.40	128.40
1	B	6	ASP	C-N-CD	5.22	139.35	128.40
1	E	6	ASP	C-N-CD	5.22	139.35	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ASP	C-N-CD	5.21	139.34	128.40
1	F	6	ASP	C-N-CD	5.21	139.34	128.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

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

5.2 Too-close contacts

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	88	0
1	B	3881	0	3848	92	0
1	C	3881	0	3848	96	0
1	D	3881	0	3848	92	0
1	E	3881	0	3848	90	0
1	F	3881	0	3848	94	0
2	A	88	0	54	22	0
2	B	88	0	54	22	0
2	C	88	0	54	23	0
2	D	88	0	54	22	0
2	E	88	0	54	23	0
2	F	88	0	54	23	0
All	All	23814	0	23412	576	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 12.

All (576) 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:F:253:GLY:HA2	2:F:601:NAI:O2A	1.49	1.13
1:C:253:GLY:HA2	2:C:601:NAI:O2A	1.49	1.13
1:E:253:GLY:HA2	2:E:601:NAI:O2A	1.49	1.11
1:D:253:GLY:HA2	2:D:601:NAI:O2A	1.49	1.10
1:A:253:GLY:HA2	2:A:601:NAI:O2A	1.49	1.10
1:B:253:GLY:HA2	2:B:601:NAI:O2A	1.49	1.10
1:D:221:HIS:O	1:D:225:ASN:ND2	1.99	0.96
1:A:221:HIS:O	1:A:225:ASN:ND2	1.99	0.95
1:D:206:GLY:N	2:D:602:NAI:H5N	1.80	0.95
1:E:221:HIS:O	1:E:225:ASN:ND2	1.99	0.95
1:E:325:ALA:O	2:E:601:NAI:H4D	1.66	0.95
1:B:221:HIS:O	1:B:225:ASN:ND2	1.99	0.95
1:B:325:ALA:O	2:B:601:NAI:H4D	1.66	0.95
1:A:206:GLY:N	2:A:602:NAI:H5N	1.80	0.95
1:B:206:GLY:N	2:B:602:NAI:H5N	1.80	0.95
1:C:206:GLY:N	2:C:602:NAI:H5N	1.80	0.95
1:E:206:GLY:N	2:E:602:NAI:H5N	1.80	0.95
1:F:206:GLY:N	2:F:602:NAI:H5N	1.80	0.95
1:C:325:ALA:O	2:C:601:NAI:H4D	1.66	0.95
1:F:325:ALA:O	2:F:601:NAI:H4D	1.66	0.95
1:C:221:HIS:O	1:C:225:ASN:ND2	1.99	0.94
1:A:325:ALA:O	2:A:601:NAI:H4D	1.66	0.94
1:F:221:HIS:O	1:F:225:ASN:ND2	1.99	0.94
1:D:325:ALA:O	2:D:601:NAI:H4D	1.66	0.94
1:C:253:GLY:CA	2:C:601:NAI:O2A	2.16	0.94
1:F:253:GLY:CA	2:F:601:NAI:O2A	2.16	0.94
1:D:253:GLY:CA	2:D:601:NAI:O2A	2.16	0.93
1:A:253:GLY:CA	2:A:601:NAI:O2A	2.16	0.93
1:E:253:GLY:CA	2:E:601:NAI:O2A	2.16	0.93
1:B:253:GLY:CA	2:B:601:NAI:O2A	2.16	0.93
1:A:350:GLY:N	1:A:370:ASP:OD2	2.08	0.87
1:D:350:GLY:N	1:D:370:ASP:OD2	2.08	0.87
1:E:350:GLY:N	1:E:370:ASP:OD2	2.08	0.87
1:B:350:GLY:N	1:B:370:ASP:OD2	2.08	0.86
1:F:272:THR:OG1	1:F:280:ILE:O	1.94	0.86
1:C:272:THR:OG1	1:C:280:ILE:O	1.94	0.86
1:C:350:GLY:N	1:C:370:ASP:OD2	2.08	0.86
2:A:602:NAI:PN	2:A:602:NAI:H52A	2.16	0.86
2:D:602:NAI:H52A	2:D:602:NAI:PN	2.16	0.86
1:F:350:GLY:N	1:F:370:ASP:OD2	2.08	0.86
1:A:272:THR:OG1	1:A:280:ILE:O	1.93	0.86
2:B:602:NAI:H52A	2:B:602:NAI:PN	2.16	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:602:NAI:H52A	2:E:602:NAI:PN	2.16	0.85
1:D:272:THR:OG1	1:D:280:ILE:O	1.93	0.85
1:E:272:THR:OG1	1:E:280:ILE:O	1.94	0.85
1:B:272:THR:OG1	1:B:280:ILE:O	1.94	0.85
2:F:602:NAI:PN	2:F:602:NAI:H52A	2.16	0.85
2:C:602:NAI:H52A	2:C:602:NAI:PN	2.16	0.85
1:A:206:GLY:CA	2:A:602:NAI:H5N	2.09	0.82
1:D:206:GLY:CA	2:D:602:NAI:H5N	2.09	0.82
1:C:206:GLY:CA	2:C:602:NAI:H5N	2.09	0.81
1:F:206:GLY:CA	2:F:602:NAI:H5N	2.09	0.81
1:B:206:GLY:CA	2:B:602:NAI:H5N	2.09	0.81
1:E:206:GLY:CA	2:E:602:NAI:H5N	2.09	0.81
1:A:6:ASP:HB3	1:A:7:PRO:HD3	1.64	0.79
1:D:6:ASP:HB3	1:D:7:PRO:HD3	1.64	0.79
1:C:6:ASP:HB3	1:C:7:PRO:HD3	1.64	0.78
1:F:6:ASP:HB3	1:F:7:PRO:HD3	1.64	0.78
1:B:325:ALA:O	2:B:601:NAI:H51N	1.84	0.78
1:A:497:GLY:O	1:A:499:THR:N	2.17	0.78
1:D:497:GLY:O	1:D:499:THR:N	2.17	0.78
1:E:325:ALA:O	2:E:601:NAI:H51N	1.84	0.78
1:F:325:ALA:O	2:F:601:NAI:H51N	1.84	0.78
1:C:325:ALA:O	2:C:601:NAI:H51N	1.84	0.78
1:A:325:ALA:O	2:A:601:NAI:H51N	1.84	0.77
1:D:325:ALA:O	2:D:601:NAI:H51N	1.84	0.77
1:E:6:ASP:HB3	1:E:7:PRO:HD3	1.64	0.77
1:B:6:ASP:HB3	1:B:7:PRO:HD3	1.64	0.77
1:E:497:GLY:O	1:E:499:THR:N	2.17	0.77
1:B:497:GLY:O	1:B:499:THR:N	2.17	0.77
1:C:497:GLY:O	1:C:499:THR:N	2.17	0.77
1:F:497:GLY:O	1:F:499:THR:N	2.17	0.77
1:B:325:ALA:O	2:B:601:NAI:C5D	2.34	0.76
1:E:325:ALA:O	2:E:601:NAI:C5D	2.34	0.76
1:A:325:ALA:O	2:A:601:NAI:C5D	2.34	0.75
1:F:325:ALA:O	2:F:601:NAI:C5D	2.34	0.75
1:D:325:ALA:O	2:D:601:NAI:C5D	2.34	0.75
1:C:325:ALA:O	2:C:601:NAI:C5D	2.34	0.75
1:A:325:ALA:O	2:A:601:NAI:C4D	2.35	0.75
1:D:325:ALA:O	2:D:601:NAI:C4D	2.35	0.75
1:C:325:ALA:O	2:C:601:NAI:C4D	2.35	0.74
1:F:325:ALA:O	2:F:601:NAI:C4D	2.35	0.74
1:B:325:ALA:O	2:B:601:NAI:C4D	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ALA:O	2:E:601:NAI:C4D	2.35	0.73
2:C:602:NAI:O1N	2:C:602:NAI:H52A	1.89	0.73
2:F:602:NAI:O1N	2:F:602:NAI:H52A	1.89	0.73
2:E:602:NAI:H52A	2:E:602:NAI:O1N	1.88	0.73
2:B:602:NAI:O1N	2:B:602:NAI:H52A	1.88	0.73
2:A:602:NAI:O1N	2:A:602:NAI:H52A	1.88	0.72
2:D:602:NAI:H52A	2:D:602:NAI:O1N	1.88	0.72
1:D:495:GLU:OE1	1:E:204:SER:OG	2.06	0.71
1:A:204:SER:OG	1:C:495:GLU:OE1	2.06	0.70
1:A:90:LYS:O	1:A:125:ALA:N	2.24	0.69
1:E:90:LYS:O	1:E:125:ALA:N	2.24	0.69
1:B:90:LYS:O	1:B:125:ALA:N	2.24	0.69
1:D:90:LYS:O	1:D:125:ALA:N	2.24	0.69
1:C:90:LYS:O	1:C:125:ALA:N	2.24	0.69
1:F:90:LYS:O	1:F:125:ALA:N	2.24	0.69
2:B:601:NAI:PN	2:B:601:NAI:H71N	2.16	0.69
2:E:601:NAI:PN	2:E:601:NAI:H71N	2.16	0.69
2:C:601:NAI:PN	2:C:601:NAI:H71N	2.16	0.68
2:F:601:NAI:H71N	2:F:601:NAI:PN	2.16	0.68
2:D:601:NAI:H71N	2:D:601:NAI:PN	2.16	0.68
2:A:601:NAI:PN	2:A:601:NAI:H71N	2.16	0.68
1:C:16:PHE:HB3	1:C:482:TYR:HE2	1.59	0.67
1:F:16:PHE:HB3	1:F:482:TYR:HE2	1.59	0.67
1:D:16:PHE:HB3	1:D:482:TYR:HE2	1.60	0.67
1:A:16:PHE:HB3	1:A:482:TYR:HE2	1.60	0.66
1:E:16:PHE:HB3	1:E:482:TYR:HE2	1.60	0.66
1:B:16:PHE:HB3	1:B:482:TYR:HE2	1.60	0.66
2:A:601:NAI:O1N	2:A:601:NAI:H2N	1.99	0.63
2:D:601:NAI:O1N	2:D:601:NAI:H2N	1.99	0.63
2:E:601:NAI:O1N	2:E:601:NAI:H2N	1.99	0.63
2:B:601:NAI:O1N	2:B:601:NAI:H2N	1.99	0.63
1:D:420:LYS:NZ	1:F:425:GLY:O	2.28	0.63
2:F:601:NAI:H2N	2:F:601:NAI:O1N	1.99	0.63
2:C:601:NAI:H2N	2:C:601:NAI:O1N	1.99	0.62
1:A:420:LYS:NZ	1:C:425:GLY:O	2.28	0.62
1:B:371:LEU:HD11	1:B:482:TYR:CE1	2.36	0.61
1:E:425:GLY:O	1:F:420:LYS:NZ	2.28	0.61
1:E:371:LEU:HD11	1:E:482:TYR:CE1	2.36	0.61
1:B:425:GLY:O	1:C:420:LYS:NZ	2.28	0.61
1:A:217:ARG:HH12	1:A:450:HIS:CD2	2.19	0.61
1:A:371:LEU:HD11	1:A:482:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HH12	1:D:450:HIS:CD2	2.19	0.61
1:D:371:LEU:HD11	1:D:482:TYR:CE1	2.36	0.61
1:F:217:ARG:HH12	1:F:450:HIS:CD2	2.19	0.60
1:C:217:ARG:HH12	1:C:450:HIS:CD2	2.19	0.60
1:C:371:LEU:HD11	1:C:482:TYR:CE1	2.36	0.60
1:F:371:LEU:HD11	1:F:482:TYR:CE1	2.36	0.60
1:A:495:GLU:OE1	1:B:204:SER:OG	2.06	0.60
1:D:204:SER:OG	1:F:495:GLU:OE1	2.06	0.59
1:B:201:LYS:O	1:B:211:ARG:NH1	2.35	0.59
1:B:217:ARG:HH12	1:B:450:HIS:CD2	2.19	0.59
1:A:201:LYS:O	1:A:211:ARG:NH1	2.35	0.59
1:E:201:LYS:O	1:E:211:ARG:NH1	2.35	0.59
1:D:201:LYS:O	1:D:211:ARG:NH1	2.35	0.59
1:E:217:ARG:HH12	1:E:450:HIS:CD2	2.19	0.59
1:C:201:LYS:O	1:C:211:ARG:NH1	2.35	0.58
1:F:201:LYS:O	1:F:211:ARG:NH1	2.35	0.58
1:C:372:TYR:CZ	1:C:461:ALA:HB2	2.39	0.58
1:F:372:TYR:CZ	1:F:461:ALA:HB2	2.39	0.58
2:A:601:NAI:O2N	2:A:601:NAI:N7N	2.37	0.58
2:D:601:NAI:N7N	2:D:601:NAI:O2N	2.37	0.58
2:F:601:NAI:O2N	2:F:601:NAI:N7N	2.37	0.57
2:C:601:NAI:N7N	2:C:601:NAI:O2N	2.37	0.57
1:B:372:TYR:CZ	1:B:461:ALA:HB2	2.39	0.57
1:E:372:TYR:CZ	1:E:461:ALA:HB2	2.39	0.57
1:E:96:SER:OG	1:E:98:ASP:OD1	2.15	0.57
1:A:372:TYR:CZ	1:A:461:ALA:HB2	2.39	0.57
1:D:425:GLY:O	1:E:420:LYS:NZ	2.28	0.57
1:D:372:TYR:CZ	1:D:461:ALA:HB2	2.39	0.57
2:B:601:NAI:O2N	2:B:601:NAI:N7N	2.37	0.57
2:E:601:NAI:O2N	2:E:601:NAI:N7N	2.37	0.57
1:A:106:ALA:O	1:A:109:SER:OG	2.19	0.56
1:F:291:LEU:HA	1:F:294:PHE:CE2	2.40	0.56
1:C:291:LEU:HA	1:C:294:PHE:CE2	2.40	0.56
1:D:106:ALA:O	1:D:109:SER:OG	2.19	0.56
1:A:291:LEU:HA	1:A:294:PHE:CE2	2.40	0.56
1:D:291:LEU:HA	1:D:294:PHE:CE2	2.40	0.56
1:A:425:GLY:O	1:B:420:LYS:NZ	2.28	0.56
1:B:106:ALA:O	1:B:109:SER:OG	2.19	0.56
1:B:206:GLY:HA2	2:B:602:NAI:H5N	1.86	0.56
1:E:206:GLY:HA2	2:E:602:NAI:H5N	1.86	0.56
1:E:371:LEU:HD11	1:E:482:TYR:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:HB3	1:A:482:TYR:CE2	2.41	0.56
1:B:371:LEU:HD11	1:B:482:TYR:HE1	1.71	0.56
1:D:16:PHE:HB3	1:D:482:TYR:CE2	2.41	0.56
1:E:106:ALA:O	1:E:109:SER:OG	2.19	0.56
1:C:206:GLY:CA	2:C:602:NAI:C5N	2.84	0.56
1:B:291:LEU:HA	1:B:294:PHE:CE2	2.40	0.56
1:F:206:GLY:CA	2:F:602:NAI:C5N	2.84	0.56
1:B:16:PHE:HB3	1:B:482:TYR:CE2	2.41	0.55
1:F:371:LEU:HD11	1:F:482:TYR:HE1	1.71	0.55
1:C:371:LEU:HD11	1:C:482:TYR:HE1	1.71	0.55
1:E:16:PHE:HB3	1:E:482:TYR:CE2	2.41	0.55
1:E:291:LEU:HA	1:E:294:PHE:CE2	2.40	0.55
1:A:371:LEU:HD11	1:A:482:TYR:HE1	1.71	0.55
1:B:206:GLY:CA	2:B:602:NAI:C5N	2.84	0.55
1:B:294:PHE:CE1	1:B:301:ILE:HA	2.42	0.55
1:D:371:LEU:HD11	1:D:482:TYR:HE1	1.71	0.55
1:E:206:GLY:CA	2:E:602:NAI:C5N	2.84	0.55
1:E:294:PHE:CE1	1:E:301:ILE:HA	2.42	0.55
1:B:495:GLU:OE1	1:C:204:SER:OG	2.06	0.55
1:D:206:GLY:HA2	2:D:602:NAI:H5N	1.86	0.55
1:A:206:GLY:CA	2:A:602:NAI:C5N	2.84	0.55
1:C:16:PHE:HB3	1:C:482:TYR:CE2	2.41	0.55
1:A:206:GLY:HA2	2:A:602:NAI:H5N	1.86	0.55
1:D:206:GLY:CA	2:D:602:NAI:C5N	2.84	0.55
1:D:83:SER:OG	1:D:85:HIS:ND1	2.22	0.55
1:B:349:ASN:ND2	2:B:601:NAI:O2D	2.40	0.55
1:E:349:ASN:ND2	2:E:601:NAI:O2D	2.40	0.55
1:F:16:PHE:HB3	1:F:482:TYR:CE2	2.41	0.55
1:F:294:PHE:CE1	1:F:301:ILE:HA	2.42	0.55
1:B:392:VAL:N	2:B:602:NAI:O3D	2.40	0.55
1:C:294:PHE:CE1	1:C:301:ILE:HA	2.42	0.55
1:C:392:VAL:N	2:C:602:NAI:O3D	2.40	0.55
1:D:294:PHE:CE1	1:D:301:ILE:HA	2.42	0.55
1:F:392:VAL:N	2:F:602:NAI:O3D	2.40	0.55
1:E:392:VAL:N	2:E:602:NAI:O3D	2.40	0.54
1:A:294:PHE:CE1	1:A:301:ILE:HA	2.42	0.54
1:A:90:LYS:HD3	1:A:122:PHE:CD2	2.43	0.54
1:D:90:LYS:HD3	1:D:122:PHE:CD2	2.43	0.54
1:E:83:SER:OG	1:E:85:HIS:ND1	2.22	0.54
1:A:83:SER:OG	1:A:85:HIS:ND1	2.22	0.54
1:C:349:ASN:ND2	2:C:601:NAI:O2D	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:N	2:A:602:NAI:O3D	2.41	0.54
1:A:253:GLY:HA3	2:A:601:NAI:O2A	2.07	0.54
1:D:392:VAL:N	2:D:602:NAI:O3D	2.41	0.54
1:D:253:GLY:HA3	2:D:601:NAI:O2A	2.07	0.54
1:F:349:ASN:ND2	2:F:601:NAI:O2D	2.40	0.54
1:F:206:GLY:HA2	2:F:602:NAI:H5N	1.86	0.54
1:B:59:LEU:HB2	1:B:157:PHE:HE2	1.73	0.54
1:B:83:SER:OG	1:B:85:HIS:ND1	2.22	0.54
1:C:59:LEU:HB2	1:C:157:PHE:HE2	1.73	0.54
1:F:59:LEU:HB2	1:F:157:PHE:HE2	1.73	0.54
1:E:59:LEU:HB2	1:E:157:PHE:HE2	1.73	0.54
1:B:90:LYS:HD3	1:B:122:PHE:CD2	2.43	0.53
1:C:206:GLY:HA2	2:C:602:NAI:H5N	1.86	0.53
1:D:349:ASN:ND2	2:D:601:NAI:O2D	2.40	0.53
1:F:251:GLY:N	1:F:274:GLY:O	2.41	0.53
1:A:349:ASN:ND2	2:A:601:NAI:O2D	2.40	0.53
2:A:602:NAI:PN	2:A:602:NAI:C5B	2.94	0.53
1:C:251:GLY:N	1:C:274:GLY:O	2.41	0.53
2:D:602:NAI:PN	2:D:602:NAI:C5B	2.94	0.53
1:E:90:LYS:HD3	1:E:122:PHE:CD2	2.43	0.53
1:D:251:GLY:N	1:D:274:GLY:O	2.41	0.53
1:F:106:ALA:O	1:F:109:SER:OG	2.19	0.53
1:A:251:GLY:N	1:A:274:GLY:O	2.41	0.53
1:A:59:LEU:HB2	1:A:157:PHE:HE2	1.73	0.53
1:D:59:LEU:HB2	1:D:157:PHE:HE2	1.73	0.53
2:E:602:NAI:PN	2:E:602:NAI:C5B	2.94	0.53
1:F:90:LYS:HD3	1:F:122:PHE:CD2	2.43	0.53
1:C:90:LYS:HD3	1:C:122:PHE:CD2	2.43	0.53
1:F:253:GLY:HA3	2:F:601:NAI:O2A	2.07	0.52
2:B:602:NAI:C5B	2:B:602:NAI:PN	2.94	0.52
1:C:253:GLY:HA3	2:C:601:NAI:O2A	2.07	0.52
1:E:251:GLY:N	1:E:274:GLY:O	2.41	0.52
1:B:119:ASP:OD1	1:B:488:LYS:NZ	2.37	0.52
1:E:495:GLU:OE1	1:F:204:SER:OG	2.06	0.52
1:B:251:GLY:N	1:B:274:GLY:O	2.41	0.52
1:E:119:ASP:OD1	1:E:488:LYS:NZ	2.37	0.52
1:B:253:GLY:HA3	2:B:601:NAI:O2A	2.07	0.51
1:A:220:PHE:HD1	1:A:263:LEU:HD23	1.75	0.51
1:D:220:PHE:HD1	1:D:263:LEU:HD23	1.75	0.51
1:E:253:GLY:HA3	2:E:601:NAI:O2A	2.07	0.51
1:C:294:PHE:O	1:C:298:HIS:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:PHE:O	1:F:298:HIS:N	2.42	0.51
1:B:86:ARG:HD3	1:B:121:PRO:HA	1.93	0.51
1:E:86:ARG:HD3	1:E:121:PRO:HA	1.93	0.51
2:C:602:NAI:C5B	2:C:602:NAI:PN	2.94	0.51
2:F:602:NAI:PN	2:F:602:NAI:C5B	2.94	0.51
1:D:86:ARG:HD3	1:D:121:PRO:HA	1.93	0.50
1:A:86:ARG:HD3	1:A:121:PRO:HA	1.93	0.50
1:F:86:ARG:HD3	1:F:121:PRO:HA	1.93	0.50
1:C:86:ARG:HD3	1:C:121:PRO:HA	1.93	0.50
1:D:294:PHE:O	1:D:298:HIS:N	2.42	0.50
1:B:220:PHE:HD1	1:B:263:LEU:HD23	1.75	0.50
1:A:294:PHE:O	1:A:298:HIS:N	2.42	0.50
1:E:220:PHE:HD1	1:E:263:LEU:HD23	1.75	0.50
1:E:294:PHE:O	1:E:298:HIS:N	2.42	0.50
1:F:220:PHE:HD1	1:F:263:LEU:HD23	1.75	0.49
1:C:220:PHE:HD1	1:C:263:LEU:HD23	1.75	0.49
1:B:294:PHE:O	1:B:298:HIS:N	2.42	0.49
1:C:63:PHE:CZ	1:C:148:PHE:HA	2.47	0.49
1:F:119:ASP:OD1	1:F:488:LYS:NZ	2.37	0.49
1:F:63:PHE:CZ	1:F:148:PHE:HA	2.47	0.49
1:A:63:PHE:CZ	1:A:148:PHE:HA	2.47	0.49
1:D:255:VAL:O	1:D:259:SER:OG	2.23	0.49
1:E:63:PHE:CZ	1:E:148:PHE:HA	2.47	0.49
1:B:63:PHE:CZ	1:B:148:PHE:HA	2.47	0.49
1:D:63:PHE:CZ	1:D:148:PHE:HA	2.47	0.49
1:A:255:VAL:O	1:A:259:SER:OG	2.23	0.49
1:B:6:ASP:HB3	1:B:7:PRO:CD	2.38	0.49
1:C:90:LYS:CD	1:C:122:PHE:CD2	2.96	0.49
1:E:6:ASP:HB3	1:E:7:PRO:CD	2.38	0.49
1:F:90:LYS:CD	1:F:122:PHE:CD2	2.96	0.49
1:B:346:GLU:OE1	1:B:478:ARG:NH2	2.43	0.48
1:E:346:GLU:OE1	1:E:478:ARG:NH2	2.43	0.48
1:A:90:LYS:CD	1:A:122:PHE:CD2	2.96	0.48
1:D:90:LYS:CD	1:D:122:PHE:CD2	2.96	0.48
1:F:96:SER:OG	1:F:98:ASP:OD1	2.15	0.48
1:A:372:TYR:CG	1:A:372:TYR:O	2.67	0.48
1:D:372:TYR:CG	1:D:372:TYR:O	2.67	0.48
1:B:372:TYR:O	1:B:372:TYR:CG	2.67	0.48
1:E:372:TYR:CG	1:E:372:TYR:O	2.67	0.48
1:F:6:ASP:HB3	1:F:7:PRO:CD	2.38	0.48
2:A:601:NAI:PN	2:A:601:NAI:H2N	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:C	2:A:602:NAI:H5N	2.32	0.48
1:C:6:ASP:HB3	1:C:7:PRO:CD	2.38	0.48
2:D:601:NAI:H2N	2:D:601:NAI:PN	2.54	0.48
1:C:418:GLU:O	1:C:422:GLY:N	2.46	0.48
1:C:96:SER:OG	1:C:98:ASP:OD1	2.15	0.48
1:D:418:GLU:O	1:D:422:GLY:N	2.46	0.48
1:D:205:GLN:C	2:D:602:NAI:H5N	2.32	0.48
1:F:418:GLU:O	1:F:422:GLY:N	2.46	0.48
1:A:63:PHE:O	1:A:74:VAL:HA	2.14	0.48
1:B:418:GLU:O	1:B:422:GLY:N	2.46	0.48
1:E:418:GLU:O	1:E:422:GLY:N	2.46	0.48
1:A:418:GLU:O	1:A:422:GLY:N	2.46	0.47
1:D:63:PHE:O	1:D:74:VAL:HA	2.14	0.47
2:B:601:NAI:PN	2:B:601:NAI:H2N	2.54	0.47
1:C:63:PHE:O	1:C:74:VAL:HA	2.14	0.47
1:C:372:TYR:CG	1:C:372:TYR:O	2.67	0.47
2:E:601:NAI:H2N	2:E:601:NAI:PN	2.54	0.47
1:F:63:PHE:O	1:F:74:VAL:HA	2.14	0.47
1:B:90:LYS:CD	1:B:122:PHE:CD2	2.96	0.47
1:B:220:PHE:CD2	1:B:262:TYR:HE2	2.33	0.47
1:E:220:PHE:CD2	1:E:262:TYR:HE2	2.33	0.47
1:F:372:TYR:O	1:F:372:TYR:CG	2.67	0.47
1:A:272:THR:OG1	1:A:273:VAL:N	2.48	0.47
1:D:272:THR:OG1	1:D:273:VAL:N	2.48	0.47
1:E:90:LYS:CD	1:E:122:PHE:CD2	2.96	0.47
1:C:205:GLN:C	2:C:602:NAI:H5N	2.32	0.47
1:F:205:GLN:C	2:F:602:NAI:H5N	2.32	0.47
1:F:83:SER:OG	1:F:85:HIS:ND1	2.22	0.47
1:F:220:PHE:CD2	1:F:262:TYR:HE2	2.32	0.47
1:C:220:PHE:CD2	1:C:262:TYR:HE2	2.32	0.47
2:C:601:NAI:H2N	2:C:601:NAI:PN	2.54	0.47
2:F:601:NAI:H2N	2:F:601:NAI:PN	2.54	0.47
1:C:227:ILE:HG13	1:C:242:PHE:HE1	1.80	0.46
1:D:346:GLU:OE1	1:D:478:ARG:NH2	2.43	0.46
1:F:227:ILE:HG13	1:F:242:PHE:HE1	1.80	0.46
1:A:220:PHE:CD2	1:A:262:TYR:HE2	2.33	0.46
1:A:346:GLU:OE1	1:A:478:ARG:NH2	2.43	0.46
1:B:63:PHE:O	1:B:74:VAL:HA	2.14	0.46
1:C:83:SER:OG	1:C:85:HIS:ND1	2.22	0.46
1:D:220:PHE:CD2	1:D:262:TYR:HE2	2.33	0.46
1:A:114:LYS:HE3	1:A:378:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LYS:HE3	1:D:378:VAL:HG21	1.98	0.46
1:E:63:PHE:O	1:E:74:VAL:HA	2.14	0.46
1:F:272:THR:OG1	1:F:273:VAL:N	2.48	0.46
1:C:272:THR:OG1	1:C:273:VAL:N	2.48	0.46
1:E:205:GLN:C	2:E:602:NAI:H5N	2.32	0.46
1:A:147:ARG:NH1	1:E:499:THR:OG1	2.49	0.46
1:A:372:TYR:O	1:A:372:TYR:CD2	2.69	0.46
1:B:499:THR:OG1	1:D:147:ARG:NH1	2.49	0.46
1:B:205:GLN:C	2:B:602:NAI:H5N	2.32	0.46
1:C:147:ARG:NH1	1:F:499:THR:OG1	2.49	0.46
1:C:114:LYS:HE3	1:C:378:VAL:HG21	1.98	0.46
1:D:372:TYR:CD2	1:D:372:TYR:O	2.69	0.46
1:F:114:LYS:HE3	1:F:378:VAL:HG21	1.98	0.46
1:C:499:THR:OG1	1:F:147:ARG:NH1	2.49	0.46
1:A:499:THR:OG1	1:E:147:ARG:NH1	2.49	0.46
1:B:147:ARG:NH1	1:D:499:THR:OG1	2.49	0.46
1:E:372:TYR:O	1:E:372:TYR:CD2	2.69	0.46
1:B:272:THR:OG1	1:B:273:VAL:N	2.48	0.46
1:B:372:TYR:CD2	1:B:372:TYR:O	2.69	0.46
1:E:227:ILE:HG13	1:E:242:PHE:HE1	1.80	0.46
1:E:272:THR:OG1	1:E:273:VAL:N	2.48	0.46
1:B:227:ILE:HG13	1:B:242:PHE:HE1	1.80	0.45
1:A:148:PHE:O	1:A:152:LEU:HD13	2.17	0.45
1:A:200:GLY:HA2	1:A:211:ARG:HD2	1.98	0.45
1:C:372:TYR:CD2	1:C:372:TYR:O	2.69	0.45
1:D:148:PHE:O	1:D:152:LEU:HD13	2.17	0.45
1:F:200:GLY:HA2	1:F:211:ARG:HD2	1.98	0.45
1:F:372:TYR:O	1:F:372:TYR:CD2	2.69	0.45
1:C:200:GLY:HA2	1:C:211:ARG:HD2	1.98	0.45
1:D:200:GLY:HA2	1:D:211:ARG:HD2	1.98	0.45
1:A:246:THR:HA	1:A:269:LYS:O	2.17	0.45
1:F:148:PHE:O	1:F:152:LEU:HD13	2.17	0.45
1:B:114:LYS:HE3	1:B:378:VAL:HG21	1.98	0.45
1:C:148:PHE:O	1:C:152:LEU:HD13	2.17	0.45
1:D:246:THR:HA	1:D:269:LYS:O	2.17	0.45
1:A:404:ASP:OD1	1:A:405:SER:N	2.50	0.45
1:B:372:TYR:OH	1:B:461:ALA:HB2	2.16	0.45
1:D:404:ASP:OD1	1:D:405:SER:N	2.50	0.45
1:E:372:TYR:OH	1:E:461:ALA:HB2	2.16	0.45
1:E:114:LYS:HE3	1:E:378:VAL:HG21	1.98	0.45
1:C:198:VAL:O	1:C:201:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:VAL:O	1:F:201:LYS:NZ	2.49	0.45
1:F:372:TYR:OH	1:F:461:ALA:HB2	2.16	0.45
1:C:246:THR:HA	1:C:269:LYS:O	2.17	0.45
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.16	0.45
1:D:119:ASP:OD1	1:D:488:LYS:NZ	2.37	0.45
1:F:246:THR:HA	1:F:269:LYS:O	2.17	0.45
1:B:200:GLY:HA2	1:B:211:ARG:HD2	1.98	0.45
1:C:404:ASP:OD1	1:C:405:SER:N	2.50	0.45
1:D:18:ASP:OD1	1:D:53:LYS:NZ	2.32	0.45
1:F:404:ASP:OD1	1:F:405:SER:N	2.50	0.45
1:B:404:ASP:OD1	1:B:405:SER:N	2.50	0.44
1:B:62:SER:HA	1:B:75:ILE:O	2.16	0.44
1:C:62:SER:HA	1:C:75:ILE:O	2.17	0.44
1:E:200:GLY:HA2	1:E:211:ARG:HD2	1.98	0.44
1:E:246:THR:HA	1:E:269:LYS:O	2.17	0.44
1:E:404:ASP:OD1	1:E:405:SER:N	2.50	0.44
1:E:62:SER:HA	1:E:75:ILE:O	2.16	0.44
1:A:227:ILE:HG13	1:A:242:PHE:HE1	1.80	0.44
1:B:246:THR:HA	1:B:269:LYS:O	2.17	0.44
1:F:62:SER:HA	1:F:75:ILE:O	2.17	0.44
1:A:198:VAL:O	1:A:201:LYS:NZ	2.49	0.44
1:D:227:ILE:HG13	1:D:242:PHE:HE1	1.80	0.44
1:A:372:TYR:OH	1:A:461:ALA:HB2	2.16	0.44
1:A:62:SER:HA	1:A:75:ILE:O	2.17	0.44
1:C:206:GLY:HA2	2:C:602:NAI:C5N	2.48	0.44
1:C:239:THR:O	1:C:245:LYS:NZ	2.36	0.44
1:D:198:VAL:O	1:D:201:LYS:NZ	2.49	0.44
1:D:62:SER:HA	1:D:75:ILE:O	2.17	0.44
1:D:372:TYR:OH	1:D:461:ALA:HB2	2.16	0.44
1:F:206:GLY:HA2	2:F:602:NAI:C5N	2.48	0.44
1:F:239:THR:O	1:F:245:LYS:NZ	2.36	0.44
1:A:272:THR:HB	1:A:281:TRP:HD1	1.82	0.44
1:C:346:GLU:OE1	1:C:478:ARG:NH2	2.43	0.44
1:C:45:VAL:HG23	1:C:46:ARG:N	2.33	0.44
1:A:206:GLY:HA2	2:A:602:NAI:C5N	2.48	0.44
1:B:355:GLU:O	1:B:358:LYS:N	2.51	0.44
1:C:28:LEU:HD11	1:C:490:PHE:CD2	2.53	0.44
1:E:148:PHE:O	1:E:152:LEU:HD13	2.17	0.44
1:E:355:GLU:O	1:E:358:LYS:N	2.51	0.44
1:F:272:THR:HB	1:F:281:TRP:HD1	1.82	0.44
1:F:346:GLU:OE1	1:F:478:ARG:NH2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:VAL:HG23	1:F:46:ARG:N	2.33	0.44
1:A:45:VAL:HG23	1:A:46:ARG:N	2.33	0.43
1:B:148:PHE:O	1:B:152:LEU:HD13	2.17	0.43
1:B:372:TYR:OH	1:B:457:MET:O	2.27	0.43
1:C:119:ASP:OD1	1:C:488:LYS:NZ	2.37	0.43
1:C:272:THR:HB	1:C:281:TRP:HD1	1.82	0.43
1:C:355:GLU:O	1:C:358:LYS:N	2.51	0.43
1:D:206:GLY:HA2	2:D:602:NAI:C5N	2.48	0.43
1:D:272:THR:HB	1:D:281:TRP:HD1	1.82	0.43
1:D:45:VAL:HG23	1:D:46:ARG:N	2.33	0.43
1:F:28:LEU:HD11	1:F:490:PHE:CD2	2.53	0.43
1:F:355:GLU:O	1:F:358:LYS:N	2.51	0.43
1:A:355:GLU:O	1:A:358:LYS:N	2.51	0.43
1:B:45:VAL:HG23	1:B:46:ARG:N	2.33	0.43
1:B:28:LEU:HD11	1:B:490:PHE:CD2	2.53	0.43
1:D:355:GLU:O	1:D:358:LYS:N	2.51	0.43
1:E:45:VAL:HG23	1:E:46:ARG:N	2.33	0.43
1:E:28:LEU:HD11	1:E:490:PHE:CD2	2.53	0.43
1:E:372:TYR:OH	1:E:457:MET:O	2.27	0.43
1:B:255:VAL:O	1:B:259:SER:OG	2.23	0.43
1:B:272:THR:HB	1:B:281:TRP:HD1	1.82	0.43
1:B:17:PHE:CE1	1:B:486:ILE:HG12	2.54	0.43
1:E:17:PHE:CE1	1:E:486:ILE:HG12	2.54	0.43
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.54	0.43
1:E:206:GLY:HA2	2:E:602:NAI:C5N	2.48	0.43
1:E:272:THR:HB	1:E:281:TRP:HD1	1.82	0.43
1:A:479:THR:O	1:A:483:VAL:HG23	2.19	0.43
1:B:206:GLY:HA2	2:B:602:NAI:C5N	2.48	0.43
1:C:52:ILE:HG12	1:C:493:TYR:CE2	2.54	0.43
1:D:17:PHE:CE1	1:D:486:ILE:HG12	2.54	0.43
1:D:479:THR:O	1:D:483:VAL:HG23	2.19	0.43
1:F:52:ILE:HG12	1:F:493:TYR:CE2	2.54	0.43
1:A:28:LEU:HD11	1:A:490:PHE:CD2	2.53	0.43
1:A:52:ILE:HG12	1:A:493:TYR:CE2	2.54	0.43
1:E:90:LYS:HD2	1:E:122:PHE:CE2	2.54	0.43
1:B:90:LYS:HD2	1:B:122:PHE:CE2	2.54	0.42
1:D:28:LEU:HD11	1:D:490:PHE:CD2	2.53	0.42
1:D:52:ILE:HG12	1:D:493:TYR:CE2	2.54	0.42
1:B:479:THR:O	1:B:483:VAL:HG23	2.19	0.42
1:F:255:VAL:O	1:F:259:SER:OG	2.23	0.42
1:B:198:VAL:O	1:B:201:LYS:NZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:HD2	1:C:122:PHE:CE2	2.54	0.42
1:C:346:GLU:OE2	1:C:352:THR:OG1	2.28	0.42
1:E:479:THR:O	1:E:483:VAL:HG23	2.19	0.42
1:A:250:GLN:HB3	1:A:324:PRO:HA	2.02	0.42
1:D:250:GLN:HB3	1:D:324:PRO:HA	2.02	0.42
1:E:198:VAL:O	1:E:201:LYS:NZ	2.49	0.42
1:F:90:LYS:HD2	1:F:122:PHE:CE2	2.54	0.42
1:D:90:LYS:HD2	1:D:122:PHE:CE2	2.54	0.42
1:A:90:LYS:HD2	1:A:122:PHE:CE2	2.54	0.42
1:C:255:VAL:O	1:C:259:SER:OG	2.23	0.42
1:C:17:PHE:CE1	1:C:486:ILE:HG12	2.54	0.42
1:F:479:THR:O	1:F:483:VAL:HG23	2.19	0.42
1:F:17:PHE:CE1	1:F:486:ILE:HG12	2.54	0.42
1:F:212:ILE:HG13	1:F:213:SER:N	2.34	0.42
1:B:121:PRO:HD2	1:B:382:TYR:CE1	2.55	0.42
1:B:345:ALA:HA	1:B:368:ILE:HB	2.02	0.42
1:C:212:ILE:HG13	1:C:213:SER:N	2.34	0.42
1:C:479:THR:O	1:C:483:VAL:HG23	2.19	0.42
1:E:121:PRO:HD2	1:E:382:TYR:CE1	2.55	0.42
1:F:250:GLN:HB3	1:F:324:PRO:HA	2.02	0.42
1:B:212:ILE:HG13	1:B:213:SER:N	2.34	0.42
1:B:8:ASN:HD22	1:B:11:LYS:HG3	1.85	0.42
1:C:250:GLN:HB3	1:C:324:PRO:HA	2.02	0.42
1:E:345:ALA:HA	1:E:368:ILE:HB	2.02	0.42
1:B:52:ILE:HG12	1:B:493:TYR:CE2	2.54	0.41
1:C:385:TRP:O	1:C:389:LEU:HG	2.20	0.41
1:D:6:ASP:HB3	1:D:7:PRO:CD	2.38	0.41
1:E:212:ILE:HG13	1:E:213:SER:N	2.34	0.41
1:E:52:ILE:HG12	1:E:493:TYR:CE2	2.54	0.41
1:E:8:ASN:HD22	1:E:11:LYS:HG3	1.85	0.41
1:F:385:TRP:O	1:F:389:LEU:HG	2.20	0.41
1:A:8:ASN:HD22	1:A:11:LYS:HG3	1.85	0.41
1:B:239:THR:O	1:B:245:LYS:NZ	2.36	0.41
1:E:250:GLN:HB3	1:E:324:PRO:HA	2.02	0.41
1:B:250:GLN:HB3	1:B:324:PRO:HA	2.02	0.41
1:C:345:ALA:HA	1:C:368:ILE:HB	2.02	0.41
1:D:121:PRO:HD2	1:D:382:TYR:CE1	2.55	0.41
1:D:212:ILE:HG13	1:D:213:SER:N	2.35	0.41
1:D:8:ASN:HD22	1:D:11:LYS:HG3	1.85	0.41
1:E:142:GLU:HB2	1:E:146:ARG:NH1	2.36	0.41
1:F:121:PRO:HD2	1:F:382:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:HD2	1:A:382:TYR:CE1	2.55	0.41
1:A:272:THR:HB	1:A:281:TRP:CD1	2.55	0.41
1:B:142:GLU:HB2	1:B:146:ARG:NH1	2.36	0.41
1:C:121:PRO:HD2	1:C:382:TYR:CE1	2.55	0.41
1:C:85:HIS:HB3	1:C:493:TYR:CE1	2.55	0.41
1:D:272:THR:HB	1:D:281:TRP:CD1	2.55	0.41
1:D:345:ALA:HA	1:D:368:ILE:HB	2.02	0.41
1:E:85:HIS:HB3	1:E:493:TYR:CE1	2.55	0.41
1:A:212:ILE:HG13	1:A:213:SER:N	2.35	0.41
1:A:345:ALA:HA	1:A:368:ILE:HB	2.02	0.41
1:B:181:ASP:O	1:B:185:SER:OG	2.31	0.41
1:B:85:HIS:HB3	1:B:493:TYR:CE1	2.55	0.41
1:F:345:ALA:HA	1:F:368:ILE:HB	2.02	0.41
1:F:85:HIS:HB3	1:F:493:TYR:CE1	2.55	0.41
1:A:6:ASP:HB3	1:A:7:PRO:CD	2.38	0.41
1:C:272:THR:HB	1:C:281:TRP:CD1	2.55	0.41
1:F:272:THR:HB	1:F:281:TRP:CD1	2.55	0.41
1:E:239:THR:O	1:E:245:LYS:NZ	2.36	0.41
1:F:333:LYS:HD2	1:F:355:GLU:HB3	2.03	0.41
1:A:333:LYS:HD2	1:A:355:GLU:HB3	2.03	0.41
1:B:385:TRP:O	1:B:389:LEU:HG	2.20	0.41
1:C:333:LYS:HD2	1:C:355:GLU:HB3	2.03	0.41
1:D:142:GLU:HB2	1:D:146:ARG:NH1	2.36	0.41
1:A:142:GLU:HB2	1:A:146:ARG:NH1	2.36	0.41
1:A:165:PRO:HD2	1:A:197:CYS:O	2.21	0.41
1:D:165:PRO:HD2	1:D:197:CYS:O	2.21	0.41
1:D:333:LYS:HD2	1:D:355:GLU:HB3	2.03	0.41
1:C:241:GLY:O	1:C:245:LYS:HG2	2.21	0.41
1:C:32:LEU:HD13	1:C:494:ASN:HD21	1.86	0.41
1:E:272:THR:HB	1:E:281:TRP:CD1	2.55	0.41
1:E:385:TRP:O	1:E:389:LEU:HG	2.20	0.41
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.86	0.41
1:F:241:GLY:O	1:F:245:LYS:HG2	2.21	0.41
1:A:79:ARG:HH21	1:A:163:ASP:CG	2.24	0.41
1:A:339:VAL:HG13	1:A:340:LYS:N	2.36	0.41
1:B:165:PRO:HD2	1:B:197:CYS:O	2.21	0.41
1:B:339:VAL:HG13	1:B:340:LYS:N	2.36	0.41
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.86	0.41
1:C:165:PRO:HD2	1:C:197:CYS:O	2.21	0.41
1:D:241:GLY:O	1:D:245:LYS:HG2	2.21	0.41
1:D:32:LEU:HD13	1:D:494:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:VAL:HG13	1:D:340:LYS:N	2.36	0.41
1:D:79:ARG:HH21	1:D:163:ASP:CG	2.24	0.41
1:E:165:PRO:HD2	1:E:197:CYS:O	2.21	0.41
1:F:165:PRO:HD2	1:F:197:CYS:O	2.21	0.41
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.86	0.41
1:A:32:LEU:HD13	1:A:494:ASN:HD21	1.86	0.40
1:B:272:THR:HB	1:B:281:TRP:CD1	2.55	0.40
1:C:272:THR:HG1	1:C:273:VAL:H	1.69	0.40
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.86	0.40
1:E:339:VAL:HG13	1:E:340:LYS:N	2.36	0.40
1:F:32:LEU:HD13	1:F:494:ASN:HD21	1.86	0.40
1:A:241:GLY:O	1:A:245:LYS:HG2	2.21	0.40
1:C:142:GLU:HB2	1:C:146:ARG:NH1	2.36	0.40
1:D:385:TRP:O	1:D:389:LEU:HG	2.20	0.40
1:D:85:HIS:HB3	1:D:493:TYR:CE1	2.55	0.40
1:F:79:ARG:HH21	1:F:163:ASP:CG	2.24	0.40
1:A:85:HIS:HB3	1:A:493:TYR:CE1	2.55	0.40
1:B:241:GLY:O	1:B:245:LYS:HG2	2.21	0.40
1:C:106:ALA:O	1:C:109:SER:OG	2.19	0.40
1:C:17:PHE:HD2	1:C:53:LYS:HE2	1.87	0.40
1:C:25:GLU:O	1:C:29:VAL:HG23	2.22	0.40
1:C:79:ARG:HH21	1:C:163:ASP:CG	2.24	0.40
1:F:8:ASN:HD22	1:F:11:LYS:HG3	1.85	0.40
1:F:17:PHE:HD2	1:F:53:LYS:HE2	1.87	0.40
1:F:25:GLU:O	1:F:29:VAL:HG23	2.22	0.40
1:A:25:GLU:O	1:A:29:VAL:HG23	2.22	0.40
1:A:385:TRP:O	1:A:389:LEU:HG	2.20	0.40
1:B:32:LEU:HD13	1:B:494:ASN:HD21	1.86	0.40
1:C:415:GLU:OE1	1:C:419:ARG:NH2	2.55	0.40
1:D:86:ARG:NH1	2:E:602:NAI:C2N	2.84	0.40
1:E:241:GLY:O	1:E:245:LYS:HG2	2.21	0.40
1:E:32:LEU:HD13	1:E:494:ASN:HD21	1.86	0.40
1:F:142:GLU:HB2	1:F:146:ARG:NH1	2.36	0.40
1:F:415:GLU:OE1	1:F:419:ARG:NH2	2.55	0.40
1:B:17:PHE:HD2	1:B:53:LYS:HE2	1.87	0.40
1:B:86:ARG:NH1	2:C:602:NAI:C2N	2.84	0.40
1:C:8:ASN:HD22	1:C:11:LYS:HG3	1.85	0.40
1:C:339:VAL:HG13	1:C:340:LYS:N	2.36	0.40
1:D:25:GLU:O	1:D:29:VAL:HG23	2.22	0.40
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.86	0.40
1:E:86:ARG:NH1	2:F:602:NAI:C2N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:339:VAL:HG13	1:F:340:LYS:N	2.36	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%)	453 (92%)	40 (8%)	1 (0%)	52	85
1	B	494/501 (99%)	453 (92%)	40 (8%)	1 (0%)	52	85
1	C	494/501 (99%)	452 (92%)	41 (8%)	1 (0%)	52	85
1	D	494/501 (99%)	453 (92%)	40 (8%)	1 (0%)	52	85
1	E	494/501 (99%)	453 (92%)	40 (8%)	1 (0%)	52	85
1	F	494/501 (99%)	452 (92%)	41 (8%)	1 (0%)	52	85
All	All	2964/3006 (99%)	2716 (92%)	242 (8%)	6 (0%)	56	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	VAL
1	B	498	VAL
1	C	498	VAL
1	D	498	VAL
1	E	498	VAL
1	F	498	VAL

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%)	416 (100%)	0	100	100
1	B	416/420 (99%)	416 (100%)	0	100	100
1	C	416/420 (99%)	416 (100%)	0	100	100
1	D	416/420 (99%)	416 (100%)	0	100	100
1	E	416/420 (99%)	416 (100%)	0	100	100
1	F	416/420 (99%)	416 (100%)	0	100	100
All	All	2496/2520 (99%)	2496 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	349	ASN
1	A	450	HIS
1	B	8	ASN
1	B	84	GLN
1	B	349	ASN
1	B	450	HIS
1	C	8	ASN
1	C	84	GLN
1	C	349	ASN
1	C	450	HIS
1	C	494	ASN
1	D	8	ASN
1	D	84	GLN
1	D	349	ASN
1	D	450	HIS
1	E	8	ASN
1	E	84	GLN
1	E	349	ASN
1	E	450	HIS
1	F	8	ASN
1	F	84	GLN
1	F	349	ASN

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Mol	Chain	Res	Type
1	F	450	HIS
1	F	494	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 ⓘ

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	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	A	602	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	B	601	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	B	602	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	C	601	-	41,48,48	1.04	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	C	602	-	41,48,48	1.06	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	D	601	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	D	602	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	E	601	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	E	602	-	41,48,48	1.05	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	F	601	-	41,48,48	1.04	2 (4%)	46,73,73	1.39	2 (4%)
2	NAI	F	602	-	41,48,48	1.06	2 (4%)	46,73,73	1.39	2 (4%)

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
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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAI	C5A-C4A	3.08	1.47	1.40
2	F	601	NAI	C5A-C4A	3.08	1.47	1.40
2	E	601	NAI	C5A-C4A	3.09	1.47	1.40
2	B	601	NAI	C5A-C4A	3.09	1.47	1.40
2	D	602	NAI	C5A-C4A	3.10	1.47	1.40
2	A	602	NAI	C5A-C4A	3.10	1.47	1.40
2	B	602	NAI	C5A-C4A	3.10	1.47	1.40
2	E	602	NAI	C5A-C4A	3.10	1.47	1.40
2	D	601	NAI	C5A-C4A	3.12	1.47	1.40
2	A	601	NAI	C5A-C4A	3.12	1.47	1.40
2	C	602	NAI	C5A-C4A	3.14	1.47	1.40
2	F	602	NAI	C5A-C4A	3.14	1.47	1.40
2	D	601	NAI	C6N-C5N	3.37	1.39	1.33
2	A	601	NAI	C6N-C5N	3.37	1.39	1.33
2	E	601	NAI	C6N-C5N	3.40	1.39	1.33
2	B	601	NAI	C6N-C5N	3.40	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAI	C6N-C5N	3.41	1.39	1.33
2	F	601	NAI	C6N-C5N	3.41	1.39	1.33
2	B	602	NAI	C6N-C5N	3.43	1.39	1.33
2	E	602	NAI	C6N-C5N	3.43	1.39	1.33
2	D	602	NAI	C6N-C5N	3.44	1.39	1.33
2	A	602	NAI	C6N-C5N	3.44	1.39	1.33
2	C	602	NAI	C6N-C5N	3.47	1.39	1.33
2	F	602	NAI	C6N-C5N	3.47	1.39	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAI	N3A-C2A-N1A	-6.66	123.64	128.87
2	A	601	NAI	N3A-C2A-N1A	-6.66	123.64	128.87
2	E	601	NAI	N3A-C2A-N1A	-6.65	123.64	128.87
2	B	601	NAI	N3A-C2A-N1A	-6.65	123.64	128.87
2	C	601	NAI	N3A-C2A-N1A	-6.64	123.66	128.87
2	F	601	NAI	N3A-C2A-N1A	-6.64	123.66	128.87
2	B	602	NAI	N3A-C2A-N1A	-6.60	123.69	128.87
2	E	602	NAI	N3A-C2A-N1A	-6.60	123.69	128.87
2	C	602	NAI	N3A-C2A-N1A	-6.59	123.69	128.87
2	F	602	NAI	N3A-C2A-N1A	-6.59	123.69	128.87
2	D	602	NAI	N3A-C2A-N1A	-6.58	123.70	128.87
2	A	602	NAI	N3A-C2A-N1A	-6.58	123.70	128.87
2	C	601	NAI	C3D-C2D-C1D	2.27	106.00	101.44
2	F	601	NAI	C3D-C2D-C1D	2.27	106.00	101.44
2	D	601	NAI	C3D-C2D-C1D	2.28	106.01	101.44
2	A	601	NAI	C3D-C2D-C1D	2.28	106.01	101.44
2	E	601	NAI	C3D-C2D-C1D	2.28	106.02	101.44
2	B	601	NAI	C3D-C2D-C1D	2.28	106.02	101.44
2	C	602	NAI	C3D-C2D-C1D	2.42	106.29	101.44
2	F	602	NAI	C3D-C2D-C1D	2.42	106.29	101.44
2	B	602	NAI	C3D-C2D-C1D	2.42	106.30	101.44
2	E	602	NAI	C3D-C2D-C1D	2.42	106.30	101.44
2	D	602	NAI	C3D-C2D-C1D	2.42	106.30	101.44
2	A	602	NAI	C3D-C2D-C1D	2.42	106.30	101.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 135 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAI	12	0
2	A	602	NAI	10	0
2	B	601	NAI	12	0
2	B	602	NAI	10	0
2	C	601	NAI	12	0
2	C	602	NAI	11	0
2	D	601	NAI	12	0
2	D	602	NAI	10	0
2	E	601	NAI	12	0
2	E	602	NAI	11	0
2	F	601	NAI	12	0
2	F	602	NAI	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.