wwPDB EM Map/Model Validation Report (i)

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
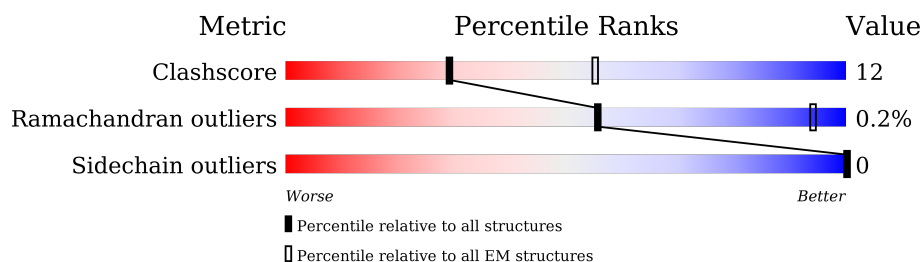http://wwpdb.org/validation/2016/EMValidationReportHelp

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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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	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: $C_{21}H_{29}N_7O_{14}P_2$).
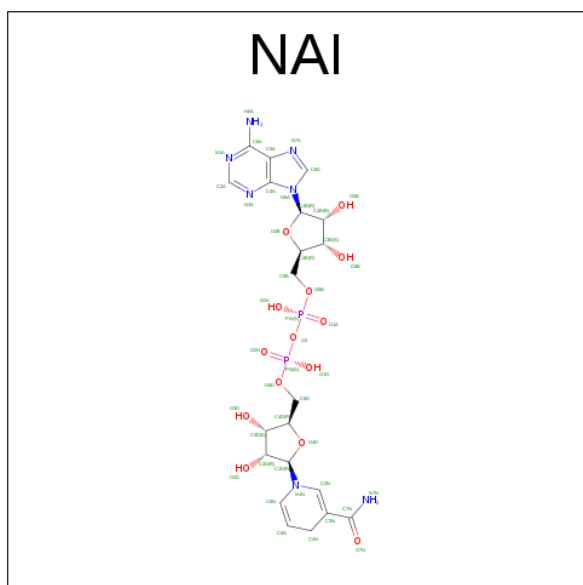
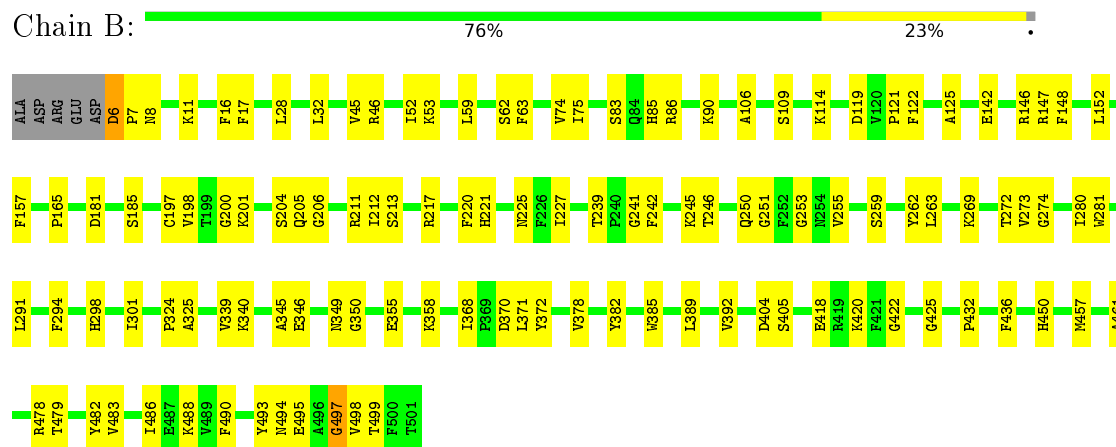| Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	A	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	B	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	C	1	Total	C	N	O	P	0
			88	42	14	28	4	
2	D	1	Total	C	N	O	P	0
			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 ⓘ

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.
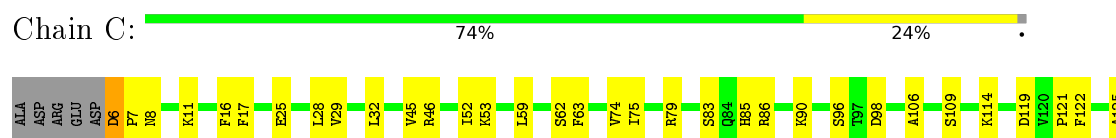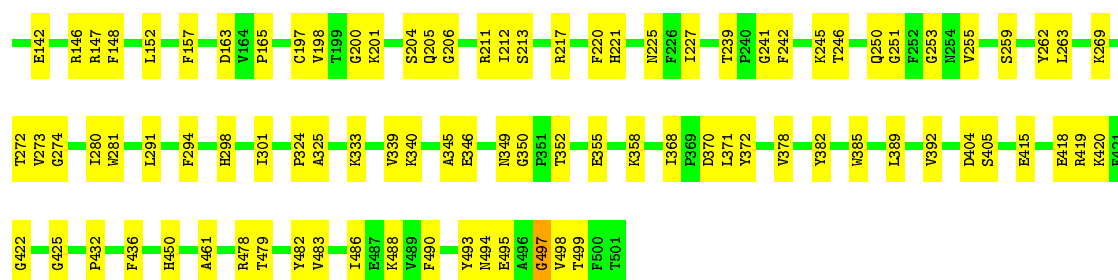
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

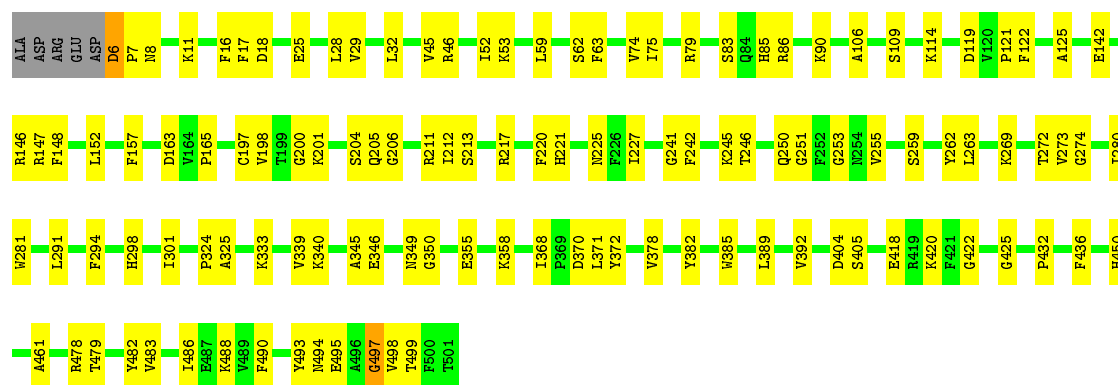- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

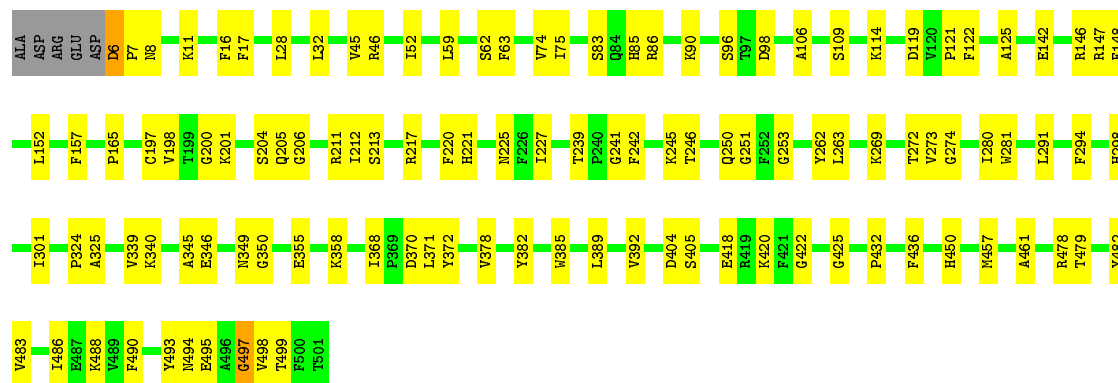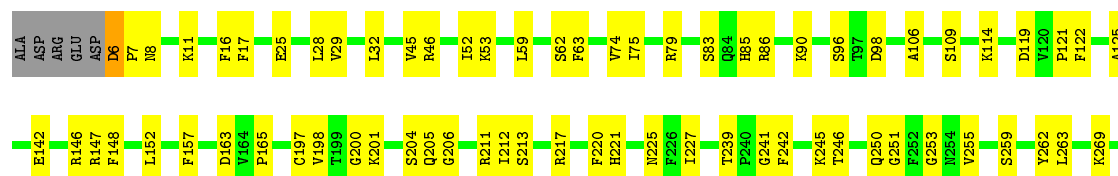- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

E142 R146 R147 F148 L152 F157 D163 V164 P165 C197 V198 T199 G200 K201 S204 Q205 G206 R211 I212 S213 R217 F220 H221 N225 E226 I227 T239 P240 G241 F242 K245 T246 Q250 G251 F252 G253 N254 V255 S259 Y262 L263 K269

T272 V273 G274 I280 W281 L291 F294 H298 I301 P324 A325 K333 V339 K340 A345 E346 N349 G350 P351 T352 E355 K358 I368 P369 D370 L371 Y372 V378 Y382 W385 L389 V392 D404 S405 E415 E418 R419 K420 F421

G422 G425 P432 F436 H450 A461 R478 T479 Y482 V483 I486 E487 K488 V489 F490 Y493 N494 E495 A496 G497 V498 T499 F500 T501

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D: 75% 23%

ALA ASP ARG GLU ASP D6 P7 N8 K11 F16 F17 D18 E25 L28 V29 L32 V45 R46 I52 K53 L59 S62 F63 V74 I75 R79 S83 Q84 H85 R86 K90 A106 S109 K114 D119 V120 P121 F122 A125 E142

R146 R147 F148 L152 F157 D163 V164 P165 C197 V198 T199 G200 K201 S204 Q205 G206 R211 I212 S213 R217 F220 H221 N225 E226 I227 G241 F242 K245 T246 Q250 G251 F252 G253 N254 V255 S259 Y262 L263 K269 T272 V273 G274 I280

W281 L291 F294 H298 I301 P324 A325 K333 V339 K340 A345 E346 N349 G350 E355 K358 I368 P369 D370 L371 Y372 V378 Y382 W385 L389 V392 D404 S405 E418 R419 K420 F421 G422 G425 P432 F436 H450

A461 R478 T479 Y482 V483 I486 E487 K488 V489 F490 Y493 N494 E495 A496 G497 V498 T499 F500 T501

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain E: 76% 22%

ALA ASP ARG GLU ASP D6 P7 N8 K11 F16 F17 L28 L32 V45 R46 I52 L59 S62 F63 V74 I75 S83 Q84 H85 R86 K90 S96 T97 D98 A106 S109 K114 D119 V120 P121 F122 A125 E142 R146 R147 F148

L152 F157 P165 C197 V198 T199 G200 K201 S204 Q205 G206 R211 I212 S213 R217 F220 H221 N225 F226 I227 T239 P240 G241 F242 K245 T246 Q250 G251 F252 G253 Y262 L263 K269 T272 V273 G274 I280 W281 L291 F294 H298

I301 P324 A325 V339 K340 A345 E346 N349 G350 E355 K358 I368 P369 D370 L371 Y372 V378 Y382 W385 L389 V392 D404 S405 E418 R419 K420 F421 G422 G425 P432 F436 H450 M457 A461 R478 T479 Y482

V483 I486 E487 K488 V489 F490 Y493 N494 E495 A496 G497 V498 T499 F500 T501

• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F: 74% 24%

ALA ASP ARG GLU ASP D6 P7 N8 K11 F16 F17 E25 L28 V29 L32 V45 R46 I52 K53 L59 S62 F63 V74 I75 R79 S83 Q84 H85 R86 K90 S96 T97 D98 A106 S109 K114 D119 V120 P121 F122 A125

E142 R146 R147 F148 L152 F157 D163 V164 P165 C197 V198 T199 G200 K201 S204 Q205 G206 R211 I212 S213 R217 F220 H221 N225 F226 I227 T239 P240 G241 F242 K245 T246 Q250 G251 F252 G253 N254 V255 S259 Y262 L263 K269

4 Experimental information (i)

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 $(e^-/\text{Å}^2)$	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	0.63	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.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

5.2   Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

The worst 5 of 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

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

5 of 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

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. 5 of 25 such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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%)
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

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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

The worst 5 of 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

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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.