wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:59 AM GMT

PDB ID	:	2VHW
Title	:	CRYSTAL STRUCTURE OF HOLO L-ALANINE DEHYDROGENASE FROM MYCOBACTERIUM TUBERCULOSIS IN THE OPEN AND CLOSED CONFORMATION
Authors	:	Agren, D.; Schneider, G.
Deposited on	:	2007-11-26
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

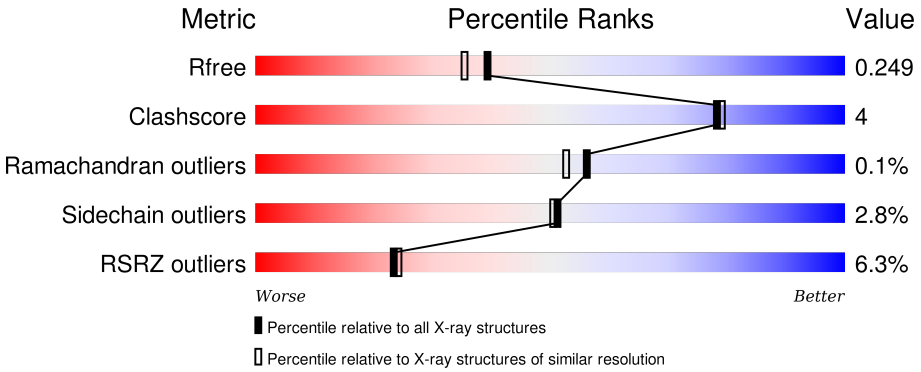
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	6% 88% 9%
1	B	377	2% 91% 7%
1	C	377	9% 87% 10%
1	D	377	% 90% 7%
1	E	377	13% 92% 6%

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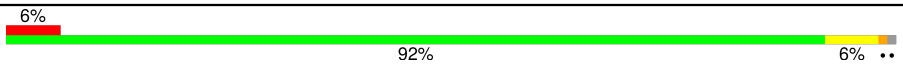
Mol	Chain	Length	Quality of chain
1	F	377	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

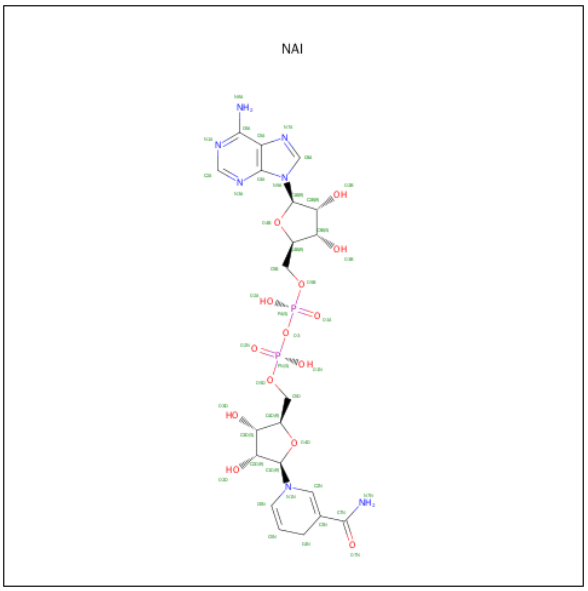
- Molecule 1 is a protein called ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2719	1710	479	517	13			
1	B	370	Total	C	N	O	S	0	3	0
			2730	1717	479	521	13			
1	C	371	Total	C	N	O	S	0	0	0
			2719	1710	479	517	13			
1	D	370	Total	C	N	O	S	0	0	0
			2714	1707	478	516	13			
1	E	373	Total	C	N	O	S	0	1	0
			2747	1727	488	519	13			
1	F	373	Total	C	N	O	S	0	2	0
			2752	1730	488	521	13			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

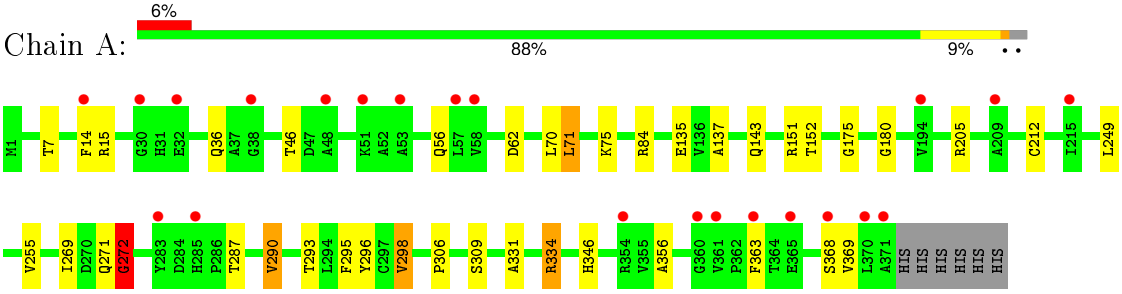
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	219	Total	O	0	0
			219	219		
4	B	310	Total	O	0	0
			310	310		
4	C	211	Total	O	0	0
			211	211		
4	D	297	Total	O	0	0
			297	297		
4	E	195	Total	O	0	0
			195	195		
4	F	280	Total	O	0	0
			280	280		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

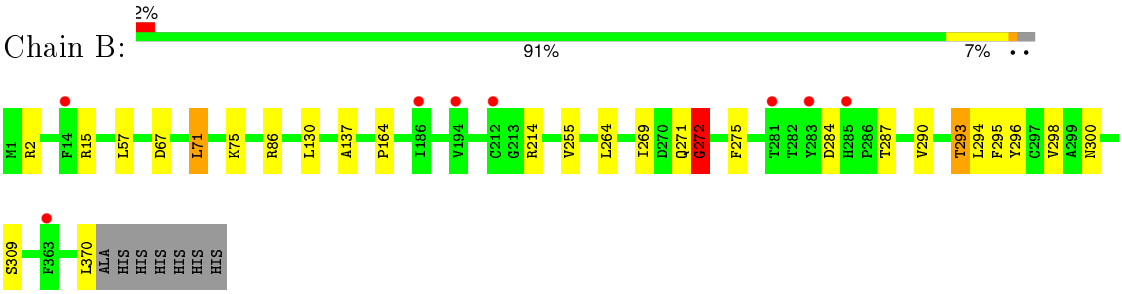
- Molecule 1: ALANINE DEHYDROGENASE

Chain A:



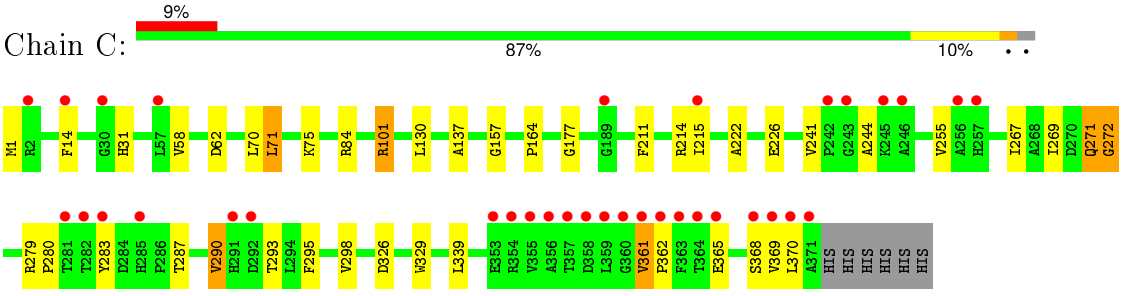
- Molecule 1: ALANINE DEHYDROGENASE

Chain B:



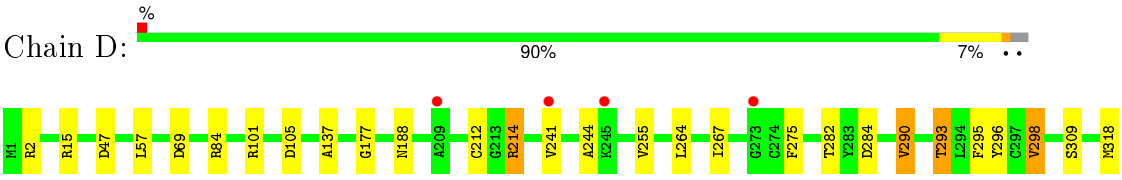
- Molecule 1: ALANINE DEHYDROGENASE

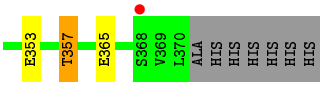
Chain C:



- Molecule 1: ALANINE DEHYDROGENASE

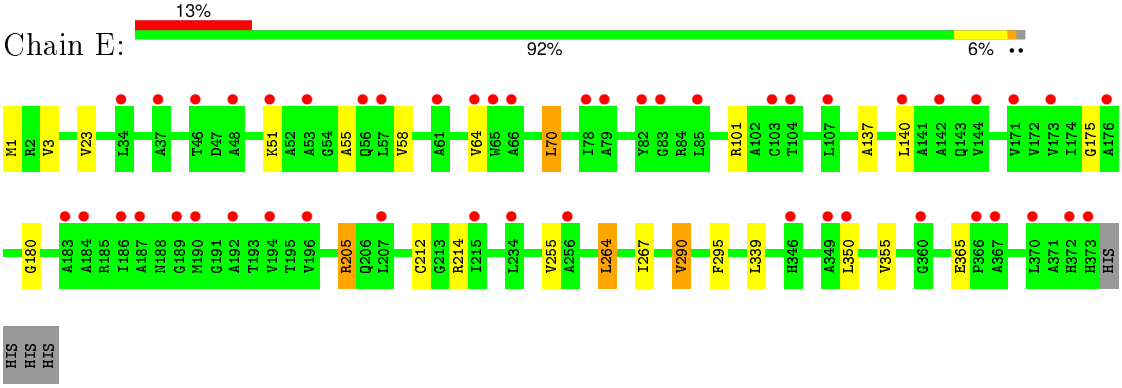
Chain D:





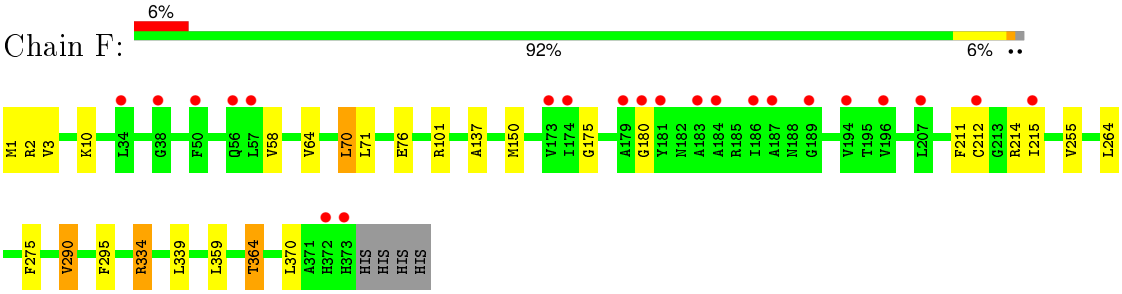
• Molecule 1: ALANINE DEHYDROGENASE

Chain E:



• Molecule 1: ALANINE DEHYDROGENASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	177.03Å 172.01Å 98.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 49.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 94.6 (49.56-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.212 0.220 , 0.249	Depositor DCC
R_{free} test set	9699 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 191725 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18159	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	1/2769 (0.0%)	0.72	3/3773 (0.1%)
1	B	0.60	0/2789	0.76	4/3800 (0.1%)
1	C	0.53	0/2769	0.66	2/3773 (0.1%)
1	D	0.58	0/2764	0.67	1/3766 (0.0%)
1	E	0.52	0/2802	0.67	3/3817 (0.1%)
1	F	0.56	0/2810	0.68	1/3828 (0.0%)
All	All	0.56	1/16703 (0.0%)	0.69	14/22757 (0.1%)

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
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	CB-OG1	-5.76	1.31	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	GLY	N-CA-C	-10.27	87.42	113.10
1	B	272	GLY	N-CA-C	-8.68	91.39	113.10
1	E	205	ARG	NE-CZ-NH2	-8.31	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	272	GLY	N-CA-C	-7.83	93.51	113.10
1	E	205	ARG	NE-CZ-NH1	7.65	124.13	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	GLN	Peptide
1	B	271	GLN	Peptide
1	C	271	GLN	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	2719	0	2732	21	0
1	B	2730	0	2743	14	0
1	C	2719	0	2732	32	0
1	D	2714	0	2727	23	0
1	E	2747	0	2759	19	0
1	F	2752	0	2763	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	27	1	0
3	B	44	0	27	1	0
3	C	44	0	27	3	0
3	D	44	0	27	3	0
3	E	44	0	27	2	0
3	F	44	0	27	1	0
4	A	219	0	0	0	0
4	B	310	0	0	1	0
4	C	211	0	0	1	0
4	D	297	0	0	3	0
4	E	195	0	0	3	0
4	F	280	0	0	3	0
All	All	18159	0	16618	120	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 4.

The worst 5 of 120 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:C:101:ARG:HG3	1:C:101:ARG:HH21	1.18	1.04
1:C:241:VAL:HG23	1:C:244:ALA:HB3	1.57	0.87
1:C:101:ARG:CG	1:C:101:ARG:HH21	1.87	0.86
1:D:282:THR:HG22	1:D:284:ASP:H	1.43	0.83
1:B:255:VAL:HG11	1:B:290:VAL:HG22	1.63	0.78

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/377 (98%)	362 (98%)	6 (2%)	1 (0%)	46	41
1	B	371/377 (98%)	364 (98%)	6 (2%)	1 (0%)	46	41
1	C	369/377 (98%)	361 (98%)	8 (2%)	0	100	100
1	D	368/377 (98%)	364 (99%)	4 (1%)	0	100	100
1	E	372/377 (99%)	366 (98%)	6 (2%)	0	100	100
1	F	373/377 (99%)	368 (99%)	5 (1%)	0	100	100
All	All	2222/2262 (98%)	2185 (98%)	35 (2%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLY
1	B	272	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/282 (98%)	265 (96%)	11 (4%)	38	33
1	B	279/282 (99%)	273 (98%)	6 (2%)	60	62
1	C	276/282 (98%)	264 (96%)	12 (4%)	35	30
1	D	276/282 (98%)	270 (98%)	6 (2%)	60	62
1	E	279/282 (99%)	273 (98%)	6 (2%)	60	62
1	F	280/282 (99%)	274 (98%)	6 (2%)	61	63
All	All	1666/1692 (98%)	1619 (97%)	47 (3%)	51	50

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	130	LEU
1	C	339	LEU
1	F	71	LEU
1	C	290	VAL
1	C	361	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	121	GLN
1	C	148	HIS
1	E	148	HIS
1	C	31	HIS
1	E	56	GLN

5.3.3 RNA

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)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAI	A	1373	-	38,48,48	1.19	3 (7%)	48,73,73	1.91	12 (25%)
3	NAI	B	1372	-	38,48,48	1.21	3 (7%)	48,73,73	1.86	11 (22%)
3	NAI	C	1372	-	38,48,48	1.22	4 (10%)	48,73,73	1.74	8 (16%)
3	NAI	D	1371	-	38,48,48	1.29	4 (10%)	48,73,73	1.98	8 (16%)
3	NAI	E	1374	-	38,48,48	1.26	5 (13%)	48,73,73	1.80	7 (14%)
3	NAI	F	1374	-	38,48,48	1.26	4 (10%)	48,73,73	1.74	9 (18%)

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
3	NAI	A	1373	-	-	0/25/72/72	0/5/5/5
3	NAI	B	1372	-	-	0/25/72/72	0/5/5/5
3	NAI	C	1372	-	-	0/25/72/72	0/5/5/5
3	NAI	D	1371	-	-	0/25/72/72	0/5/5/5
3	NAI	E	1374	-	-	0/25/72/72	0/5/5/5
3	NAI	F	1374	-	-	0/25/72/72	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1373	NAI	C4N-C5N	-4.67	1.39	1.49
3	B	1372	NAI	C4N-C5N	-4.13	1.40	1.49
3	E	1374	NAI	C4N-C5N	-4.01	1.40	1.49
3	D	1371	NAI	C4N-C5N	-3.99	1.40	1.49
3	C	1372	NAI	C4N-C5N	-3.61	1.41	1.49

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1373	NAI	N3A-C2A-N1A	-8.31	122.53	128.89
3	E	1374	NAI	N3A-C2A-N1A	-7.92	122.83	128.89
3	D	1371	NAI	N3A-C2A-N1A	-7.70	123.00	128.89
3	B	1372	NAI	N3A-C2A-N1A	-6.97	123.56	128.89
3	C	1372	NAI	N3A-C2A-N1A	-6.73	123.74	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1373	NAI	1	0
3	B	1372	NAI	1	0
3	C	1372	NAI	3	0
3	D	1371	NAI	3	0
3	E	1374	NAI	2	0
3	F	1374	NAI	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	371/377 (98%)	0.56	22 (5%) 26 27	26, 46, 56, 68	0
1	B	370/377 (98%)	0.19	8 (2%) 65 66	25, 40, 51, 58	0
1	C	371/377 (98%)	0.63	35 (9%) 11 11	26, 47, 61, 70	0
1	D	370/377 (98%)	0.17	5 (1%) 78 78	25, 40, 52, 57	0
1	E	373/377 (98%)	0.85	48 (12%) 5 5	27, 50, 65, 76	0
1	F	373/377 (98%)	0.50	22 (5%) 26 27	26, 42, 49, 66	0
All	All	2228/2262 (98%)	0.48	140 (6%) 23 24	25, 44, 57, 76	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	372	HIS	5.3
1	C	283	TYR	5.2
1	C	363	PHE	4.6
1	C	243	GLY	4.3
1	C	368	SER	4.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAI	C	1372	44/44	0.96	0.13	-0.04	36,41,46,47	0
3	NAI	D	1371	44/44	0.97	0.10	-0.73	30,34,39,43	0
3	NAI	A	1373	44/44	0.96	0.09	-1.60	30,34,39,43	0
3	NAI	E	1374	44/44	0.97	0.10	-1.71	27,31,40,41	0
3	NAI	F	1374	44/44	0.98	0.09	-1.93	20,24,29,31	0
3	NAI	B	1372	44/44	0.98	0.07	-2.13	23,29,33,36	0
2	MG	A	1372	1/1	0.92	0.11	-	48,48,48,48	0
2	MG	B	1371	1/1	0.98	0.03	-	45,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.