wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 01:18 am GMT

PDB ID	:	4BHY
Title	:	Structure of alanine racemase from Aeromonas hydrophila
Authors	:	Otero, L.H.; Carrasco-Lopez, C.; Bernardo-Garcia, N.; Hermoso, J.A.
Deposited on	:	2013-04-09
Resolution	:	3.25 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

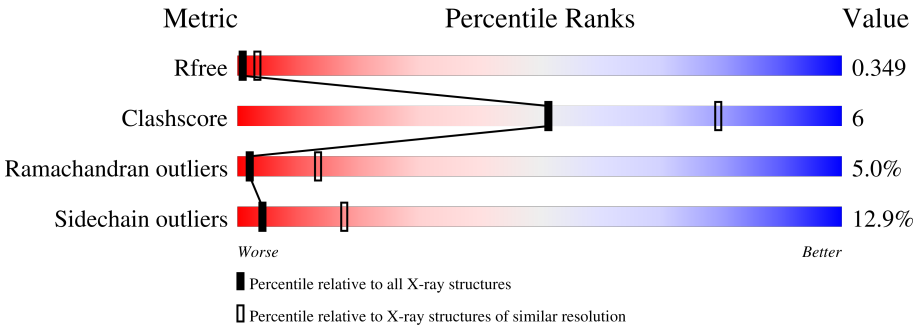
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.25 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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	378	67% 18% • 14%
1	B	378	61% 19% • • 15%
1	C	378	61% 19% • • 16%
1	D	378	66% 18% • • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10083 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 RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2493	1600	423	457	13			
1	B	320	Total	C	N	O	S	0	0	0
			2473	1582	424	454	13			
1	C	317	Total	C	N	O	S	0	0	0
			2412	1542	411	444	15			
1	D	336	Total	C	N	O	S	0	0	0
			2570	1644	436	476	14			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP A0KH11
A	-19	HIS	-	expression tag	UNP A0KH11
A	-18	HIS	-	expression tag	UNP A0KH11
A	-17	HIS	-	expression tag	UNP A0KH11
A	-16	HIS	-	expression tag	UNP A0KH11
A	-15	HIS	-	expression tag	UNP A0KH11
A	-14	HIS	-	expression tag	UNP A0KH11
A	-13	ASP	-	expression tag	UNP A0KH11
A	-12	TYR	-	expression tag	UNP A0KH11
A	-11	ASP	-	expression tag	UNP A0KH11
A	-10	ILE	-	expression tag	UNP A0KH11
A	-9	PRO	-	expression tag	UNP A0KH11
A	-8	THR	-	expression tag	UNP A0KH11
A	-7	THR	-	expression tag	UNP A0KH11
A	-6	GLU	-	expression tag	UNP A0KH11
A	-5	ASN	-	expression tag	UNP A0KH11
A	-4	LEU	-	expression tag	UNP A0KH11
A	-3	TYR	-	expression tag	UNP A0KH11
A	-2	PHE	-	expression tag	UNP A0KH11
A	-1	GLN	-	expression tag	UNP A0KH11
A	0	SER	-	expression tag	UNP A0KH11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP A0KH11
B	-19	HIS	-	expression tag	UNP A0KH11
B	-18	HIS	-	expression tag	UNP A0KH11
B	-17	HIS	-	expression tag	UNP A0KH11
B	-16	HIS	-	expression tag	UNP A0KH11
B	-15	HIS	-	expression tag	UNP A0KH11
B	-14	HIS	-	expression tag	UNP A0KH11
B	-13	ASP	-	expression tag	UNP A0KH11
B	-12	TYR	-	expression tag	UNP A0KH11
B	-11	ASP	-	expression tag	UNP A0KH11
B	-10	ILE	-	expression tag	UNP A0KH11
B	-9	PRO	-	expression tag	UNP A0KH11
B	-8	THR	-	expression tag	UNP A0KH11
B	-7	THR	-	expression tag	UNP A0KH11
B	-6	GLU	-	expression tag	UNP A0KH11
B	-5	ASN	-	expression tag	UNP A0KH11
B	-4	LEU	-	expression tag	UNP A0KH11
B	-3	TYR	-	expression tag	UNP A0KH11
B	-2	PHE	-	expression tag	UNP A0KH11
B	-1	GLN	-	expression tag	UNP A0KH11
B	0	SER	-	expression tag	UNP A0KH11
C	-20	MET	-	expression tag	UNP A0KH11
C	-19	HIS	-	expression tag	UNP A0KH11
C	-18	HIS	-	expression tag	UNP A0KH11
C	-17	HIS	-	expression tag	UNP A0KH11
C	-16	HIS	-	expression tag	UNP A0KH11
C	-15	HIS	-	expression tag	UNP A0KH11
C	-14	HIS	-	expression tag	UNP A0KH11
C	-13	ASP	-	expression tag	UNP A0KH11
C	-12	TYR	-	expression tag	UNP A0KH11
C	-11	ASP	-	expression tag	UNP A0KH11
C	-10	ILE	-	expression tag	UNP A0KH11
C	-9	PRO	-	expression tag	UNP A0KH11
C	-8	THR	-	expression tag	UNP A0KH11
C	-7	THR	-	expression tag	UNP A0KH11
C	-6	GLU	-	expression tag	UNP A0KH11
C	-5	ASN	-	expression tag	UNP A0KH11
C	-4	LEU	-	expression tag	UNP A0KH11
C	-3	TYR	-	expression tag	UNP A0KH11
C	-2	PHE	-	expression tag	UNP A0KH11
C	-1	GLN	-	expression tag	UNP A0KH11
C	0	SER	-	expression tag	UNP A0KH11

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP A0KH11
D	-19	HIS	-	expression tag	UNP A0KH11
D	-18	HIS	-	expression tag	UNP A0KH11
D	-17	HIS	-	expression tag	UNP A0KH11
D	-16	HIS	-	expression tag	UNP A0KH11
D	-15	HIS	-	expression tag	UNP A0KH11
D	-14	HIS	-	expression tag	UNP A0KH11
D	-13	ASP	-	expression tag	UNP A0KH11
D	-12	TYR	-	expression tag	UNP A0KH11
D	-11	ASP	-	expression tag	UNP A0KH11
D	-10	ILE	-	expression tag	UNP A0KH11
D	-9	PRO	-	expression tag	UNP A0KH11
D	-8	THR	-	expression tag	UNP A0KH11
D	-7	THR	-	expression tag	UNP A0KH11
D	-6	GLU	-	expression tag	UNP A0KH11
D	-5	ASN	-	expression tag	UNP A0KH11
D	-4	LEU	-	expression tag	UNP A0KH11
D	-3	TYR	-	expression tag	UNP A0KH11
D	-2	PHE	-	expression tag	UNP A0KH11
D	-1	GLN	-	expression tag	UNP A0KH11
D	0	SER	-	expression tag	UNP A0KH11

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	A	2	Total O 2 2	0	0
2	A	1	Total O 1 1	0	0
2	B	34	Total O 34 34	0	0
2	B	1	Total O 1 1	0	0
2	B	2	Total O 2 2	0	0
2	B	1	Total O 1 1	0	0
2	B	2	Total O 2 2	0	0
2	B	1	Total O 1 1	0	0

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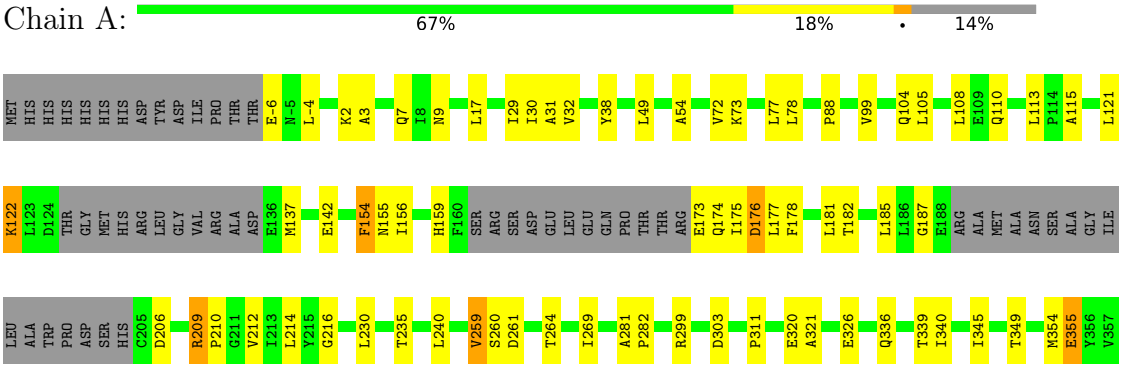
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0
2	C	30	Total O 30 30	0	0
2	C	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0
2	C	2	Total O 2 2	0	0
2	C	1	Total O 1 1	0	0
2	D	26	Total O 26 26	0	0
2	D	3	Total O 3 3	0	0
2	D	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

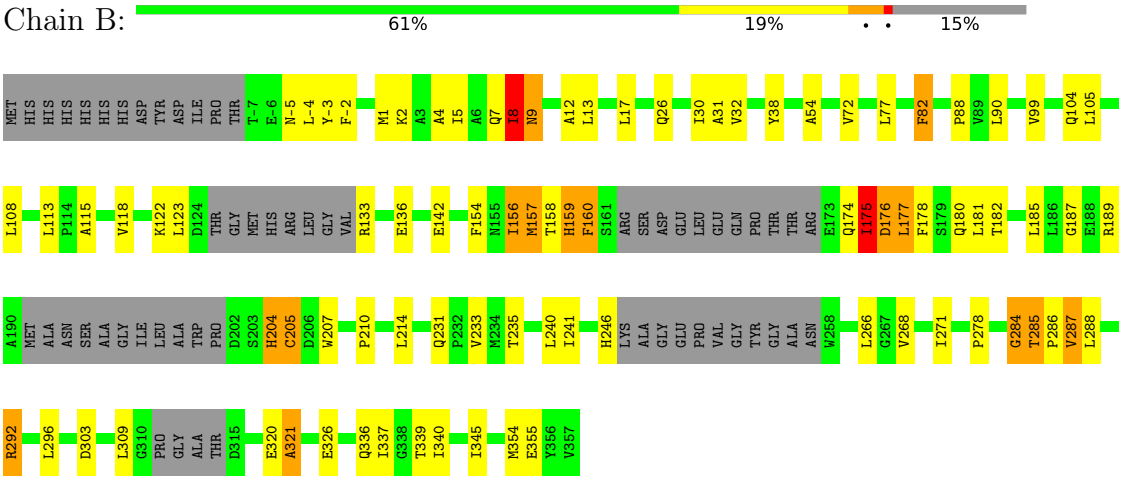
- Molecule 1: ALANINE RACEMASE

Chain A:



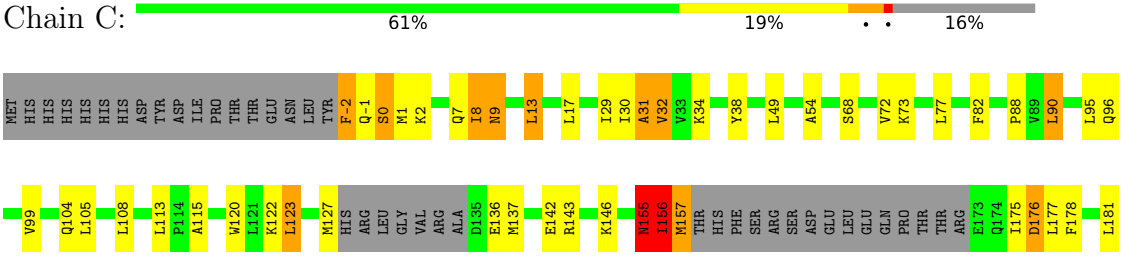
- Molecule 1: ALANINE RACEMASE

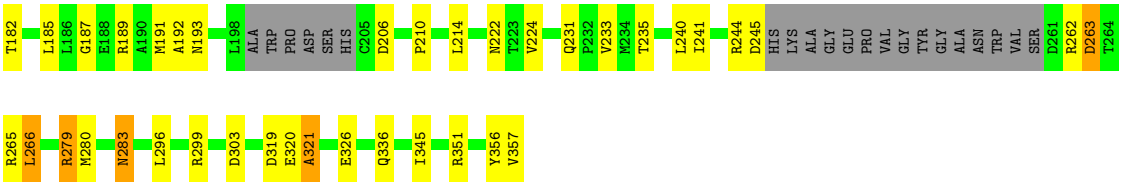
Chain B:



- Molecule 1: ALANINE RACEMASE

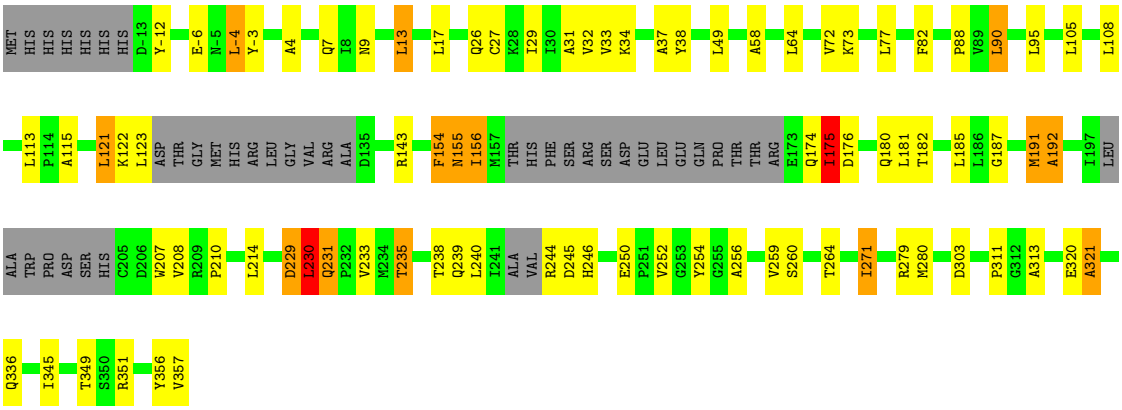
Chain C:





• Molecule 1: ALANINE RACEMASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.80Å 134.74Å 192.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 3.25 47.99 – 3.25	Depositor EDS
% Data completeness (in resolution range)	92.5 (47.32-3.25) 92.5 (47.99-3.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.256 , 0.292 0.302 , 0.349	Depositor DCC
R_{free} test set	2171 reflections (10.20%)	wwPDB-VP
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 132.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10083	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: KCX

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	0.43	0/2532	0.62	1/3453 (0.0%)
1	B	0.46	0/2508	0.69	6/3415 (0.2%)
1	C	0.45	0/2442	0.69	4/3325 (0.1%)
1	D	0.44	0/2607	0.65	4/3552 (0.1%)
All	All	0.44	0/10089	0.66	15/13745 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	ALA	C-N-CA	7.54	140.54	121.70
1	B	156	ILE	C-N-CA	6.62	138.25	121.70
1	D	154	PHE	C-N-CA	6.30	137.44	121.70
1	B	31	ALA	C-N-CA	6.28	137.41	121.70
1	A	31	ALA	C-N-CA	6.23	137.28	121.70

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	2493	0	2521	19	0
1	B	2473	0	2496	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2412	0	2461	35	0
1	D	2570	0	2593	37	0
2	A	26	0	0	0	0
2	B	42	0	0	0	0
2	C	35	0	0	0	0
2	D	32	0	0	0	0
All	All	10083	0	10071	113	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 6.

The worst 5 of 113 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:B:204:HIS:HA	1:B:205:CYS:HB2	1.29	1.13
1:D:229:ASP:HA	1:D:230:LEU:HB2	1.39	1.01
1:B:8:ILE:HA	1:B:9:ASN:HB2	1.60	0.84
1:D:245:ASP:H	1:D:246:HIS:HA	1.43	0.83
1:C:155:ASN:HA	1:C:156:ILE:HG22	1.61	0.83

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	316/378 (84%)	275 (87%)	27 (8%)	14 (4%)	2 15
1	B	307/378 (81%)	253 (82%)	34 (11%)	20 (6%)	1 9
1	C	306/378 (81%)	259 (85%)	33 (11%)	14 (5%)	2 15
1	D	323/378 (85%)	273 (84%)	35 (11%)	15 (5%)	2 15
All	All	1252/1512 (83%)	1060 (85%)	129 (10%)	63 (5%)	2 13

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	154	PHE
1	A	155	ASN
1	A	282	PRO
1	B	32	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 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	262/307 (85%)	229 (87%)	33 (13%)	4	18
1	B	262/307 (85%)	228 (87%)	34 (13%)	4	17
1	C	254/307 (83%)	219 (86%)	35 (14%)	3	16
1	D	270/307 (88%)	237 (88%)	33 (12%)	5	20
All	All	1048/1228 (85%)	913 (87%)	135 (13%)	4	18

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	LEU
1	D	156	ILE
1	D	271	ILE
1	B	123	LEU
1	B	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	GLN
1	B	180	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	D	122	1	9,11,12	0.63	0	5,12,14	1.57	1 (20%)
1	KCX	B	122	1	9,11,12	0.58	0	5,12,14	1.23	0
1	KCX	C	122	1	9,11,12	0.66	0	5,12,14	1.17	0
1	KCX	A	122	1	9,11,12	0.78	0	5,12,14	1.95	1 (20%)

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
1	KCX	D	122	1	-	4/9/10/12	-
1	KCX	B	122	1	-	4/9/10/12	-
1	KCX	C	122	1	-	4/9/10/12	-
1	KCX	A	122	1	-	4/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	KCX	OQ1-CX-NZ	-3.75	119.14	124.96
1	D	122	KCX	OQ1-CX-NZ	-3.49	119.55	124.96

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	122	KCX	N-CA-CB-CG
1	A	122	KCX	C-CA-CB-CG
1	C	122	KCX	N-CA-CB-CG
1	C	122	KCX	C-CA-CB-CG
1	D	122	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	122	KCX	2	0
1	C	122	KCX	2	0
1	A	122	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	252:VAL	C	253:GLY	N	3.75

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.