wwPDB X-ray Structure Validation Summary Report (i)

Sep 4, 2023 – 11:57 PM EDT

PDB ID	:	3U4F
Title	:	Crystal structure of a mandelate racemase (muconate lactonizing enzyme family protein) from Roseovarius nubinhibens
Authors	:	Eswaramoorthy, S.; Kumaran, D.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-10-07
Resolution	:	1.90 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:

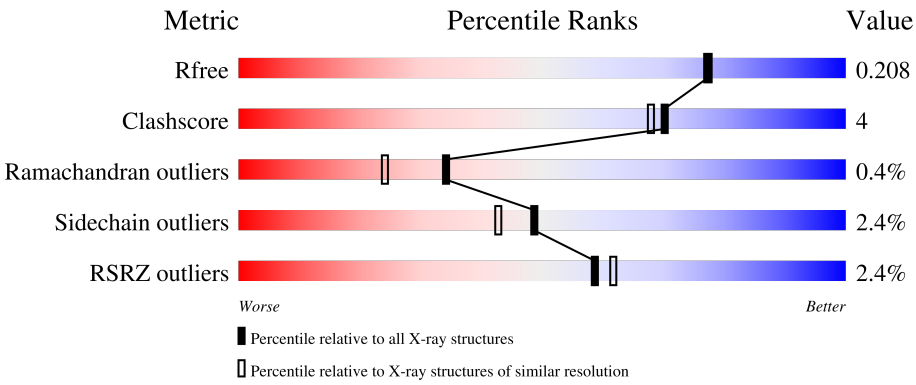
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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% 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	388	4%, 88%, 7%, •
1	B	388	2%, 86%, 8%, • •
1	C	388	2%, 86%, 8%, • 5%
1	D	388	2%, 87%, 8%, • •

Validation Pipeline (wwPDB-VP) : 2.35

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12194 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 Mandelate racemase/muconate lactonizing enzyme family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	371	2920	1834	513	554	8	11	0	0	0
1	B	371	2920	1834	513	554	8	11	0	0	0
1	C	369	2903	1822	511	551	8	11	0	0	0
1	D	371	2920	1834	513	554	8	11	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	expression tag	UNP A3SMJ4
A	-20	HIS	-	expression tag	UNP A3SMJ4
A	-19	HIS	-	expression tag	UNP A3SMJ4
A	-18	HIS	-	expression tag	UNP A3SMJ4
A	-17	HIS	-	expression tag	UNP A3SMJ4
A	-16	HIS	-	expression tag	UNP A3SMJ4
A	-15	HIS	-	expression tag	UNP A3SMJ4
A	-14	SER	-	expression tag	UNP A3SMJ4
A	-13	SER	-	expression tag	UNP A3SMJ4
A	-12	GLY	-	expression tag	UNP A3SMJ4
A	-11	VAL	-	expression tag	UNP A3SMJ4
A	-10	ASP	-	expression tag	UNP A3SMJ4
A	-9	LEU	-	expression tag	UNP A3SMJ4
A	-8	GLY	-	expression tag	UNP A3SMJ4
A	-7	THR	-	expression tag	UNP A3SMJ4
A	-6	GLU	-	expression tag	UNP A3SMJ4
A	-5	ASN	-	expression tag	UNP A3SMJ4
A	-4	LEU	-	expression tag	UNP A3SMJ4
A	-3	TYR	-	expression tag	UNP A3SMJ4
A	-2	PHE	-	expression tag	UNP A3SMJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP A3SMJ4
A	0	SER	-	expression tag	UNP A3SMJ4
B	-21	MSE	-	expression tag	UNP A3SMJ4
B	-20	HIS	-	expression tag	UNP A3SMJ4
B	-19	HIS	-	expression tag	UNP A3SMJ4
B	-18	HIS	-	expression tag	UNP A3SMJ4
B	-17	HIS	-	expression tag	UNP A3SMJ4
B	-16	HIS	-	expression tag	UNP A3SMJ4
B	-15	HIS	-	expression tag	UNP A3SMJ4
B	-14	SER	-	expression tag	UNP A3SMJ4
B	-13	SER	-	expression tag	UNP A3SMJ4
B	-12	GLY	-	expression tag	UNP A3SMJ4
B	-11	VAL	-	expression tag	UNP A3SMJ4
B	-10	ASP	-	expression tag	UNP A3SMJ4
B	-9	LEU	-	expression tag	UNP A3SMJ4
B	-8	GLY	-	expression tag	UNP A3SMJ4
B	-7	THR	-	expression tag	UNP A3SMJ4
B	-6	GLU	-	expression tag	UNP A3SMJ4
B	-5	ASN	-	expression tag	UNP A3SMJ4
B	-4	LEU	-	expression tag	UNP A3SMJ4
B	-3	TYR	-	expression tag	UNP A3SMJ4
B	-2	PHE	-	expression tag	UNP A3SMJ4
B	-1	GLN	-	expression tag	UNP A3SMJ4
B	0	SER	-	expression tag	UNP A3SMJ4
C	-21	MSE	-	expression tag	UNP A3SMJ4
C	-20	HIS	-	expression tag	UNP A3SMJ4
C	-19	HIS	-	expression tag	UNP A3SMJ4
C	-18	HIS	-	expression tag	UNP A3SMJ4
C	-17	HIS	-	expression tag	UNP A3SMJ4
C	-16	HIS	-	expression tag	UNP A3SMJ4
C	-15	HIS	-	expression tag	UNP A3SMJ4
C	-14	SER	-	expression tag	UNP A3SMJ4
C	-13	SER	-	expression tag	UNP A3SMJ4
C	-12	GLY	-	expression tag	UNP A3SMJ4
C	-11	VAL	-	expression tag	UNP A3SMJ4
C	-10	ASP	-	expression tag	UNP A3SMJ4
C	-9	LEU	-	expression tag	UNP A3SMJ4
C	-8	GLY	-	expression tag	UNP A3SMJ4
C	-7	THR	-	expression tag	UNP A3SMJ4
C	-6	GLU	-	expression tag	UNP A3SMJ4
C	-5	ASN	-	expression tag	UNP A3SMJ4
C	-4	LEU	-	expression tag	UNP A3SMJ4

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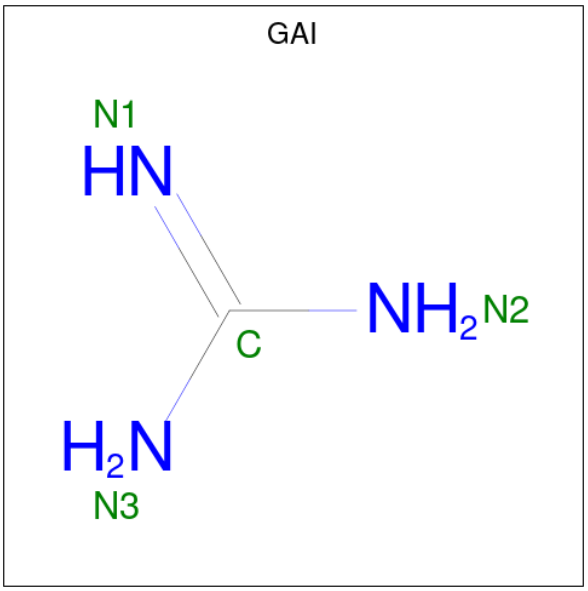
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP A3SMJ4
C	-2	PHE	-	expression tag	UNP A3SMJ4
C	-1	GLN	-	expression tag	UNP A3SMJ4
C	0	SER	-	expression tag	UNP A3SMJ4
D	-21	MSE	-	expression tag	UNP A3SMJ4
D	-20	HIS	-	expression tag	UNP A3SMJ4
D	-19	HIS	-	expression tag	UNP A3SMJ4
D	-18	HIS	-	expression tag	UNP A3SMJ4
D	-17	HIS	-	expression tag	UNP A3SMJ4
D	-16	HIS	-	expression tag	UNP A3SMJ4
D	-15	HIS	-	expression tag	UNP A3SMJ4
D	-14	SER	-	expression tag	UNP A3SMJ4
D	-13	SER	-	expression tag	UNP A3SMJ4
D	-12	GLY	-	expression tag	UNP A3SMJ4
D	-11	VAL	-	expression tag	UNP A3SMJ4
D	-10	ASP	-	expression tag	UNP A3SMJ4
D	-9	LEU	-	expression tag	UNP A3SMJ4
D	-8	GLY	-	expression tag	UNP A3SMJ4
D	-7	THR	-	expression tag	UNP A3SMJ4
D	-6	GLU	-	expression tag	UNP A3SMJ4
D	-5	ASN	-	expression tag	UNP A3SMJ4
D	-4	LEU	-	expression tag	UNP A3SMJ4
D	-3	TYR	-	expression tag	UNP A3SMJ4
D	-2	PHE	-	expression tag	UNP A3SMJ4
D	-1	GLN	-	expression tag	UNP A3SMJ4
D	0	SER	-	expression tag	UNP A3SMJ4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	3	3	3	0	0

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	4	1	3	0	0
3	B	1	4	1	3	0	0
3	C	1	4	1	3	0	0
3	D	1	4	1	3	0	0

- Molecule 4 is water.

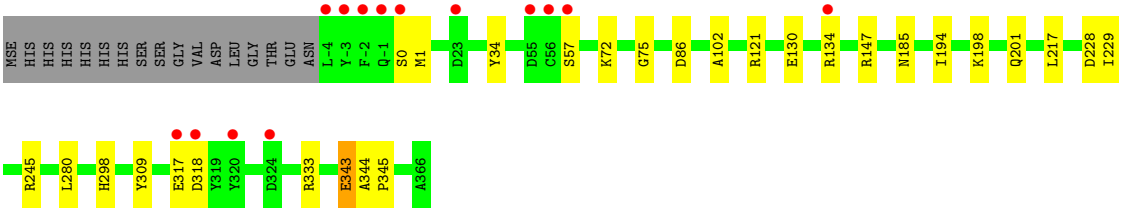
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	140	140	140	0	0
4	B	107	107	107	0	0
4	C	123	123	123	0	0
4	D	136	136	136	0	0

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 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.

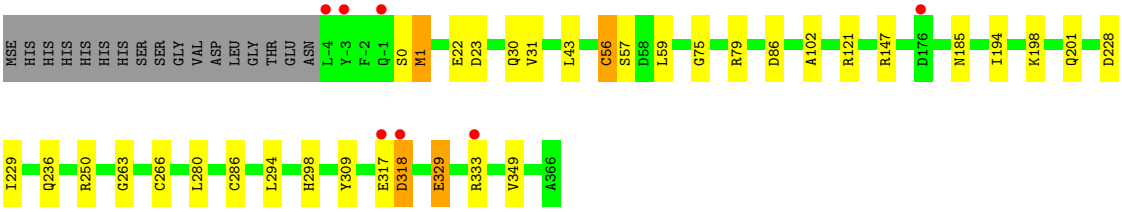
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain A:



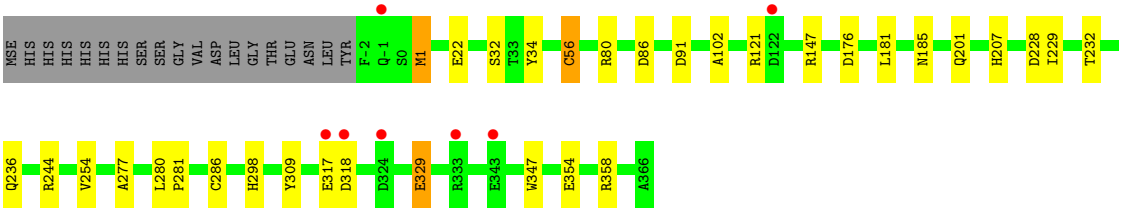
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain B:



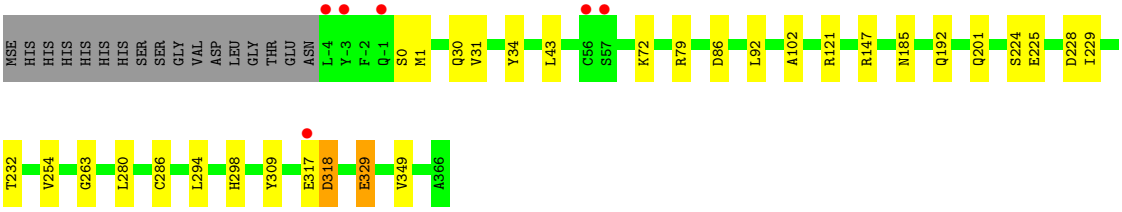
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain C:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain D:


MSE
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
VAL
ASP
LEU
GLY
THR
GLU
ASN
L-4
Y-3
F-2
Q-1
S0
M1
Q30
V31
Y34
L43
C56
S57
K72
R79
D86
L92
A102
R121
R147
N185
Q192
Q201
S224
E225
D228
I229
T232
V254
G263
L280
C286
L294
H298
Y309
E317
D318
E329
V349
A366

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	125.87Å 125.87Å 98.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.63 – 1.90 47.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.63-1.90) 100.0 (47.63-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.09 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.180 , 0.207 0.181 , 0.208	Depositor DCC
R_{free} test set	6875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l 0.020 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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 (i)

5.1 Standard geometry (i)

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

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	0.70	0/2977	0.71	0/4020
1	B	0.70	1/2977 (0.0%)	0.69	0/4020
1	C	0.72	2/2959 (0.1%)	0.73	1/3995 (0.0%)
1	D	0.71	1/2977 (0.0%)	0.70	0/4020
All	All	0.71	4/11890 (0.0%)	0.71	1/16055 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	CYS	CB-SG	-6.07	1.72	1.82
1	B	329	GLU	CG-CD	5.38	1.60	1.51
1	C	329	GLU	CG-CD	5.18	1.59	1.51
1	D	329	GLU	CG-CD	5.17	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	244	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2920	0	2819	24	0
1	B	2920	0	2819	24	0
1	C	2903	0	2808	18	0
1	D	2920	0	2819	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	2	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
4	A	140	0	0	0	0
4	B	107	0	0	2	0
4	C	123	0	0	1	0
4	D	136	0	0	3	0
All	All	12194	0	11276	82	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 82 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:D:192:GLN:HG3	4:D:417:HOH:O	1.34	1.26
1:D:225:GLU:HG2	4:D:460:HOH:O	1.52	1.06
1:A:121:ARG:HH22	1:A:185:ASN:HD22	1.00	0.99
1:D:147:ARG:HH11	1:D:185:ASN:HD21	1.18	0.91
1:C:121:ARG:HH22	1:C:185:ASN:HD22	1.05	0.90

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	369/388 (95%)	362 (98%)	6 (2%)	1 (0%)	41	31
1	B	369/388 (95%)	361 (98%)	7 (2%)	1 (0%)	41	31
1	C	367/388 (95%)	357 (97%)	8 (2%)	2 (0%)	29	18
1	D	369/388 (95%)	355 (96%)	12 (3%)	2 (0%)	29	18
All	All	1474/1552 (95%)	1435 (97%)	33 (2%)	6 (0%)	34	24

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	ASP
1	C	318	ASP
1	D	318	ASP
1	A	34	TYR
1	C	34	TYR

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	303/307 (99%)	298 (98%)	5 (2%)	60	57
1	B	303/307 (99%)	294 (97%)	9 (3%)	41	33
1	C	302/307 (98%)	294 (97%)	8 (3%)	46	39
1	D	303/307 (99%)	296 (98%)	7 (2%)	50	45
All	All	1211/1228 (99%)	1182 (98%)	29 (2%)	49	43

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	MSE
1	D	309	TYR
1	C	280	LEU
1	D	86	ASP
1	C	176	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	185	ASN
1	C	298	HIS
1	C	236	GLN
1	D	46	GLN
1	A	298	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	GAI	A	372	-	3,3,3	0.87	0	3,3,3	0.70	0
3	GAI	D	372	-	3,3,3	0.62	0	3,3,3	0.88	0
3	GAI	C	372	-	3,3,3	0.83	0	3,3,3	1.07	0
3	GAI	B	372	-	3,3,3	0.24	0	3,3,3	0.53	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	360/388 (92%)	-0.22	14 (3%)	39	42	5, 12, 27, 61	0
1	B	360/388 (92%)	-0.16	7 (1%)	66	69	6, 14, 28, 49	0
1	C	358/388 (92%)	-0.22	7 (1%)	65	68	6, 13, 28, 43	0
1	D	360/388 (92%)	-0.26	6 (1%)	70	72	7, 12, 29, 54	0
All	All	1438/1552 (92%)	-0.22	34 (2%)	59	62	5, 13, 28, 61	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	TYR	12.2
1	A	-4	LEU	9.0
1	A	57	SER	5.1
1	A	56	CYS	4.6
1	C	317	GLU	4.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
3	GAI	A	372	4/4	0.89	0.12	7,7,7,9	0
3	GAI	D	372	4/4	0.89	0.13	8,9,9,10	0
3	GAI	C	372	4/4	0.91	0.12	10,11,11,12	0
3	GAI	B	372	4/4	0.94	0.12	9,9,12,13	0
2	MG	D	379	1/1	0.98	0.05	25,25,25,25	0
2	MG	D	371	1/1	0.99	0.05	11,11,11,11	0
2	MG	D	374	1/1	0.99	0.07	11,11,11,11	0
2	MG	A	371	1/1	0.99	0.05	9,9,9,9	0
2	MG	A	374	1/1	0.99	0.04	14,14,14,14	0
2	MG	B	374	1/1	0.99	0.04	15,15,15,15	0
2	MG	C	371	1/1	0.99	0.06	12,12,12,12	0
2	MG	C	374	1/1	0.99	0.06	14,14,14,14	0
2	MG	B	371	1/1	1.00	0.04	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.