



# Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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)

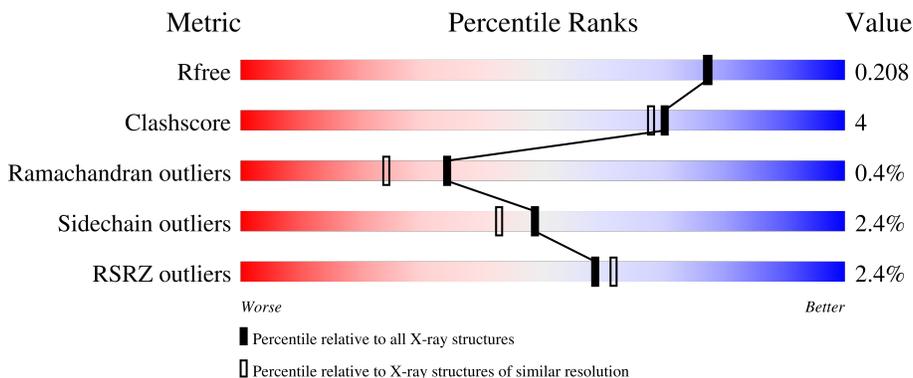
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

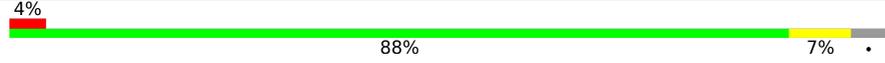
The reported resolution of this entry is 1.90 Å.

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  $\geq 3$ , 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  $\leq 5\%$ . 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% . .

## 2 Entry composition

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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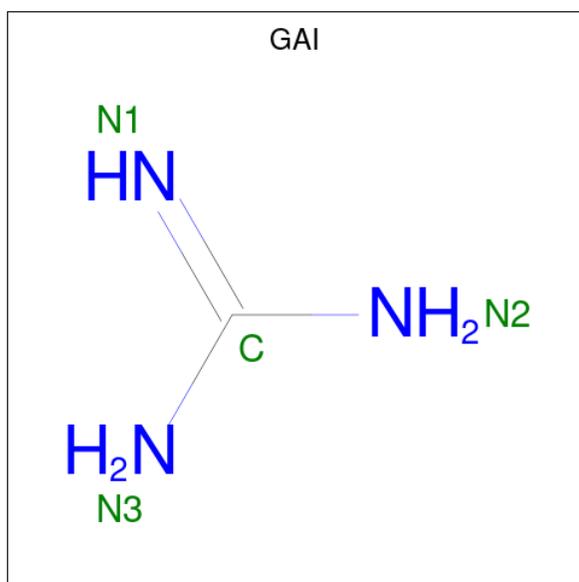
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP A3SMJ4
C	-2	PHE	-	expression tag	UNP A3SMJ4
C	-1	GLN	-	expression tag	UNP A3SMJ4
C	0	SER	-	expression tag	UNP A3SMJ4
D	-21	MSE	-	expression tag	UNP A3SMJ4
D	-20	HIS	-	expression 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
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	3	Total Mg 3 3	0	0

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula: CH<sub>5</sub>N<sub>3</sub>).



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

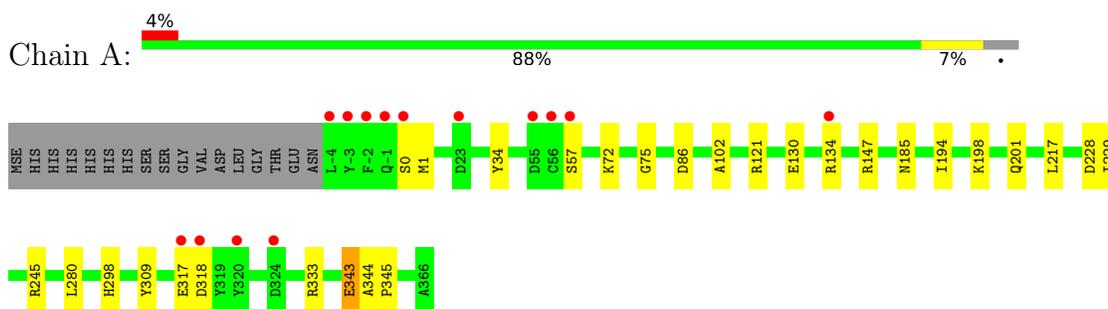
- Molecule 4 is water.

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

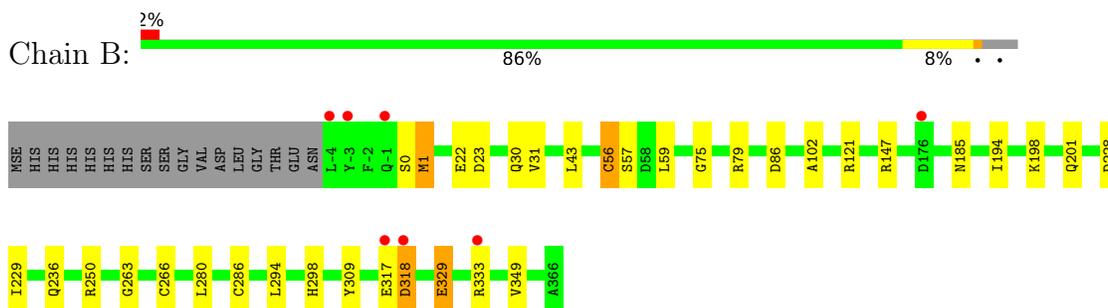
### 3 Residue-property plots [i](#)

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.

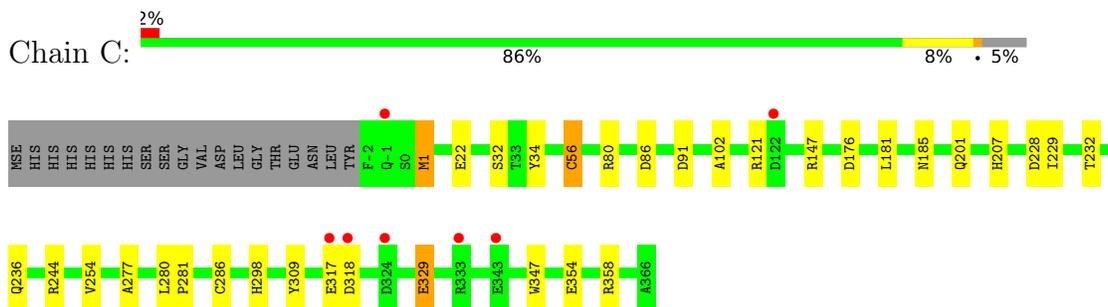
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein



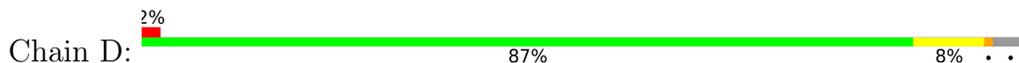
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

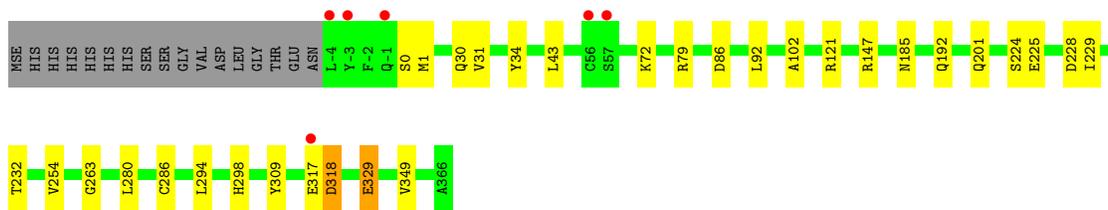


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein



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





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.09 (at 1.90Å)	Xtrriage
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 <sup>2</sup> )	15.1	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for -h,-k,l 0.020 for h,-h-k,-l 0.012 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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(°)	Ideal(°)
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.

All (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
1:B:121:ARG:HH22	1:B:185:ASN:HD22	1.12	0.90
1:A:147:ARG:HH11	1:A:185:ASN:HD21	1.20	0.89
1:A:201:GLN:HE21	1:A:229:ILE:H	1.21	0.87
1:C:201:GLN:HE21	1:C:229:ILE:H	1.23	0.86
1:B:147:ARG:HH11	1:B:185:ASN:HD21	1.17	0.86
1:D:121:ARG:HH22	1:D:185:ASN:HD22	1.21	0.86
1:B:201:GLN:HE21	1:B:229:ILE:H	1.28	0.79
1:C:102:ALA:H	1:C:298:HIS:HD2	1.30	0.77
1:B:102:ALA:H	1:B:298:HIS:HD2	1.30	0.77
1:A:343:GLU:H	1:A:343:GLU:CD	1.87	0.77
1:A:217:LEU:HD12	1:A:245:ARG:NH1	2.01	0.76
1:D:201:GLN:HE21	1:D:229:ILE:H	1.35	0.75
1:A:201:GLN:HE22	1:A:228:ASP:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ARG:HH11	1:C:185:ASN:HD21	1.40	0.70
1:D:102:ALA:H	1:D:298:HIS:HD2	1.39	0.68
1:A:102:ALA:H	1:A:298:HIS:HD2	1.42	0.68
1:B:201:GLN:HE22	1:B:228:ASP:H	1.41	0.68
1:A:121:ARG:NH2	1:A:185:ASN:HD22	1.84	0.64
1:C:201:GLN:HE22	1:C:228:ASP:H	1.44	0.64
1:C:121:ARG:NH2	1:C:185:ASN:HD22	1.87	0.64
1:B:147:ARG:NH1	1:B:185:ASN:HD21	1.95	0.63
1:B:317:GLU:O	1:B:318:ASP:HB3	1.98	0.62
1:B:294:LEU:CD2	1:B:349:VAL:HG21	2.33	0.58
1:A:201:GLN:NE2	1:A:228:ASP:H	2.02	0.58
1:B:333:ARG:HG3	4:B:400:HOH:O	2.04	0.57
1:C:201:GLN:NE2	1:C:228:ASP:H	2.03	0.56
1:B:22:GLU:HG2	4:B:398:HOH:O	2.04	0.56
1:B:0:SER:HA	1:B:57:SER:HB3	1.88	0.55
1:B:294:LEU:CD2	1:B:349:VAL:CG2	2.85	0.55
1:C:254:VAL:HG22	1:C:281:PRO:HG2	1.88	0.54
1:A:217:LEU:HD12	1:A:245:ARG:HH11	1.73	0.54
1:C:22:GLU:HG2	4:C:467:HOH:O	2.08	0.54
1:D:317:GLU:O	1:D:318:ASP:CB	2.55	0.54
1:A:147:ARG:NH1	1:A:185:ASN:HD21	2.00	0.53
1:D:201:GLN:HE22	1:D:228:ASP:H	1.55	0.53
1:B:1:MSE:HE3	1:B:56:CYS:HB2	1.91	0.52
1:C:1:MSE:HE3	1:C:56:CYS:HB3	1.92	0.51
1:A:201:GLN:NE2	1:A:229:ILE:H	2.01	0.51
1:C:32:SER:HB3	1:C:80:ARG:HG2	1.93	0.51
1:B:294:LEU:HD22	1:B:349:VAL:HG21	1.94	0.49
1:D:317:GLU:O	1:D:318:ASP:HB3	2.12	0.49
1:C:232:THR:HG22	1:C:254:VAL:HB	1.93	0.49
1:D:232:THR:HG22	1:D:254:VAL:HB	1.94	0.49
1:B:317:GLU:O	1:B:318:ASP:CB	2.61	0.48
1:C:91:ASP:HB2	1:C:347:TRP:CD1	2.48	0.48
1:C:236:GLN:HE21	1:D:72:LYS:HD3	1.79	0.48
1:B:201:GLN:NE2	1:B:228:ASP:H	2.07	0.48
1:B:194:ILE:O	1:B:198:LYS:HG2	2.14	0.48
1:A:72:LYS:HD3	1:B:236:GLN:HE21	1.77	0.48
1:A:0:SER:HA	1:A:57:SER:HB3	1.97	0.47
1:C:354:GLU:OE2	1:C:358:ARG:NE	2.39	0.46
1:D:147:ARG:NH1	1:D:185:ASN:HD21	1.99	0.46
1:A:317:GLU:N	1:A:317:GLU:OE1	2.50	0.45
1:C:181:LEU:HG	1:C:207:HIS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HD2	1:C:277:ALA:HB2	1.98	0.45
1:D:79:ARG:O	1:D:263:GLY:HA2	2.16	0.45
1:D:294:LEU:HD22	1:D:349:VAL:HG21	1.99	0.45
1:A:75:GLY:HA3	1:B:75:GLY:HA3	1.97	0.45
1:B:79:ARG:O	1:B:263:GLY:HA2	2.16	0.45
1:D:30:GLN:HG2	1:D:31:VAL:O	2.17	0.45
1:B:43:LEU:HD23	1:B:43:LEU:C	2.39	0.44
1:D:92:LEU:C	1:D:92:LEU:HD23	2.39	0.43
1:D:224:SER:HB3	4:D:432:HOH:O	2.18	0.43
1:A:194:ILE:O	1:A:198:LYS:HG2	2.18	0.43
1:A:121:ARG:HH22	1:A:185:ASN:ND2	1.85	0.43
1:D:201:GLN:NE2	1:D:228:ASP:H	2.17	0.42
1:A:130:GLU:O	1:A:134:ARG:HG2	2.20	0.42
1:D:317:GLU:O	1:D:318:ASP:OD1	2.38	0.42
1:A:344:ALA:HA	1:A:345:PRO:HD3	1.96	0.42
1:B:317:GLU:H	1:B:317:GLU:CD	2.23	0.42
1:D:43:LEU:C	1:D:43:LEU:HD23	2.39	0.42
1:A:201:GLN:NE2	1:A:228:ASP:N	2.66	0.41
1:B:30:GLN:HG2	1:B:31:VAL:O	2.20	0.41
1:A:201:GLN:HE22	1:A:228:ASP:N	2.10	0.41
1:B:59:LEU:HD23	1:B:266:CYS:SG	2.61	0.41
1:C:1:MSE:HE3	1:C:56:CYS:CB	2.50	0.40
1:A:317:GLU:O	1:A:318:ASP:C	2.60	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 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	D	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

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	86	ASP
1	A	280	LEU
1	A	309	TYR
1	A	343	GLU
1	B	1	MSE

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Mol	Chain	Res	Type
1	B	23	ASP
1	B	56	CYS
1	B	86	ASP
1	B	250	ARG
1	B	280	LEU
1	B	286	CYS
1	B	309	TYR
1	B	329	GLU
1	C	1	MSE
1	C	86	ASP
1	C	176	ASP
1	C	280	LEU
1	C	286	CYS
1	C	309	TYR
1	C	317	GLU
1	C	329	GLU
1	D	0	SER
1	D	1	MSE
1	D	86	ASP
1	D	280	LEU
1	D	286	CYS
1	D	309	TYR
1	D	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	46	GLN
1	A	126	HIS
1	A	185	ASN
1	A	201	GLN
1	A	236	GLN
1	A	298	HIS
1	B	46	GLN
1	B	126	HIS
1	B	185	ASN
1	B	201	GLN
1	B	236	GLN
1	B	298	HIS
1	C	46	GLN
1	C	185	ASN

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Mol	Chain	Res	Type
1	C	201	GLN
1	C	236	GLN
1	C	298	HIS
1	D	46	GLN
1	D	185	ASN
1	D	201	GLN
1	D	236	GLN
1	D	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

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<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	D	-3	TYR	4.4
1	A	-1	GLN	3.9
1	D	57	SER	3.7
1	A	318	ASP	3.7
1	A	-2	PHE	3.7
1	A	317	GLU	3.7
1	C	-1	GLN	3.3
1	B	-3	TYR	3.3
1	A	0	SER	3.1
1	B	317	GLU	2.9
1	B	318	ASP	2.8
1	D	-4	LEU	2.8
1	D	317	GLU	2.8
1	D	56	CYS	2.7
1	D	-1	GLN	2.6
1	C	318	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	324	ASP	2.5
1	A	324	ASP	2.5
1	B	-4	LEU	2.4
1	A	55	ASP	2.4
1	A	23	ASP	2.3
1	C	333	ARG	2.3
1	A	320	TYR	2.2
1	C	343	GLU	2.2
1	B	-1	GLN	2.1
1	B	176	ASP	2.1
1	A	134	ARG	2.0
1	B	333	ARG	2.0
1	C	122	ASP	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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.