



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 04:44 PM EST

PDB ID : 3H12
Title : Crystal structure of putative mandelate racemase from Bordetella Bronchiseptica RB50
Authors : Malashkevich, V.N.; Toro, R.; Morano, C.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-04-10
Resolution : 1.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

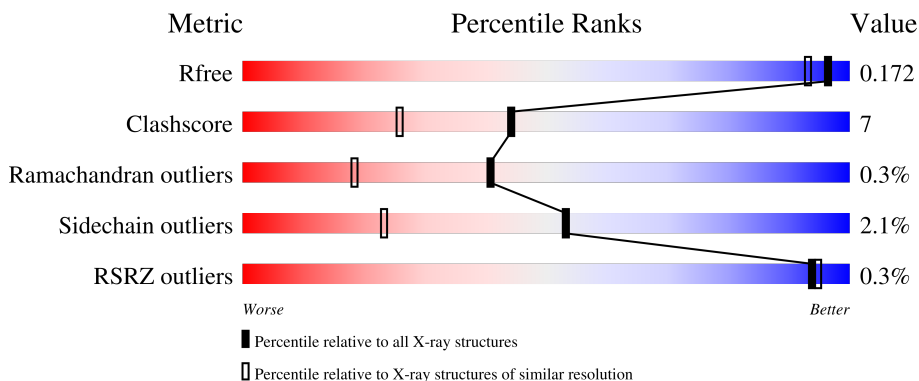
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 $\leq 5\%$. 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	397	
1	B	397	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6853 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3029	1908	553	558	10	0	2	0
1	B	392	3041	1917	554	560	10	0	3	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q7WEE8
A	2	SER	-	expression tag	UNP Q7WEE8
A	3	LEU	-	expression tag	UNP Q7WEE8
A	390	GLU	-	expression tag	UNP Q7WEE8
A	391	GLY	-	expression tag	UNP Q7WEE8
A	392	HIS	-	expression tag	UNP Q7WEE8
A	393	HIS	-	expression tag	UNP Q7WEE8
A	394	HIS	-	expression tag	UNP Q7WEE8
A	395	HIS	-	expression tag	UNP Q7WEE8
A	396	HIS	-	expression tag	UNP Q7WEE8
A	397	HIS	-	expression tag	UNP Q7WEE8
B	1	MET	-	expression tag	UNP Q7WEE8
B	2	SER	-	expression tag	UNP Q7WEE8
B	3	LEU	-	expression tag	UNP Q7WEE8
B	390	GLU	-	expression tag	UNP Q7WEE8
B	391	GLY	-	expression tag	UNP Q7WEE8
B	392	HIS	-	expression tag	UNP Q7WEE8
B	393	HIS	-	expression tag	UNP Q7WEE8
B	394	HIS	-	expression tag	UNP Q7WEE8
B	395	HIS	-	expression tag	UNP Q7WEE8
B	396	HIS	-	expression tag	UNP Q7WEE8
B	397	HIS	-	expression tag	UNP Q7WEE8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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


- Molecule 3 is water.

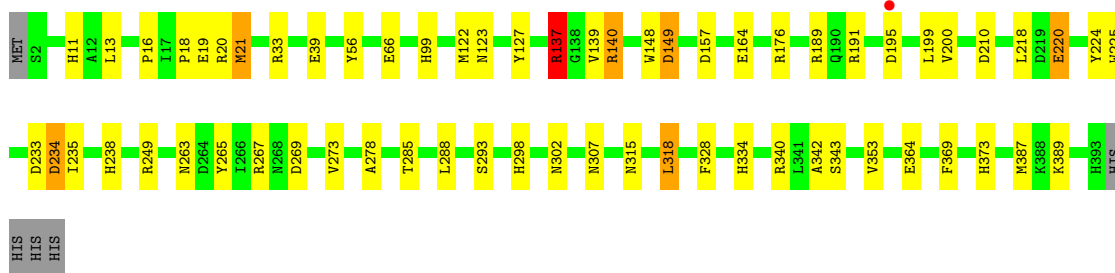
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	386	Total 386	O 386	0	0
3	B	395	Total 395	O 395	0	0

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.

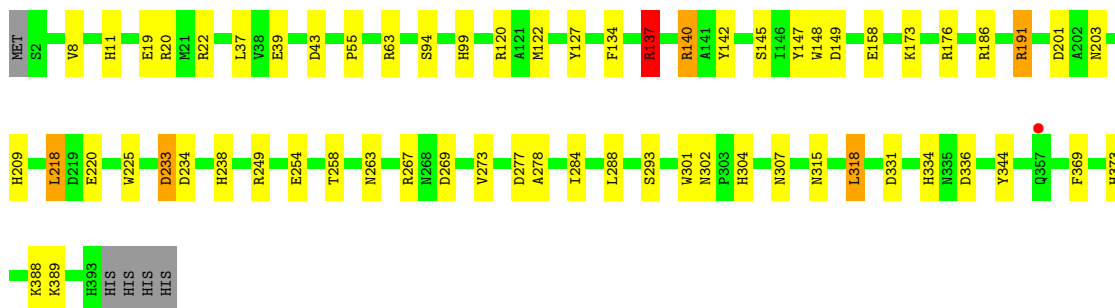
- Molecule 1: mandelate racemase

Chain A:  83% 14% ..



- Molecule 1: mandelate racemase

Chain B:  83% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	116.15Å 116.15Å 128.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.73 – 1.50 8.73 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (8.73-1.50) 95.8 (8.73-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.50Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.173 0.145 , 0.172	Depositor DCC
R_{free} test set	6483 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtrriage
Anisotropy	0.007	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for -h,k,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6853	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA

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	1.49	10/3104 (0.3%)	1.34	27/4216 (0.6%)
1	B	1.47	20/3117 (0.6%)	1.33	26/4234 (0.6%)
All	All	1.48	30/6221 (0.5%)	1.34	53/8450 (0.6%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	MET	CB-CG	12.67	1.92	1.51
1	A	21	MET	CG-SD	10.51	2.08	1.81
1	B	220	GLU	CG-CD	8.89	1.65	1.51
1	B	19	GLU	CB-CG	-8.38	1.36	1.52
1	A	293	SER	CB-OG	7.51	1.52	1.42
1	B	254	GLU	CD-OE2	-7.43	1.17	1.25
1	B	19	GLU	CG-CD	-7.40	1.40	1.51
1	A	220	GLU	CG-CD	7.28	1.62	1.51
1	B	147	TYR	CE2-CZ	6.93	1.47	1.38
1	B	158	GLU	CD-OE1	6.92	1.33	1.25
1	B	293	SER	CB-OG	6.46	1.50	1.42
1	A	140	ARG	CZ-NH1	6.26	1.41	1.33
1	B	344	TYR	CD1-CE1	5.97	1.48	1.39
1	A	56	TYR	C-O	5.85	1.34	1.23
1	A	353	VAL	CB-CG1	5.83	1.65	1.52
1	B	249	ARG	CZ-NH2	5.80	1.40	1.33
1	B	22	ARG	CZ-NH1	5.73	1.40	1.33
1	A	66	GLU	CD-OE1	5.57	1.31	1.25
1	B	147	TYR	CD2-CE2	5.42	1.47	1.39
1	A	249	ARG	CZ-NH2	5.37	1.40	1.33
1	B	301	TRP	CZ3-CH2	5.33	1.48	1.40
1	B	94	SER	CB-OG	5.28	1.49	1.42
1	B	148	TRP	CD1-NE1	5.20	1.46	1.38
1	A	189	ARG	CZ-NH2	5.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	PHE	CE2-CZ	5.06	1.47	1.37
1	B	148	TRP	CE3-CZ3	5.05	1.47	1.38
1	B	8	VAL	CB-CG2	5.03	1.63	1.52
1	B	145	SER	CB-OG	5.03	1.48	1.42
1	B	191[A]	ARG	CZ-NH1	-5.01	1.26	1.33
1	B	191[B]	ARG	CZ-NH1	-5.01	1.26	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	MET	CB-CG-SD	-10.29	81.52	112.40
1	B	176	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	A	218	LEU	CB-CG-CD2	9.00	126.30	111.00
1	A	176	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	249	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	186	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	B	63	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	20	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	A	340	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	218	LEU	CB-CG-CD1	7.77	124.21	111.00
1	B	318	LEU	CB-CG-CD1	-7.75	97.82	111.00
1	B	122	MET	CG-SD-CE	-7.71	87.87	100.20
1	B	137	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	B	147	TYR	CB-CG-CD1	-7.67	116.40	121.00
1	B	22	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	21	MET	CG-SD-CE	7.31	111.89	100.20
1	A	234	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	B	140	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	A	20	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	B	149	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	210	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	B	140	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	13	LEU	CB-CG-CD1	-6.54	99.89	111.00
1	A	195	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	B	120	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	149	ASP	CB-CG-OD2	6.32	123.98	118.30
1	B	233	ASP	CB-CG-OD1	-6.32	112.62	118.30
1	B	140	ARG	NH1-CZ-NH2	6.29	126.32	119.40
1	B	331	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	137	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	336	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	127	TYR	CG-CD2-CE2	-6.16	116.37	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	MET	CG-SD-CE	-6.11	90.43	100.20
1	B	201	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	140	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	A	269	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	127	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	139	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	A	189	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	199	LEU	CB-CG-CD2	-5.83	101.10	111.00
1	A	328	PHE	CB-CG-CD1	-5.58	116.89	120.80
1	B	43	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	269	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	149	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	B	37	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	33	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	122	MET	CG-SD-CE	-5.39	91.58	100.20
1	A	224	TYR	CZ-CE2-CD2	-5.36	114.98	119.80
1	A	157	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	142	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	B	269	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	200	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	B	147	TYR	CZ-CE2-CD2	-5.02	115.28	119.80

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	3029	0	2990	50	0
1	B	3041	0	2998	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	386	0	0	15	4
3	B	395	0	0	16	4
All	All	6853	0	5988	80	4

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 7.

All (80) 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:A:21:MET:CG	1:A:21:MET:CB	1.91	1.45
1:A:21:MET:CG	1:A:21:MET:SD	2.08	1.41
1:A:364:GLU:HB2	3:A:537:HOH:O	1.27	1.30
1:A:21:MET:HG2	3:A:749:HOH:O	1.51	1.11
1:A:288:LEU:HD23	1:A:318:LEU:HD21	1.29	1.07
1:B:318:LEU:HG	3:B:690:HOH:O	1.56	1.06
1:B:191[A]:ARG:NH2	3:B:882:HOH:O	1.86	1.06
1:B:191[A]:ARG:NE	3:B:882:HOH:O	1.99	0.96
1:B:191[A]:ARG:CZ	3:B:882:HOH:O	2.17	0.90
1:A:288:LEU:CD2	1:A:318:LEU:HD21	2.01	0.90
1:A:21:MET:SD	1:A:21:MET:CB	2.61	0.88
1:A:21:MET:HE3	1:A:334:HIS:CG	2.10	0.86
1:A:278:ALA:H	1:A:315:ASN:HD21	1.20	0.85
1:B:258:THR:HG22	3:B:811:HOH:O	1.78	0.82
1:A:21:MET:CE	1:A:21:MET:CB	2.59	0.81
1:A:21:MET:CE	1:A:334:HIS:CG	2.66	0.79
1:A:18:PRO:HD2	1:A:21:MET:CE	2.12	0.79
1:A:21:MET:HE2	1:A:21:MET:HB2	1.63	0.78
1:A:21:MET:HE3	1:A:334:HIS:CB	2.15	0.77
1:A:21:MET:HB2	1:A:21:MET:CE	2.14	0.76
1:B:278:ALA:H	1:B:315:ASN:HD21	1.28	0.76
1:A:18:PRO:HD2	1:A:21:MET:HE2	1.67	0.74
1:A:191[B]:ARG:NH2	3:A:823:HOH:O	1.99	0.74
1:A:220:GLU:HB2	3:A:704:HOH:O	1.86	0.74
1:B:334:HIS:HD2	3:B:708:HOH:O	1.74	0.70
1:A:191[B]:ARG:NE	3:A:823:HOH:O	2.21	0.69
1:A:342:ALA:O	3:A:489:HOH:O	2.13	0.67
1:A:288:LEU:HD23	1:A:318:LEU:CD2	2.19	0.66
1:B:277:ASP:OD2	1:B:304:HIS:HD2	1.78	0.66
1:B:369:PHE:O	1:B:373:HIS:HD2	1.77	0.66
1:A:285:THR:HG21	3:A:644:HOH:O	1.96	0.65
1:B:304:HIS:HE1	3:B:661:HOH:O	1.79	0.65
1:A:21:MET:HB2	1:A:21:MET:SD	2.37	0.65
1:B:209:HIS:HD2	3:B:481:HOH:O	1.80	0.63
1:A:234:ASP:O	1:A:238:HIS:HD2	1.81	0.63
1:A:99:HIS:HD2	1:B:233:ASP:OD1	1.82	0.63
1:A:364:GLU:CB	3:A:537:HOH:O	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:HG23	1:B:318:LEU:HD11	1.80	0.62
1:A:21:MET:HE3	1:A:334:HIS:HB2	1.82	0.61
3:A:406:HOH:O	1:B:99:HIS:HE1	1.84	0.60
1:A:369:PHE:O	1:A:373:HIS:HD2	1.85	0.60
1:A:233:ASP:OD1	1:B:99:HIS:HD2	1.86	0.59
1:B:234:ASP:O	1:B:238:HIS:HD2	1.86	0.58
1:B:334:HIS:HE1	3:B:459:HOH:O	1.86	0.58
1:B:137:ARG:HH21	1:B:137:ARG:HG2	1.68	0.58
1:A:99:HIS:HE1	3:B:400:HOH:O	1.86	0.58
1:A:21:MET:HE1	1:A:334:HIS:CG	2.39	0.56
1:A:364:GLU:CA	3:A:537:HOH:O	2.49	0.55
1:B:11:HIS:HE1	1:B:39:GLU:OE1	1.89	0.55
1:A:18:PRO:HD2	1:A:21:MET:HE1	1.86	0.55
1:A:11:HIS:HE1	1:A:39:GLU:OE1	1.91	0.54
1:B:20:ARG:CD	3:B:632:HOH:O	2.55	0.53
1:B:288:LEU:HD23	3:B:690:HOH:O	2.08	0.53
1:B:278:ALA:H	1:B:315:ASN:ND2	2.04	0.53
1:A:298:HIS:HE1	3:A:457:HOH:O	1.92	0.52
1:A:21:MET:CE	1:A:21:MET:HB3	2.40	0.52
1:A:238:HIS:HE1	3:A:435:HOH:O	1.94	0.51
1:B:273:VAL:HG13	1:B:302:ASN:HD22	1.75	0.51
1:A:278:ALA:H	1:A:315:ASN:ND2	2.00	0.50
1:A:21:MET:HE1	1:A:334:HIS:ND1	2.27	0.49
1:A:273:VAL:HG13	1:A:302:ASN:HD22	1.80	0.47
1:A:164:GLU:OE1	3:A:817:HOH:O	2.20	0.47
1:B:263:ASN:HD21	1:B:267[B]:ARG:HD3	1.79	0.47
1:A:220:GLU:HG2	3:A:826:HOH:O	2.15	0.47
1:B:173:LYS:NZ	1:B:203:ASN:HD21	2.14	0.46
1:B:373:HIS:HE1	3:B:670:HOH:O	1.98	0.45
1:A:21:MET:CE	1:A:334:HIS:ND1	2.79	0.45
1:B:263:ASN:ND2	1:B:267[B]:ARG:HD3	2.33	0.43
1:A:148:TRP:O	1:A:149:ASP:HB2	2.18	0.43
1:A:21:MET:HE3	1:A:21:MET:HB3	2.01	0.43
1:B:55:PRO:HA	3:B:874:HOH:O	2.17	0.43
1:B:238:HIS:HE1	3:B:413:HOH:O	2.01	0.43
1:B:388:LYS:NZ	3:B:751:HOH:O	2.52	0.42
1:A:263:ASN:ND2	1:A:267[B]:ARG:HD2	2.35	0.41
1:B:369:PHE:O	1:B:373:HIS:CD2	2.66	0.41
1:A:343:SER:OG	3:A:698:HOH:O	2.07	0.41
1:A:137:ARG:HG2	1:A:137:ARG:HH11	1.85	0.41
1:A:235:ILE:HG12	1:A:265:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:HD21	1:A:267[B]:ARG:HD2	1.86	0.40
1:B:263:ASN:O	1:B:267[B]:ARG:HG3	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:732:HOH:O	3:B:482:HOH:O[3_655]	2.04	0.16
3:A:715:HOH:O	3:B:890:HOH:O[6_555]	2.09	0.11
3:A:622:HOH:O	3:B:623:HOH:O[3_655]	2.12	0.08
3:A:461:HOH:O	3:B:834:HOH:O[3_655]	2.14	0.06

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	392/397 (99%)	375 (96%)	16 (4%)	1 (0%)	41	18
1	B	393/397 (99%)	380 (97%)	12 (3%)	1 (0%)	41	18
All	All	785/794 (99%)	755 (96%)	28 (4%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	307	ASN

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	307/310 (99%)	299 (97%)	8 (3%)	46	16
1	B	308/310 (99%)	303 (98%)	5 (2%)	62	36
All	All	615/620 (99%)	602 (98%)	13 (2%)	53	23

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	19	GLU
1	A	123	ASN
1	A	137	ARG
1	A	140	ARG
1	A	225	TRP
1	A	318	LEU
1	A	389	LYS
1	B	137	ARG
1	B	140	ARG
1	B	218	LEU
1	B	225	TRP
1	B	389	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	99	HIS
1	A	238	HIS
1	A	255	ASN
1	A	263	ASN
1	A	298	HIS
1	A	302	ASN
1	A	315	ASN
1	A	373	HIS
1	B	11	HIS
1	B	99	HIS
1	B	123	ASN
1	B	203	ASN
1	B	209	HIS

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Mol	Chain	Res	Type
1	B	238	HIS
1	B	244	GLN
1	B	255	ASN
1	B	263	ASN
1	B	302	ASN
1	B	304	HIS
1	B	307	ASN
1	B	315	ASN
1	B	334	HIS
1	B	373	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	392/397 (98%)	-0.69	1 (0%) 94 95	13, 17, 30, 53	0
1	B	392/397 (98%)	-0.73	1 (0%) 94 95	14, 17, 29, 50	0
All	All	784/794 (98%)	-0.71	2 (0%) 94 95	13, 17, 30, 53	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ASP	2.3
1	B	357	GLN	2.2

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
2	NA	B	500	1/1	1.00	0.02	17,17,17,17	0
2	NA	A	500	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.