



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:12 AM UTC

PDB ID : 3DFH / pdb_00003dfh
Title : crystal structure of putative mandelate racemase / muconate lactonizing enzyme from Vibrionales bacterium SWAT-3
Authors : Malashkevich, V.N.; Toro, R.; Wasserman, S.R.; Meyer, A.J.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-06-12
Resolution : 2.20 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

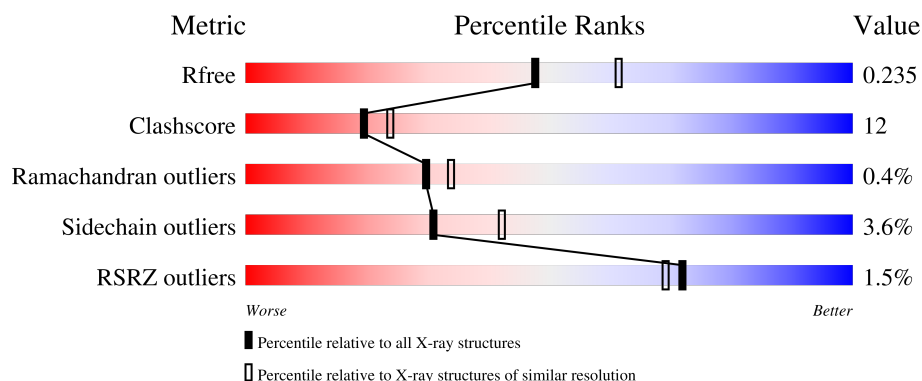
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	394	
1	B	394	
1	C	394	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8955 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
1	A	359	Total	C	N	O	S	0	1	0
			2863	1825	494	528	16			
1	B	359	Total	C	N	O	S	0	0	0
			2857	1821	494	526	16			
1	C	359	Total	C	N	O	S	0	0	0
			2857	1821	494	526	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A5KUH4
A	2	SER	-	expression tag	UNP A5KUH4
A	3	LEU	-	expression tag	UNP A5KUH4
A	388	GLY	-	expression tag	UNP A5KUH4
A	389	HIS	-	expression tag	UNP A5KUH4
A	390	HIS	-	expression tag	UNP A5KUH4
A	391	HIS	-	expression tag	UNP A5KUH4
A	392	HIS	-	expression tag	UNP A5KUH4
A	393	HIS	-	expression tag	UNP A5KUH4
A	394	HIS	-	expression tag	UNP A5KUH4
B	1	MET	-	expression tag	UNP A5KUH4
B	2	SER	-	expression tag	UNP A5KUH4
B	3	LEU	-	expression tag	UNP A5KUH4
B	388	GLY	-	expression tag	UNP A5KUH4
B	389	HIS	-	expression tag	UNP A5KUH4
B	390	HIS	-	expression tag	UNP A5KUH4
B	391	HIS	-	expression tag	UNP A5KUH4
B	392	HIS	-	expression tag	UNP A5KUH4
B	393	HIS	-	expression tag	UNP A5KUH4
B	394	HIS	-	expression tag	UNP A5KUH4
C	1	MET	-	expression tag	UNP A5KUH4
C	2	SER	-	expression tag	UNP A5KUH4
C	3	LEU	-	expression tag	UNP A5KUH4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	388	GLY	-	expression tag	UNP A5KUH4
C	389	HIS	-	expression tag	UNP A5KUH4
C	390	HIS	-	expression tag	UNP A5KUH4
C	391	HIS	-	expression tag	UNP A5KUH4
C	392	HIS	-	expression tag	UNP A5KUH4
C	393	HIS	-	expression tag	UNP A5KUH4
C	394	HIS	-	expression tag	UNP A5KUH4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

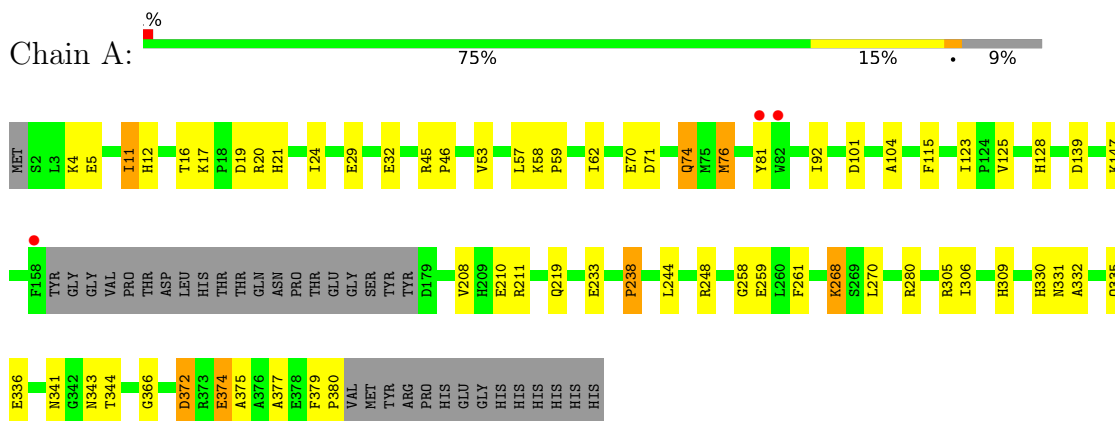
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total 135	O 135	0	0
3	B	113	Total 113	O 113	0	0
3	C	127	Total 127	O 127	0	0

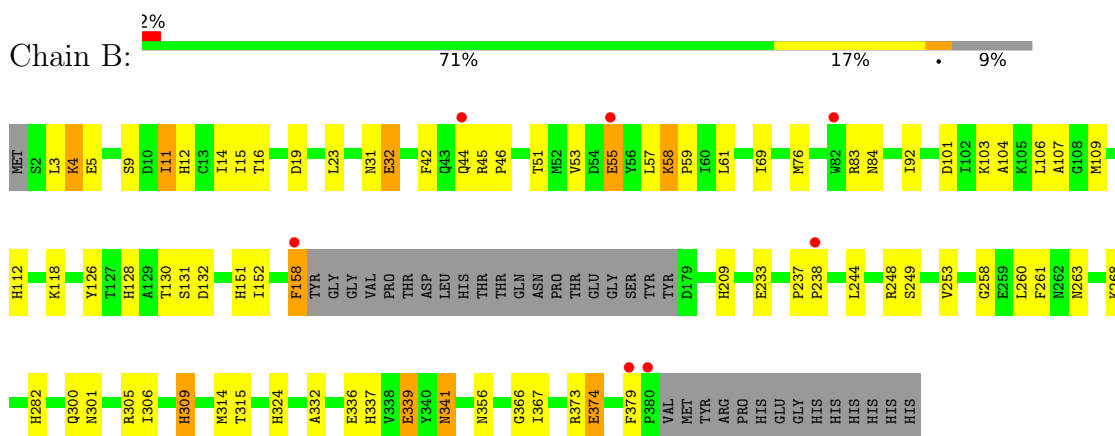
3 Residue-property plots

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.

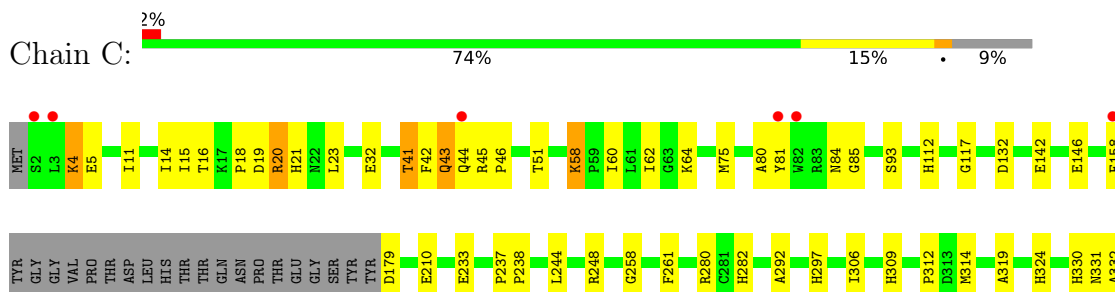
• Molecule 1: mandelate racemase



• Molecule 1: mandelate racemase



• Molecule 1: mandelate racemase



E336	E339	Y340	N341	F348	I367	I371	D372	R373	E374	A377	P380	VAL	MET	TYR	ARG	PRO	HIS	GLU	GLY	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.84Å 121.84Å 319.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.59 – 2.20 41.59 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.59-2.20) 99.7 (41.59-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	96.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.234 0.173 , 0.235	Depositor DCC
R_{free} test set	3113 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8955	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

5.1 Standard geometry

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	1.01	1/2937 (0.0%)	1.10	7/3988 (0.2%)
1	B	1.04	2/2928 (0.1%)	1.14	7/3976 (0.2%)
1	C	1.05	1/2928 (0.0%)	1.09	7/3976 (0.2%)
All	All	1.04	4/8793 (0.0%)	1.11	21/11940 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	ALA	CA-CB	5.60	1.62	1.53
1	A	115	PHE	CA-C	-5.49	1.45	1.52
1	B	263	ASN	CA-C	5.44	1.57	1.52
1	B	253	VAL	CA-CB	5.43	1.59	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	MET	CG-SD-CE	-10.02	78.85	100.90
1	B	237	PRO	CA-C-N	-7.56	113.03	120.52
1	B	237	PRO	C-N-CA	-7.56	113.03	120.52
1	C	85	GLY	CA-C-N	6.70	126.15	118.85
1	C	85	GLY	C-N-CA	6.70	126.15	118.85
1	C	280	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	B	300	GLN	N-CA-C	6.37	117.88	111.07
1	A	123	ILE	CA-C-N	-5.97	114.12	120.03
1	A	123	ILE	C-N-CA	-5.97	114.12	120.03
1	A	280	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	B	249	SER	N-CA-C	-5.51	106.56	113.28
1	A	238	PRO	N-CA-C	-5.34	103.46	111.57
1	B	101	ASP	N-CA-C	-5.32	105.38	111.07
1	A	101	ASP	N-CA-C	-5.17	105.53	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	348	PHE	CA-C-N	5.13	125.06	119.78
1	C	348	PHE	C-N-CA	5.13	125.06	119.78
1	A	24	ILE	N-CA-C	5.11	115.21	107.75
1	C	117	GLY	N-CA-C	5.07	118.19	111.70
1	C	41	THR	CB-CA-C	-5.04	104.07	111.23
1	B	238	PRO	N-CA-C	-5.03	103.64	111.13
1	A	76	MET	N-CA-C	-5.02	105.89	111.36

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	2863	0	2798	55	0
1	B	2857	0	2792	78	0
1	C	2857	0	2792	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	135	0	0	6	0
3	B	113	0	0	6	0
3	C	127	0	0	3	0
All	All	8955	0	8382	197	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 12.

All (197) 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:57:LEU:HD13	1:B:76:MET:CE	1.54	1.37
1:A:11:ILE:O	1:A:58:LYS:HE2	1.29	1.30
1:B:19:ASP:CG	1:B:341:ASN:HD21	1.41	1.26
1:A:19:ASP:HB2	1:A:341:ASN:ND2	1.53	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASP:CG	1:B:341:ASN:ND2	2.01	1.16
1:A:17:LYS:HE2	1:A:20:ARG:O	1.49	1.11
1:A:57:LEU:HD13	1:A:76:MET:CE	1.80	1.11
1:C:58:LYS:HD3	1:C:62:ILE:CD1	1.86	1.05
1:B:19:ASP:CB	1:B:341:ASN:ND2	2.20	1.05
1:B:19:ASP:HB2	1:B:341:ASN:ND2	1.70	1.04
1:C:339:GLU:CD	1:C:340:TYR:H	1.63	1.03
1:C:58:LYS:HD3	1:C:62:ILE:HD12	1.41	1.03
1:B:57:LEU:HD13	1:B:76:MET:HE1	1.40	1.01
1:A:57:LEU:HD13	1:A:76:MET:HE1	1.43	1.01
1:B:11:ILE:HD11	1:B:53:VAL:CG1	1.93	0.99
1:A:76:MET:HE2	1:A:92:ILE:HG12	1.42	0.99
1:A:19:ASP:HB2	1:A:341:ASN:HD22	1.13	0.98
1:C:112:HIS:HD2	1:C:324:HIS:HD2	1.12	0.96
1:B:57:LEU:CD1	1:B:76:MET:CE	2.43	0.96
1:C:43:GLN:O	1:C:46:PRO:HD3	1.66	0.95
1:C:14:ILE:CD1	1:C:373:ARG:HD3	2.03	0.89
1:B:158:PHE:CZ	1:B:209:HIS:HE1	1.91	0.89
1:C:112:HIS:HD2	1:C:324:HIS:CD2	1.93	0.86
1:C:112:HIS:CD2	1:C:324:HIS:HD2	1.93	0.86
1:B:57:LEU:HD13	1:B:76:MET:HE3	1.56	0.85
1:A:19:ASP:CB	1:A:341:ASN:HD22	1.90	0.83
1:C:19:ASP:OD2	1:C:20:ARG:N	2.10	0.83
1:B:11:ILE:HD11	1:B:53:VAL:HG12	1.61	0.82
1:C:339:GLU:CG	1:C:340:TYR:N	2.41	0.82
1:C:233:GLU:OE2	1:C:309:HIS:HE1	1.62	0.82
1:B:57:LEU:HD13	1:B:76:MET:HE2	1.60	0.81
1:C:14:ILE:HD13	1:C:373:ARG:HD3	1.63	0.80
1:B:112:HIS:HD2	1:B:324:HIS:HD2	1.29	0.79
1:C:58:LYS:HD3	1:C:62:ILE:HD11	1.65	0.79
1:C:339:GLU:OE2	1:C:340:TYR:N	2.12	0.79
1:A:244:LEU:O	1:A:248:ARG:HG2	1.82	0.78
1:B:305:ARG:HD3	3:B:632:HOH:O	1.82	0.77
1:C:179:ASP:N	3:C:560:HOH:O	2.17	0.77
1:C:339:GLU:HG2	1:C:340:TYR:N	1.98	0.77
1:B:19:ASP:OD1	1:B:341:ASN:ND2	2.19	0.76
1:C:339:GLU:CD	1:C:340:TYR:N	2.43	0.76
1:B:112:HIS:HD2	1:B:324:HIS:CD2	2.03	0.75
1:A:268:LYS:HG2	1:B:301:ASN:HD21	1.52	0.75
1:A:57:LEU:CD1	1:A:76:MET:CE	2.65	0.74
1:A:57:LEU:HD13	1:A:76:MET:HE3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASP:HB2	1:A:341:ASN:HD21	1.53	0.73
1:B:112:HIS:CD2	1:B:324:HIS:HD2	2.07	0.72
1:C:244:LEU:O	1:C:248:ARG:HG2	1.89	0.72
1:C:374:GLU:O	1:C:377:ALA:HB3	1.91	0.70
1:C:339:GLU:CG	1:C:340:TYR:H	1.99	0.70
1:B:158:PHE:CE2	1:B:209:HIS:HE1	2.10	0.69
1:A:17:LYS:CE	1:A:20:ARG:O	2.37	0.69
1:B:244:LEU:O	1:B:248:ARG:HG2	1.92	0.69
1:B:57:LEU:CD1	1:B:76:MET:HE2	2.20	0.68
1:C:16:THR:HG22	1:C:18:PRO:HD3	1.73	0.68
1:B:32:GLU:HA	3:B:655:HOH:O	1.94	0.68
1:A:19:ASP:CB	1:A:341:ASN:ND2	2.45	0.67
1:C:210:GLU:OE1	1:C:238:PRO:HB3	1.93	0.67
1:B:233:GLU:OE2	1:B:309:HIS:HE1	1.77	0.67
1:C:309:HIS:HD2	1:C:336:GLU:OE1	1.77	0.67
1:A:341:ASN:OD1	1:A:343:ASN:N	2.29	0.66
1:C:309:HIS:CD2	1:C:336:GLU:OE1	2.49	0.66
1:A:57:LEU:HD22	1:A:76:MET:HE3	1.78	0.66
1:A:11:ILE:O	1:A:58:LYS:CE	2.24	0.66
1:A:233:GLU:OE2	1:A:309:HIS:HE1	1.79	0.65
1:C:14:ILE:HD11	1:C:373:ARG:HD3	1.76	0.65
1:B:19:ASP:HB2	1:B:341:ASN:HD22	1.61	0.64
1:C:237:PRO:O	3:C:513:HOH:O	2.15	0.64
1:B:337:HIS:CE1	1:B:339:GLU:HG2	2.33	0.64
1:B:58:LYS:HB3	1:B:59:PRO:HD3	1.80	0.63
1:B:11:ILE:CD1	1:B:53:VAL:CG1	2.72	0.63
1:C:324:HIS:HE1	1:C:367:ILE:O	1.82	0.62
1:A:58:LYS:O	1:A:62:ILE:HG12	1.99	0.61
1:A:372:ASP:OD2	1:A:375:ALA:CB	2.49	0.61
1:B:51:THR:O	1:B:55:GLU:HG3	2.01	0.61
1:B:158:PHE:CE2	1:B:209:HIS:CE1	2.89	0.61
1:C:19:ASP:HB2	1:C:341:ASN:ND2	2.16	0.60
1:B:3:LEU:HD11	1:B:106:LEU:HD13	1.85	0.59
1:C:21:HIS:CE1	1:C:312:PRO:HB2	2.38	0.59
1:C:19:ASP:HB2	1:C:341:ASN:HD21	1.68	0.59
1:A:12:HIS:NE2	1:A:29:GLU:OE2	2.28	0.58
1:C:41:THR:O	1:C:41:THR:OG1	2.21	0.58
1:C:371:ILE:O	1:C:371:ILE:HG23	2.05	0.57
1:B:19:ASP:CB	1:B:341:ASN:HD22	2.15	0.57
1:A:305:ARG:HD3	3:A:519:HOH:O	2.05	0.57
1:B:11:ILE:HD12	1:B:11:ILE:C	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:O	1:A:58:LYS:HG3	2.05	0.56
1:B:158:PHE:CZ	1:B:209:HIS:CE1	2.83	0.56
1:B:309:HIS:CD2	1:B:336:GLU:OE1	2.58	0.56
1:A:16:THR:CG2	1:A:379:PHE:HB2	2.35	0.56
1:C:60:ILE:O	1:C:64:LYS:HE2	2.04	0.56
1:B:19:ASP:CB	1:B:341:ASN:HD21	1.95	0.56
1:B:23:LEU:HB3	1:B:315:THR:HG22	1.88	0.56
1:A:309:HIS:CD2	1:A:336:GLU:OE1	2.60	0.55
1:C:19:ASP:CG	1:C:20:ARG:H	2.12	0.55
1:C:297:HIS:HE1	3:C:529:HOH:O	1.90	0.54
1:C:258:GLY:HA2	1:C:261:PHE:CE2	2.43	0.54
1:A:377:ALA:O	1:A:380:PRO:HD3	2.08	0.53
1:B:14:ILE:CD1	1:B:373:ARG:HD2	2.38	0.53
1:A:21:HIS:HD2	3:A:608:HOH:O	1.91	0.53
1:C:80:ALA:O	1:C:81:TYR:HB3	2.09	0.52
1:B:69:ILE:HD12	1:B:103:LYS:HE3	1.92	0.52
1:C:14:ILE:HD11	1:C:373:ARG:CD	2.39	0.52
1:B:19:ASP:CG	1:B:341:ASN:HD22	2.10	0.51
1:B:258:GLY:HA2	1:B:261:PHE:CD2	2.45	0.51
1:C:258:GLY:HA2	1:C:261:PHE:CD2	2.46	0.51
1:B:305:ARG:CD	3:B:632:HOH:O	2.50	0.51
1:B:128:HIS:HE1	1:B:336:GLU:OE2	1.94	0.51
1:B:11:ILE:HD12	1:B:12:HIS:N	2.26	0.50
1:B:83:ARG:HD2	3:B:588:HOH:O	2.12	0.50
1:A:104:ALA:HB3	1:A:366:GLY:HA2	1.93	0.50
1:A:128:HIS:HE1	1:A:336:GLU:OE2	1.94	0.50
1:B:309:HIS:HD2	1:B:336:GLU:OE1	1.94	0.50
1:C:43:GLN:HG2	1:C:44:GLN:N	2.25	0.50
1:A:309:HIS:CD2	3:A:538:HOH:O	2.64	0.50
1:C:19:ASP:OD1	1:C:341:ASN:ND2	2.45	0.49
1:A:16:THR:HG23	1:A:379:PHE:HB2	1.94	0.49
1:A:125:VAL:HA	1:A:335:GLN:O	2.12	0.49
1:B:306:ILE:HB	1:B:332:ALA:HA	1.93	0.49
1:B:112:HIS:HE1	1:B:118:LYS:NZ	2.11	0.49
1:C:45:ARG:N	1:C:46:PRO:HD3	2.28	0.49
1:B:11:ILE:HG13	1:B:58:LYS:HG3	1.94	0.49
1:B:112:HIS:HE1	1:B:118:LYS:HZ2	1.60	0.49
1:C:44:GLN:O	1:C:45:ARG:HD3	2.13	0.49
1:A:330:HIS:HD2	1:A:331:ASN:ND2	2.12	0.48
1:B:51:THR:HG23	1:B:55:GLU:CD	2.38	0.48
1:B:258:GLY:HA2	1:B:261:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HD13	1:B:46:PRO:HB2	1.96	0.48
1:B:16:THR:CG2	1:B:379:PHE:HB2	2.43	0.48
1:B:16:THR:HG22	1:B:379:PHE:HB2	1.95	0.48
1:B:324:HIS:HE1	1:B:367:ILE:O	1.97	0.48
1:A:372:ASP:OD2	1:A:375:ALA:HB2	2.13	0.48
1:B:104:ALA:HB3	1:B:366:GLY:HA2	1.95	0.47
1:B:356:ASN:H	1:C:20:ARG:CZ	2.26	0.47
1:A:210:GLU:OE1	1:A:238:PRO:HG3	2.15	0.47
1:C:4:LYS:H	1:C:4:LYS:HG2	1.57	0.47
1:A:258:GLY:HA2	1:A:261:PHE:CD2	2.50	0.47
1:A:306:ILE:HB	1:A:332:ALA:HA	1.96	0.47
1:C:19:ASP:CB	1:C:341:ASN:ND2	2.78	0.47
1:C:341:ASN:OD1	1:C:341:ASN:C	2.58	0.46
1:A:70[B]:GLU:HG2	1:A:71:ASP:N	2.31	0.46
1:C:306:ILE:HB	1:C:332:ALA:HA	1.96	0.46
1:C:330:HIS:HD2	1:C:331:ASN:ND2	2.14	0.46
1:C:112:HIS:CD2	1:C:324:HIS:CD2	2.81	0.46
1:A:208:VAL:O	1:A:211:ARG:HG2	2.16	0.46
1:B:337:HIS:HE1	1:B:339:GLU:HG2	1.78	0.45
3:A:545:HOH:O	1:B:268:LYS:HD2	2.16	0.45
1:A:309:HIS:HD2	1:A:336:GLU:OE1	2.00	0.45
1:A:374:GLU:HG2	1:A:375:ALA:H	1.82	0.45
1:B:11:ILE:HD11	1:B:53:VAL:HG13	1.92	0.45
1:C:282:HIS:CE1	1:C:309:HIS:CB	2.99	0.45
1:C:371:ILE:O	1:C:371:ILE:CG2	2.65	0.45
1:A:258:GLY:HA2	1:A:261:PHE:CE2	2.52	0.45
1:B:128:HIS:HD2	3:B:636:HOH:O	2.00	0.44
1:B:151:HIS:C	1:B:152:ILE:HG13	2.41	0.44
1:A:58:LYS:HB2	1:A:59:PRO:HD3	2.00	0.44
1:C:15:ILE:HA	1:C:23:LEU:O	2.18	0.44
1:B:51:THR:HG23	1:B:55:GLU:OE2	2.17	0.44
1:C:142:GLU:O	1:C:146:GLU:HG3	2.18	0.44
1:A:45:ARG:N	1:A:46:PRO:HD3	2.32	0.44
1:A:128:HIS:HD2	3:A:513:HOH:O	2.01	0.44
1:B:3:LEU:CD1	1:B:106:LEU:HD13	2.46	0.44
1:B:126:TYR:CZ	1:B:336:GLU:HG3	2.53	0.44
1:B:130:THR:HG21	1:B:158:PHE:HB2	1.99	0.44
1:B:76:MET:HB3	1:B:92:ILE:HG12	2.00	0.43
1:C:374:GLU:H	1:C:374:GLU:CD	2.25	0.43
1:B:42:PHE:CD2	1:B:45:ARG:HB2	2.54	0.43
1:C:43:GLN:O	1:C:46:PRO:CD	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLN:HG2	1:C:44:GLN:H	1.84	0.43
1:A:16:THR:HG22	1:A:17:LYS:N	2.33	0.43
1:B:107:ALA:HB1	1:B:109:MET:HG2	2.01	0.42
1:B:112:HIS:CE1	1:B:118:LYS:NZ	2.87	0.42
1:B:58:LYS:N	1:B:59:PRO:CD	2.82	0.42
1:B:4:LYS:O	1:B:5:GLU:C	2.62	0.42
1:B:112:HIS:CD2	1:B:324:HIS:CD2	2.91	0.42
1:C:11:ILE:HD12	1:C:58:LYS:HA	2.01	0.42
1:C:314:MET:HE3	1:C:319:ALA:N	2.34	0.42
1:C:314:MET:HE3	1:C:319:ALA:CA	2.50	0.42
1:A:219:GLN:HG3	3:A:582:HOH:O	2.20	0.42
1:A:341:ASN:OD1	1:A:344:THR:N	2.43	0.42
1:A:19:ASP:CG	1:A:341:ASN:HD22	2.26	0.42
1:A:57:LEU:CD2	1:A:76:MET:HE3	2.48	0.42
1:C:64:LYS:HE3	1:C:75:MET:HE1	2.02	0.42
1:B:374:GLU:H	1:B:374:GLU:HG2	1.49	0.42
1:B:9:SER:HB3	1:B:31:ASN:ND2	2.35	0.41
1:C:64:LYS:CE	1:C:75:MET:HE1	2.50	0.41
1:A:74:GLN:HE21	1:A:74:GLN:HB2	1.68	0.41
1:A:341:ASN:OD1	1:A:341:ASN:C	2.63	0.41
1:B:76:MET:HE2	1:B:92:ILE:HG12	2.03	0.41
1:C:20:ARG:HB3	1:C:21:HIS:CE1	2.56	0.41
1:A:4:LYS:O	1:A:5:GLU:C	2.63	0.41
1:B:44:GLN:O	1:B:45:ARG:HD3	2.20	0.41
1:C:282:HIS:NE2	1:C:309:HIS:HB3	2.36	0.40
1:C:4:LYS:O	1:C:5:GLU:C	2.65	0.40
1:A:374:GLU:O	1:A:375:ALA:C	2.64	0.40
1:B:282:HIS:HD2	3:B:610:HOH:O	2.04	0.40
1:C:132:ASP:OD1	1:C:158:PHE:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	356/394 (90%)	346 (97%)	9 (2%)	1 (0%)	36	42
1	B	355/394 (90%)	346 (98%)	7 (2%)	2 (1%)	21	23
1	C	355/394 (90%)	342 (96%)	12 (3%)	1 (0%)	36	42
All	All	1066/1182 (90%)	1034 (97%)	28 (3%)	4 (0%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	341	ASN
1	A	81	TYR
1	B	84	ASN
1	C	84	ASN

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	309/339 (91%)	299 (97%)	10 (3%)	34	47
1	B	308/339 (91%)	295 (96%)	13 (4%)	26	36
1	C	308/339 (91%)	298 (97%)	10 (3%)	34	47
All	All	925/1017 (91%)	892 (96%)	33 (4%)	31	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	32	GLU
1	A	74	GLN
1	A	139	ASP
1	A	147	LYS
1	A	259	GLU
1	A	268	LYS
1	A	270	LEU
1	A	372	ASP

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Mol	Chain	Res	Type
1	A	374	GLU
1	B	4	LYS
1	B	11	ILE
1	B	32	GLU
1	B	55	GLU
1	B	58	LYS
1	B	61	LEU
1	B	131	SER
1	B	132	ASP
1	B	158	PHE
1	B	260	LEU
1	B	309	HIS
1	B	339	GLU
1	B	374	GLU
1	C	4	LYS
1	C	20	ARG
1	C	32	GLU
1	C	42	PHE
1	C	43	GLN
1	C	51	THR
1	C	58	LYS
1	C	93	SER
1	C	339	GLU
1	C	373	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	22	ASN
1	A	67	ASN
1	A	90	ASN
1	A	128	HIS
1	A	186	ASN
1	A	215	ASN
1	A	301	ASN
1	A	309	HIS
1	A	326	ASN
1	A	331	ASN
1	B	22	ASN
1	B	31	ASN
1	B	112	HIS

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Mol	Chain	Res	Type
1	B	128	HIS
1	B	186	ASN
1	B	201	GLN
1	B	209	HIS
1	B	282	HIS
1	B	301	ASN
1	B	309	HIS
1	B	324	HIS
1	B	330	HIS
1	B	337	HIS
1	B	341	ASN
1	C	12	HIS
1	C	31	ASN
1	C	43	GLN
1	C	74	GLN
1	C	112	HIS
1	C	186	ASN
1	C	219	GLN
1	C	282	HIS
1	C	297	HIS
1	C	309	HIS
1	C	324	HIS
1	C	330	HIS
1	C	331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 [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	359/394 (91%)	-0.15	3 (0%) 82 80	13, 22, 42, 56	1 (0%)
1	B	359/394 (91%)	-0.32	7 (1%) 66 63	13, 22, 41, 61	0
1	C	359/394 (91%)	-0.04	6 (1%) 69 66	13, 22, 46, 61	0
All	All	1077/1182 (91%)	-0.17	16 (1%) 72 69	13, 22, 43, 61	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	TYR	5.2
1	C	158	PHE	3.6
1	C	82	TRP	3.5
1	B	380	PRO	3.1
1	B	158	PHE	2.9
1	B	55	GLU	2.5
1	C	2	SER	2.4
1	A	81	TYR	2.4
1	B	82	TRP	2.4
1	B	379	PHE	2.3
1	C	3	LEU	2.3
1	A	158	PHE	2.3
1	A	82	TRP	2.3
1	B	44	GLN	2.2
1	C	44	GLN	2.2
1	B	238	PRO	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NA	C	501	1/1	0.97	0.21	16,16,16,16	1
2	NA	A	502	1/1	0.98	0.17	19,19,19,19	1
2	NA	B	503	1/1	1.00	0.17	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.