



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:19 PM UTC

PDB ID : 7OLF / pdb_00007olf
Title : Crystal structure of FMNH2-dependent monooxygenase from *Agrobacterium tumefaciens* for oxidative desulfurization of sulfoquinovose
Authors : Sharma, M.; Davies, G.J.
Deposited on : 2021-05-19
Resolution : 3.40 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
Xtrriage (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

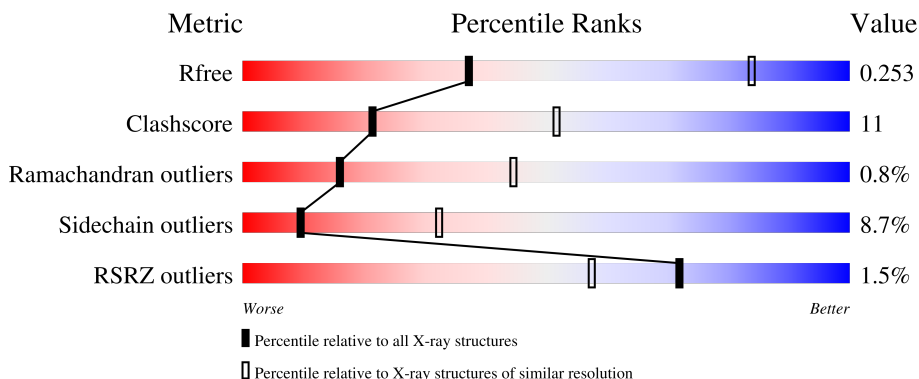
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	393	
1	B	393	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5392 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 Methanesulfonate sulfonataase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2731	1720	479	517	15	0	0	0
1	B	366	2661	1678	468	500	15	0	0	0

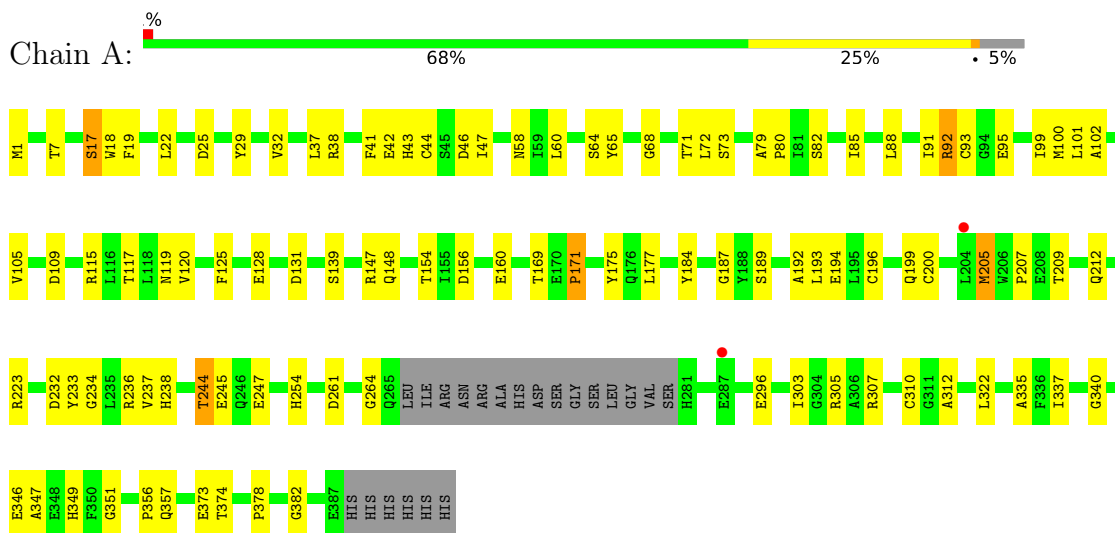
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP A9CEY7
A	387	GLU	-	expression tag	UNP A9CEY7
A	388	HIS	-	expression tag	UNP A9CEY7
A	389	HIS	-	expression tag	UNP A9CEY7
A	390	HIS	-	expression tag	UNP A9CEY7
A	391	HIS	-	expression tag	UNP A9CEY7
A	392	HIS	-	expression tag	UNP A9CEY7
A	393	HIS	-	expression tag	UNP A9CEY7
B	386	LEU	-	expression tag	UNP A9CEY7
B	387	GLU	-	expression tag	UNP A9CEY7
B	388	HIS	-	expression tag	UNP A9CEY7
B	389	HIS	-	expression tag	UNP A9CEY7
B	390	HIS	-	expression tag	UNP A9CEY7
B	391	HIS	-	expression tag	UNP A9CEY7
B	392	HIS	-	expression tag	UNP A9CEY7
B	393	HIS	-	expression tag	UNP A9CEY7

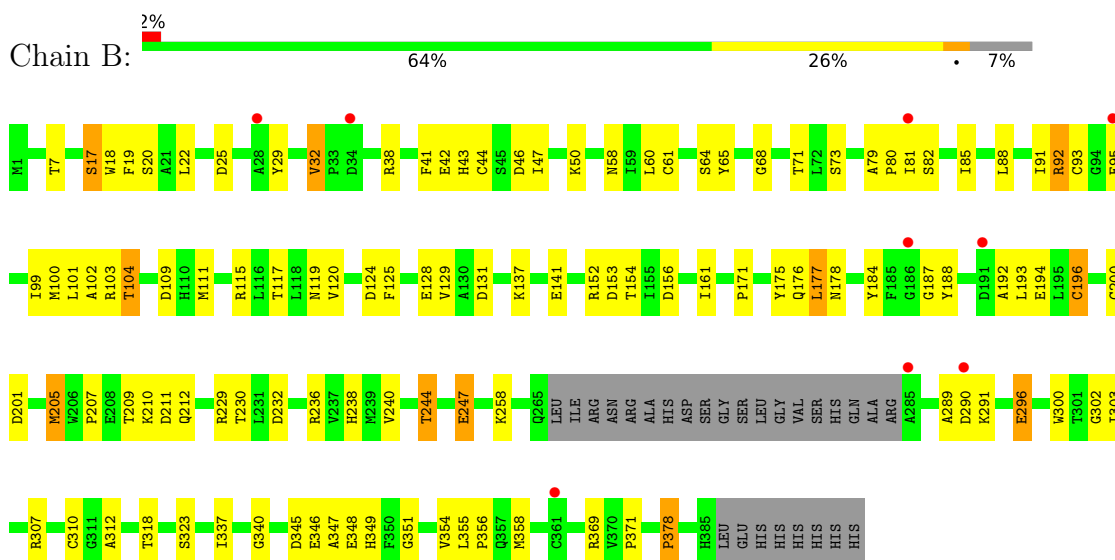
3 Residue-property plots i

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: Methanesulfonate sulfonatae



- Molecule 1: Methanesulfonate sulfonatae



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	203.76Å 203.76Å 110.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 3.40 48.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.00-3.40) 99.8 (48.00-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.261 0.219 , 0.253	Depositor DCC
R_{free} test set	1002 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtrriage
Anisotropy	1.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5392	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

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	1.11	1/2795 (0.0%)	1.56	5/3813 (0.1%)
1	B	1.14	2/2722 (0.1%)	1.57	10/3712 (0.3%)
All	All	1.12	3/5517 (0.1%)	1.57	15/7525 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLU	N-CA	5.53	1.49	1.46
1	B	296	GLU	N-CA	5.18	1.49	1.46
1	B	32	VAL	N-CA	5.12	1.50	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	TYR	CA-C-N	7.49	126.74	121.65
1	A	233	TYR	C-N-CA	7.49	126.74	121.65
1	B	25	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	196	CYS	CA-C-N	6.11	126.60	119.94
1	B	196	CYS	C-N-CA	6.11	126.60	119.94
1	A	25	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	153	ASP	CB-CA-C	-5.94	101.52	110.90
1	B	152	ARG	CA-C-N	5.61	128.07	120.44
1	B	152	ARG	C-N-CA	5.61	128.07	120.44
1	B	188	TYR	CB-CA-C	5.48	117.84	109.34
1	A	171	PRO	CA-C-N	5.08	130.52	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	PRO	C-N-CA	5.08	130.52	122.60
1	B	201	ASP	N-CA-C	-5.03	104.79	112.04
1	B	247	GLU	CA-C-N	5.01	127.25	120.44
1	B	247	GLU	C-N-CA	5.01	127.25	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide

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	2731	0	2494	56	0
1	B	2661	0	2441	63	0
All	All	5392	0	4935	112	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 11.

All (112) 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:340:GLY:HA3	1:B:346:GLU:HG2	1.66	0.78
1:A:340:GLY:HA3	1:A:346:GLU:HG2	1.65	0.77
1:B:354:VAL:HG12	1:B:358:MET:HE2	1.67	0.77
1:B:354:VAL:HG12	1:B:358:MET:CE	2.25	0.66
1:B:91:ILE:HG13	1:B:91:ILE:O	1.96	0.64
1:A:171:PRO:HB2	1:B:65:TYR:CE1	2.33	0.63
1:A:187:GLY:HA3	1:A:192:ALA:HB1	1.79	0.63
1:A:148:GLN:HE22	1:A:156:ASP:H	1.51	0.59
1:B:187:GLY:HA3	1:B:192:ALA:HB1	1.84	0.59
1:B:93:CYS:SG	1:B:120:VAL:HG13	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:NE2	1:B:310:CYS:HB3	2.20	0.56
1:B:177:LEU:HD13	1:B:177:LEU:N	2.20	0.56
1:A:65:TYR:CE1	1:B:171:PRO:HB2	2.41	0.55
1:A:18:TRP:CD1	1:A:19:PHE:H	2.25	0.54
1:B:18:TRP:CD1	1:B:19:PHE:H	2.26	0.54
1:A:238:HIS:NE2	1:A:310:CYS:HB3	2.22	0.54
1:B:340:GLY:HA3	1:B:346:GLU:CG	2.37	0.53
1:A:41:PHE:CD1	1:B:111:MET:HE2	2.44	0.53
1:A:101:LEU:O	1:A:105:VAL:HG23	2.09	0.53
1:A:236:ARG:NH1	1:A:337:ILE:O	2.42	0.53
1:B:177:LEU:N	1:B:177:LEU:CD1	2.72	0.53
1:A:244:THR:OG1	1:A:247:GLU:HB2	2.09	0.52
1:A:147:ARG:NH2	1:A:199:GLN:O	2.41	0.52
1:A:43:HIS:O	1:A:46:ASP:HB2	2.10	0.52
1:A:340:GLY:HA3	1:A:346:GLU:CG	2.37	0.52
1:B:355:LEU:HA	1:B:358:MET:HE3	1.92	0.51
1:A:18:TRP:CE2	1:A:347:ALA:HB2	2.47	0.50
1:A:100:MET:HG3	1:B:95:GLU:CD	2.36	0.50
1:B:18:TRP:CE2	1:B:347:ALA:HB2	2.46	0.50
1:A:60:LEU:HA	1:A:88:LEU:HB3	1.93	0.50
1:B:210:LYS:N	1:B:296:GLU:OE2	2.34	0.50
1:B:41:PHE:O	1:B:42:GLU:C	2.55	0.50
1:A:154:THR:HA	1:A:169:THR:HG23	1.93	0.50
1:B:43:HIS:O	1:B:46:ASP:HB2	2.11	0.49
1:B:119:ASN:C	1:B:119:ASN:OD1	2.55	0.49
1:B:244:THR:OG1	1:B:247:GLU:HB2	2.13	0.49
1:A:85:ILE:O	1:A:115:ARG:NH1	2.44	0.49
1:B:88:LEU:HD12	1:B:117:THR:O	2.13	0.49
1:A:64:SER:HA	1:A:92:ARG:HH22	1.78	0.49
1:A:82:SER:OG	1:A:115:ARG:NH2	2.39	0.48
1:B:60:LEU:HA	1:B:88:LEU:HB3	1.94	0.48
1:A:382:GLY:O	1:B:38:ARG:NH2	2.46	0.48
1:A:119:ASN:OD1	1:A:119:ASN:C	2.56	0.48
1:A:41:PHE:O	1:A:42:GLU:C	2.55	0.48
1:B:79:ALA:N	1:B:80:PRO:HD2	2.29	0.48
1:B:236:ARG:NH1	1:B:337:ILE:O	2.44	0.47
1:A:79:ALA:N	1:A:80:PRO:HD2	2.30	0.47
1:A:88:LEU:HD12	1:A:117:THR:O	2.15	0.47
1:B:209:THR:OG1	1:B:212:GLN:HB2	2.15	0.47
1:A:17:SER:HA	1:A:58:ASN:O	2.15	0.46
1:B:92:ARG:HH11	1:B:92:ARG:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:TRP:CG	1:B:19:PHE:H	2.33	0.46
1:B:177:LEU:HD21	1:B:371:PRO:HB3	1.98	0.46
1:A:209:THR:OG1	1:A:212:GLN:HB2	2.17	0.45
1:A:29:TYR:O	1:A:32:VAL:HB	2.16	0.45
1:B:85:ILE:O	1:B:115:ARG:NH1	2.47	0.45
1:B:207:PRO:HG2	1:B:312:ALA:HB3	1.97	0.45
1:A:95:GLU:CD	1:B:100:MET:HG3	2.42	0.45
1:B:29:TYR:O	1:B:32:VAL:HB	2.17	0.45
1:A:207:PRO:HG2	1:A:312:ALA:HB3	1.98	0.45
1:B:99:ILE:O	1:B:102:ALA:HB3	2.16	0.45
1:B:64:SER:HA	1:B:92:ARG:HH22	1.82	0.45
1:B:17:SER:HA	1:B:58:ASN:O	2.16	0.45
1:B:44:CYS:O	1:B:47:ILE:HB	2.18	0.44
1:A:205:MET:HE3	1:A:205:MET:HB2	1.87	0.44
1:B:176:GLN:C	1:B:177:LEU:HD13	2.43	0.44
1:A:44:CYS:O	1:A:47:ILE:HB	2.17	0.44
1:A:18:TRP:CG	1:A:19:PHE:H	2.36	0.44
1:A:193:LEU:HB3	1:A:223:ARG:HG3	2.00	0.44
1:B:109:ASP:OD2	1:B:175:TYR:N	2.51	0.44
1:A:109:ASP:OD2	1:A:175:TYR:N	2.51	0.43
1:B:196:CYS:O	1:B:200:CYS:CB	2.65	0.43
1:A:91:ILE:HG22	1:A:91:ILE:O	2.18	0.43
1:B:238:HIS:CD2	1:B:310:CYS:HB3	2.54	0.43
1:A:22:LEU:O	1:A:68:GLY:HA3	2.18	0.43
1:B:82:SER:OG	1:B:115:ARG:NH2	2.39	0.43
1:B:355:LEU:HA	1:B:355:LEU:HD12	1.90	0.43
1:A:234:GLY:HA2	1:A:335:ALA:O	2.19	0.43
1:A:193:LEU:O	1:A:194:GLU:C	2.62	0.43
1:A:72:LEU:HD21	1:A:91:ILE:HD11	2.00	0.42
1:B:355:LEU:N	1:B:356:PRO:CD	2.82	0.42
1:B:351:GLY:O	1:B:356:PRO:HD3	2.19	0.42
1:B:20:SER:OG	1:B:61:CYS:HA	2.19	0.42
1:A:93:CYS:SG	1:A:120:VAL:HG13	2.58	0.42
1:A:100:MET:O	1:A:101:LEU:C	2.62	0.42
1:A:261:ASP:CB	1:A:305:ARG:HE	2.33	0.42
1:B:124:ASP:OD1	1:B:129:VAL:HA	2.20	0.42
1:A:351:GLY:O	1:A:356:PRO:HD3	2.20	0.42
1:A:88:LEU:HA	1:A:117:THR:O	2.20	0.42
1:A:99:ILE:O	1:A:102:ALA:HB3	2.20	0.42
1:A:125:PHE:HB2	1:A:128:GLU:HB2	2.02	0.42
1:B:100:MET:O	1:B:101:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HH11	1:A:92:ARG:HB2	1.84	0.41
1:A:322:LEU:HD11	1:A:357:GLN:CB	2.49	0.41
1:B:205:MET:HE2	1:B:205:MET:HB2	1.92	0.41
1:A:93:CYS:CB	1:A:139:SER:HA	2.50	0.41
1:A:196:CYS:O	1:A:200:CYS:CB	2.69	0.41
1:B:125:PHE:HB2	1:B:128:GLU:HB2	2.01	0.41
1:A:207:PRO:HB2	1:A:312:ALA:HB3	2.03	0.41
1:A:237:VAL:HA	1:A:310:CYS:SG	2.60	0.41
1:B:103:ARG:O	1:B:104:THR:C	2.64	0.41
1:B:154:THR:HG23	1:B:156:ASP:OD2	2.21	0.41
1:A:38:ARG:HD3	1:B:378:PRO:O	2.21	0.41
1:A:223:ARG:HA	1:A:223:ARG:NE	2.36	0.41
1:B:141:GLU:CD	1:B:161:ILE:HG23	2.46	0.41
1:B:178:ASN:HB2	1:B:369:ARG:HD2	2.03	0.40
1:B:300:TRP:CE2	1:B:302:GLY:HA3	2.56	0.40
1:B:22:LEU:O	1:B:68:GLY:HA3	2.21	0.40
1:B:193:LEU:O	1:B:194:GLU:C	2.65	0.40
1:B:289:ALA:O	1:B:291:LYS:N	2.55	0.40
1:B:345:ASP:O	1:B:348:GLU:HB2	2.21	0.40
1:B:207:PRO:HB2	1:B:312:ALA:HB3	2.02	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	368/393 (94%)	318 (86%)	47 (13%)	3 (1%)	16	44
1	B	362/393 (92%)	306 (84%)	53 (15%)	3 (1%)	16	44
All	All	730/786 (93%)	624 (86%)	100 (14%)	6 (1%)	16	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ARG
1	B	290	ASP
1	B	307	ARG
1	A	264	GLY
1	A	349	HIS
1	B	349	HIS

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	257/323 (80%)	237 (92%)	20 (8%)	11	37
1	B	248/323 (77%)	224 (90%)	24 (10%)	8	28
All	All	505/646 (78%)	461 (91%)	44 (9%)	9	32

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	17	SER
1	A	37	LEU
1	A	71	THR
1	A	73	SER
1	A	92	ARG
1	A	131	ASP
1	A	160	GLU
1	A	177	LEU
1	A	184	TYR
1	A	189	SER
1	A	205	MET
1	A	232	ASP
1	A	244	THR
1	A	245	GLU
1	A	254	HIS
1	A	303	ILE
1	A	373	GLU

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Mol	Chain	Res	Type
1	A	374	THR
1	A	378	PRO
1	B	7	THR
1	B	17	SER
1	B	50	LYS
1	B	71	THR
1	B	73	SER
1	B	81	ILE
1	B	92	ARG
1	B	104	THR
1	B	131	ASP
1	B	137	LYS
1	B	177	LEU
1	B	184	TYR
1	B	205	MET
1	B	211	ASP
1	B	229	ARG
1	B	230	THR
1	B	232	ASP
1	B	240	VAL
1	B	244	THR
1	B	258	LYS
1	B	303	ILE
1	B	318	THR
1	B	323	SER
1	B	378	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	86	ASN
1	A	140	HIS
1	A	148	GLN
1	A	176	GLN
1	A	298	ASN
1	B	86	ASN
1	B	176	GLN
1	B	298	ASN
1	B	349	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 oligosaccharides 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](#)

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	372/393 (94%)	-0.18	2 (0%) 87 78	49, 78, 113, 182	0
1	B	366/393 (93%)	-0.06	9 (2%) 58 43	55, 87, 117, 154	0
All	All	738/786 (93%)	-0.12	11 (1%) 72 57	49, 83, 116, 182	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ALA	3.7
1	B	95	GLU	3.0
1	A	287	GLU	2.8
1	B	34	ASP	2.8
1	B	290	ASP	2.6
1	B	28	ALA	2.5
1	B	81	ILE	2.5
1	A	204	LEU	2.1
1	B	361	CYS	2.1
1	B	191	ASP	2.0
1	B	186	GLY	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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.