



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:04 AM UTC

PDB ID : 9J9J / pdb_00009j9j
Title : Nitrophenol monooxygenase RsPNPA from Rhodococcus sp. 21391
Authors : Yang, J.; Li, R.; Lin, S.; Long, L.
Deposited on : 2024-08-22
Resolution : 2.40 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
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

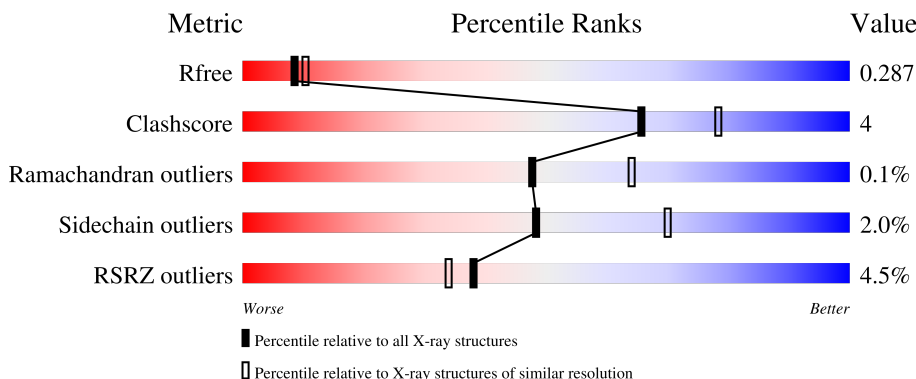
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	536	2% 81% 10% 8%
1	B	536	4% 84% 8% 8%
1	C	536	6% 80% 10% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11840 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 4-nitrophenol 4-monooxygenase/4-nitrocatechol 2-monooxygenase, oxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3932	2492	693	733	14			
1	B	491	Total	C	N	O	S	0	0	0
			3910	2477	689	730	14			
1	C	487	Total	C	N	O	S	0	0	0
			3876	2456	683	723	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	529	LEU	-	expression tag	UNP Q6F4M8
A	530	GLU	-	expression tag	UNP Q6F4M8
A	531	HIS	-	expression tag	UNP Q6F4M8
A	532	HIS	-	expression tag	UNP Q6F4M8
A	533	HIS	-	expression tag	UNP Q6F4M8
A	534	HIS	-	expression tag	UNP Q6F4M8
A	535	HIS	-	expression tag	UNP Q6F4M8
A	536	HIS	-	expression tag	UNP Q6F4M8
B	529	LEU	-	expression tag	UNP Q6F4M8
B	530	GLU	-	expression tag	UNP Q6F4M8
B	531	HIS	-	expression tag	UNP Q6F4M8
B	532	HIS	-	expression tag	UNP Q6F4M8
B	533	HIS	-	expression tag	UNP Q6F4M8
B	534	HIS	-	expression tag	UNP Q6F4M8
B	535	HIS	-	expression tag	UNP Q6F4M8
B	536	HIS	-	expression tag	UNP Q6F4M8
C	529	LEU	-	expression tag	UNP Q6F4M8
C	530	GLU	-	expression tag	UNP Q6F4M8
C	531	HIS	-	expression tag	UNP Q6F4M8
C	532	HIS	-	expression tag	UNP Q6F4M8
C	533	HIS	-	expression tag	UNP Q6F4M8
C	534	HIS	-	expression tag	UNP Q6F4M8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	535	HIS	-	expression tag	UNP Q6F4M8
C	536	HIS	-	expression tag	UNP Q6F4M8

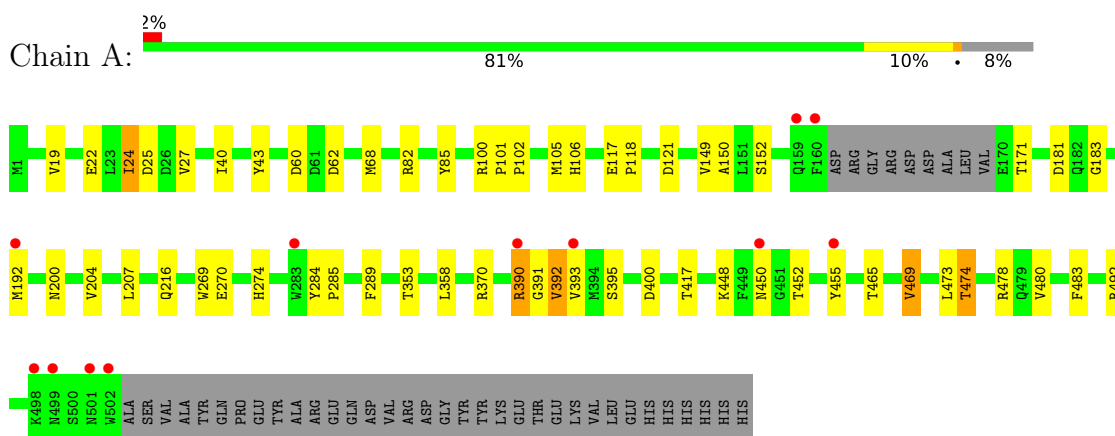
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	31	Total	O	0	0
			31	31		
2	C	17	Total	O	0	0
			17	17		

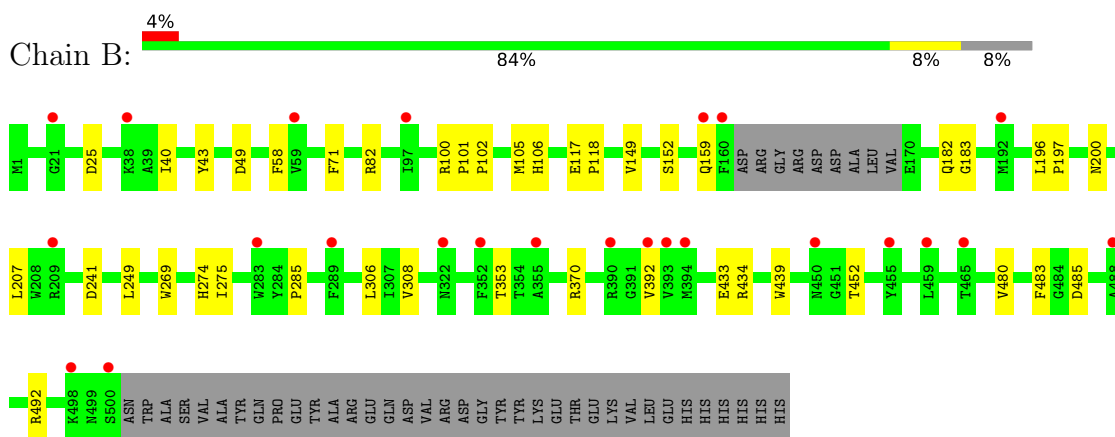
3 Residue-property plots [i](#)

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.

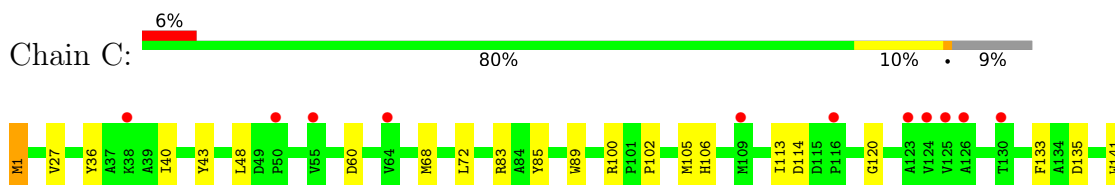
- Molecule 1: 4-nitrophenol 4-monooxygenase/4-nitrocatechol 2-monooxygenase, oxygenase component

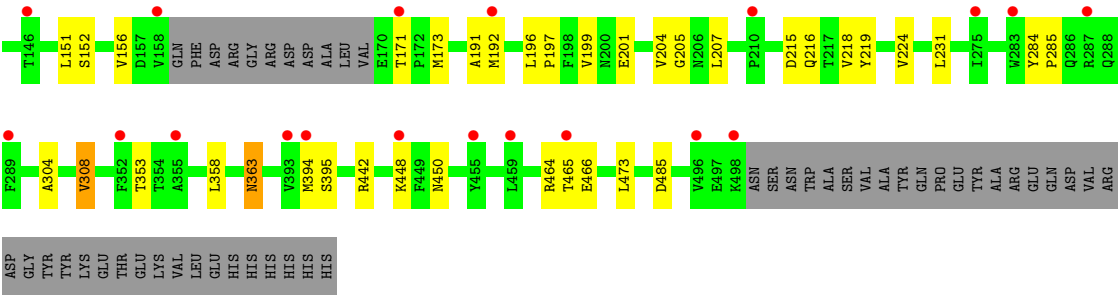


- Molecule 1: 4-nitrophenol 4-monooxygenase/4-nitrocatechol 2-monooxygenase, oxygenase component



- Molecule 1: 4-nitrophenol 4-monooxygenase/4-nitrocatechol 2-monooxygenase, oxygenase component





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.56Å 149.56Å 322.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.40 49.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.27-2.40) 99.9 (49.27-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.227 , 0.282 0.232 , 0.287	Depositor DCC
R_{free} test set	3620 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11840	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5994e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.70	0/4035	1.15	10/5494 (0.2%)
1	B	0.58	0/4011	1.10	3/5460 (0.1%)
1	C	0.56	0/3976	1.09	6/5413 (0.1%)
All	All	0.62	0/12022	1.11	19/16367 (0.1%)

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	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	49	ASP	CA-CB-CG	6.40	119.00	112.60
1	B	485	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	483	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	289	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	25	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	121	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	60	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	485	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	135	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	215	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	417	THR	CA-CB-OG1	-5.32	101.62	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	181	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	448	LYS	CB-CA-C	5.22	119.73	110.85
1	C	466	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	455	TYR	N-CA-CB	5.15	118.16	110.22
1	A	400	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	1	MET	CG-SD-CE	5.03	111.97	100.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	492	ARG	Sidechain
1	A	82	ARG	Sidechain
1	B	492	ARG	Sidechain
1	B	82	ARG	Sidechain
1	C	394	MET	Peptide
1	C	83	ARG	Sidechain

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	3932	0	3783	31	0
1	B	3910	0	3767	19	0
1	C	3876	0	3739	40	0
2	A	74	0	0	0	0
2	B	31	0	0	1	0
2	C	17	0	0	0	0
All	All	11840	0	11289	88	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 (88) 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:C:72:LEU:HD21	1:C:113:ILE:HD11	1.70	0.73
1:C:1:MET:HE3	1:C:48:LEU:HD23	1.72	0.69
1:B:370:ARG:NH2	1:B:452:THR:O	2.28	0.67
1:C:105:MET:HE2	1:C:152:SER:HA	1.79	0.65
1:B:105:MET:SD	1:B:152:SER:HB2	2.42	0.60
1:A:105:MET:SD	1:A:152:SER:HB2	2.42	0.59
1:C:1:MET:CE	1:C:48:LEU:HD23	2.33	0.58
1:B:102:PRO:HB3	1:B:106:HIS:CE1	2.38	0.58
1:C:156:VAL:HG23	1:C:191:ALA:HB3	1.87	0.56
1:A:100:ARG:NH2	1:A:450:ASN:HD21	2.04	0.55
1:B:308:VAL:HG11	1:C:473:LEU:HD21	1.88	0.55
1:A:469:VAL:O	1:A:474:THR:HG21	2.08	0.54
1:C:224:VAL:HG13	1:C:231:LEU:HD11	1.90	0.54
1:A:474:THR:CG2	1:A:478:ARG:HE	2.20	0.53
1:A:102:PRO:HB3	1:A:106:HIS:CE1	2.43	0.53
1:A:390:ARG:O	1:A:392:VAL:N	2.42	0.52
1:C:72:LEU:HD11	1:C:113:ILE:CD1	2.39	0.52
1:C:173:MET:HE2	1:C:216:GLN:HB3	1.90	0.52
1:B:117:GLU:N	1:B:118:PRO:CD	2.73	0.52
1:C:171:THR:HG22	1:C:173:MET:H	1.76	0.51
1:C:100:ARG:HH22	1:C:450:ASN:HD21	1.59	0.51
1:C:363:ASN:ND2	1:C:464:ARG:HH22	2.10	0.50
1:A:117:GLU:N	1:A:118:PRO:CD	2.75	0.50
1:A:24:ILE:HD12	1:A:24:ILE:N	2.27	0.49
1:B:149:VAL:HG13	1:B:200:ASN:HB2	1.94	0.49
1:C:304:ALA:O	1:C:308:VAL:HG12	2.13	0.49
1:A:353:THR:HA	1:A:358:LEU:O	2.14	0.48
1:A:22:GLU:O	1:A:24:ILE:CD1	2.61	0.48
1:A:390:ARG:O	1:A:393:VAL:N	2.44	0.48
1:C:353:THR:HA	1:C:358:LEU:O	2.14	0.48
1:A:22:GLU:O	1:A:24:ILE:HD12	2.14	0.47
1:A:19:VAL:HB	1:A:24:ILE:HD11	1.95	0.47
1:C:151:LEU:HD23	1:C:201:GLU:HB2	1.97	0.47
1:A:370:ARG:NH2	1:A:452:THR:O	2.40	0.47
1:B:306:LEU:HD21	1:B:434:ARG:CZ	2.45	0.47
1:B:308:VAL:CG1	1:C:473:LEU:HD21	2.45	0.47
1:C:207:LEU:HD23	1:C:285:PRO:HB2	1.96	0.47
1:C:120:GLY:HA2	1:C:133:PHE:HB2	1.96	0.46
1:B:183:GLY:HA2	1:B:269:TRP:CD1	2.50	0.46
1:C:36:TYR:CZ	1:C:40:ILE:HD11	2.50	0.46
1:A:100:ARG:HH21	1:A:450:ASN:HD21	1.62	0.46
1:B:40:ILE:O	1:B:43:TYR:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD23	1:A:285:PRO:HB2	1.98	0.45
1:A:274:HIS:CD2	1:A:274:HIS:C	2.94	0.45
1:A:68:MET:HB2	1:A:85:TYR:CE1	2.52	0.45
1:B:241:ASP:HB2	2:B:618:HOH:O	2.16	0.44
1:C:114:ASP:OD1	1:C:358:LEU:HB2	2.17	0.44
1:B:249:LEU:HB2	1:B:433:GLU:HG2	2.00	0.44
1:C:102:PRO:HB3	1:C:106:HIS:CE1	2.52	0.44
1:C:40:ILE:O	1:C:43:TYR:HB3	2.17	0.44
1:B:249:LEU:HB3	1:B:439:TRP:CH2	2.53	0.43
1:B:58:PHE:CD2	1:B:71:PHE:HD1	2.37	0.43
1:B:274:HIS:CD2	1:B:274:HIS:C	2.94	0.43
1:A:284:TYR:N	1:A:285:PRO:HD2	2.34	0.43
1:C:284:TYR:N	1:C:285:PRO:CD	2.81	0.43
1:A:390:ARG:C	1:A:392:VAL:N	2.72	0.43
1:A:100:ARG:N	1:A:101:PRO:CD	2.82	0.42
1:C:72:LEU:HD11	1:C:113:ILE:HD11	2.00	0.42
1:C:105:MET:HE1	1:C:152:SER:HB2	2.00	0.42
1:A:171:THR:HG21	1:A:216:GLN:NE2	2.34	0.42
1:B:100:ARG:N	1:B:101:PRO:CD	2.83	0.42
1:B:207:LEU:HD13	1:B:285:PRO:HB2	2.01	0.42
1:A:183:GLY:HA2	1:A:269:TRP:CD1	2.54	0.42
1:A:149:VAL:HG12	1:A:150:ALA:N	2.35	0.42
1:A:474:THR:CG2	1:A:478:ARG:NE	2.81	0.42
1:C:89:TRP:CE3	1:C:89:TRP:HA	2.55	0.42
1:A:149:VAL:HG13	1:A:200:ASN:HB2	2.01	0.42
1:A:390:ARG:O	1:A:391:GLY:C	2.63	0.42
1:C:151:LEU:HA	1:C:201:GLU:O	2.19	0.42
1:C:105:MET:CE	1:C:152:SER:HA	2.49	0.41
1:A:390:ARG:C	1:A:392:VAL:H	2.28	0.41
1:C:72:LEU:HD11	1:C:113:ILE:HD12	2.01	0.41
1:A:473:LEU:O	1:A:473:LEU:HG	2.20	0.41
1:C:105:MET:HE1	1:C:199:VAL:HG11	2.01	0.41
1:C:196:LEU:N	1:C:197:PRO:CD	2.84	0.41
1:C:363:ASN:CG	1:C:464:ARG:HH22	2.28	0.41
1:A:40:ILE:O	1:A:43:TYR:HB3	2.19	0.41
1:C:113:ILE:HD12	1:C:141:TRP:CE2	2.56	0.41
1:C:68:MET:HB2	1:C:85:TYR:CE1	2.56	0.41
1:C:204:VAL:O	1:C:219:TYR:HA	2.21	0.41
1:C:205:GLY:HA2	1:C:218:VAL:O	2.20	0.41
1:C:442:ARG:C	1:C:442:ARG:HD3	2.46	0.41
1:C:100:ARG:NH2	1:C:450:ASN:HD21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:N	1:A:24:ILE:CD1	2.84	0.40
1:B:196:LEU:N	1:B:197:PRO:CD	2.84	0.40
1:B:274:HIS:CD2	1:B:275:ILE:N	2.89	0.40
1:C:105:MET:CE	1:C:152:SER:CB	3.00	0.40
1:C:113:ILE:HD13	1:C:141:TRP:CE3	2.56	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	489/536 (91%)	480 (98%)	8 (2%)	1 (0%)	43	58
1	B	487/536 (91%)	478 (98%)	9 (2%)	0	100	100
1	C	483/536 (90%)	476 (99%)	7 (1%)	0	100	100
All	All	1459/1608 (91%)	1434 (98%)	24 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP

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	416/453 (92%)	404 (97%)	12 (3%)	37	60
1	B	414/453 (91%)	408 (99%)	6 (1%)	59	79
1	C	410/453 (90%)	403 (98%)	7 (2%)	53	74
All	All	1240/1359 (91%)	1215 (98%)	25 (2%)	48	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	27	VAL
1	A	192	MET
1	A	204	VAL
1	A	270	GLU
1	A	390	ARG
1	A	392	VAL
1	A	395	SER
1	A	465	THR
1	A	469	VAL
1	A	474	THR
1	A	480	VAL
1	B	159	GLN
1	B	182	GLN
1	B	353	THR
1	B	392	VAL
1	B	480	VAL
1	B	483	PHE
1	C	27	VAL
1	C	192	MET
1	C	308	VAL
1	C	363	ASN
1	C	395	SER
1	C	448	LYS
1	C	465	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	216	GLN
1	A	237	ASN
1	A	293	HIS

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Mol	Chain	Res	Type
1	A	450	ASN
1	B	92	HIS
1	B	293	HIS
1	B	300	HIS
1	B	316	ASN
1	B	383	GLN
1	C	92	HIS
1	C	237	ASN
1	C	438	GLN
1	C	450	ASN
1	C	468	GLN

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

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, 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	493/536 (91%)	-0.01	12 (2%) 59 55	29, 41, 67, 112	0
1	B	491/536 (91%)	0.42	24 (4%) 35 31	45, 59, 82, 122	0
1	C	487/536 (90%)	0.46	30 (6%) 26 23	43, 63, 94, 119	0
All	All	1471/1608 (91%)	0.29	66 (4%) 38 34	29, 56, 86, 122	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	PHE	5.5
1	B	283	TRP	4.9
1	A	160	PHE	4.5
1	B	192	MET	4.5
1	C	393	VAL	4.4
1	B	393	VAL	4.3
1	A	502	TRP	4.3
1	C	394	MET	3.8
1	C	158	VAL	3.7
1	B	352	PHE	3.7
1	C	352	PHE	3.6
1	C	126	ALA	3.6
1	A	393	VAL	3.5
1	C	289	PHE	3.4
1	C	283	TRP	3.4
1	B	450	ASN	3.4
1	A	159	GLN	3.3
1	A	499	ASN	3.2
1	B	209	ARG	3.2
1	B	488	ALA	3.2
1	C	455	TYR	3.2
1	B	159	GLN	3.1
1	B	455	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	390	ARG	3.0
1	A	498	LYS	3.0
1	C	355	ALA	2.9
1	C	116	PRO	2.9
1	B	322	ASN	2.8
1	B	500	SER	2.8
1	A	283	TRP	2.7
1	C	130	THR	2.7
1	C	124	VAL	2.7
1	B	459	LEU	2.7
1	B	59	VAL	2.7
1	B	289	PHE	2.7
1	C	123	ALA	2.7
1	C	38	LYS	2.6
1	C	125	VAL	2.6
1	C	192	MET	2.6
1	B	38	LYS	2.6
1	C	465	THR	2.5
1	C	448	LYS	2.5
1	A	390	ARG	2.5
1	C	498	LYS	2.4
1	C	64	VAL	2.4
1	B	392	VAL	2.4
1	C	55	VAL	2.4
1	A	501	ASN	2.4
1	B	97	ILE	2.3
1	B	394	MET	2.3
1	C	109	MET	2.3
1	C	210	PRO	2.3
1	C	171	THR	2.2
1	C	275	ILE	2.2
1	B	21	GLY	2.2
1	C	50	PRO	2.2
1	C	496	VAL	2.2
1	A	450	ASN	2.1
1	A	192	MET	2.1
1	B	355	ALA	2.1
1	C	459	LEU	2.1
1	A	455	TYR	2.1
1	B	498	LYS	2.1
1	C	287	ARG	2.1
1	B	465	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	146	THR	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.