W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 08:19 PM JST

PDB ID	:	7DBW
Title	:	PnpA1, the oxygenase component of a two-component para-nitrophenol hydroxylase from Rhodococcus imtechensis RKJ300
Authors	:	Guo, Y.; Zheng, J.T.; Zhou, N.Y.
Deposited on	:	2020-10-22
Resolution	:	2.50 Å(reported)

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

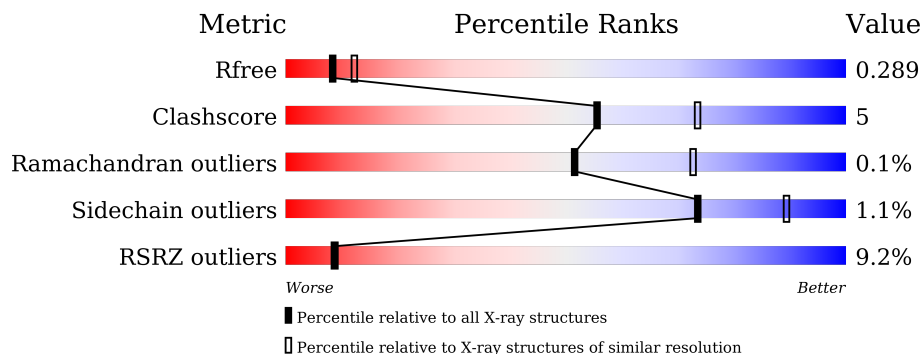|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	Percentile Ranks	Value
Rfree		0.289
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		1.1%
RSRZ outliers		9.2%

Worse ——— Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	528	11% 80% 14% • 6%
1	B	528	11% 83% 12% 6%
1	C	528	4% 85% 9% 6%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11969 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-hydroxyphenylacetate 3-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	498	Total 3965	C 2512	N 698	O 741	S 14	0	0	0
1	A	498	Total 3965	C 2512	N 698	O 741	S 14	0	0	0
1	B	498	Total 3965	C 2512	N 698	O 741	S 14	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	52	Total 52	O 52	0	0
2	A	12	Total 12	O 12	0	0
2	B	10	Total 10	O 10	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.
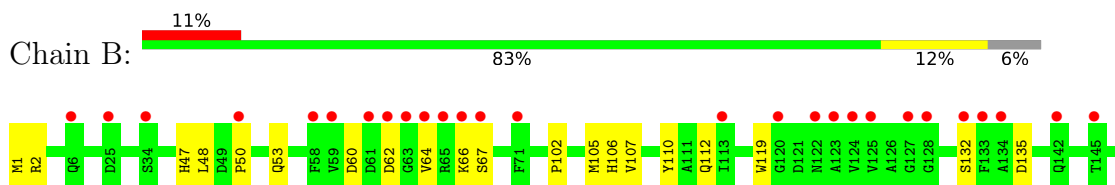
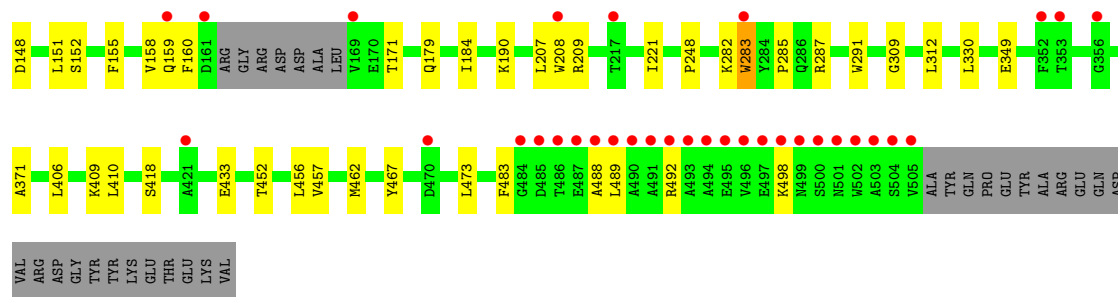- Molecule 1: 4-hydroxyphenylacetate 3-hydroxylase
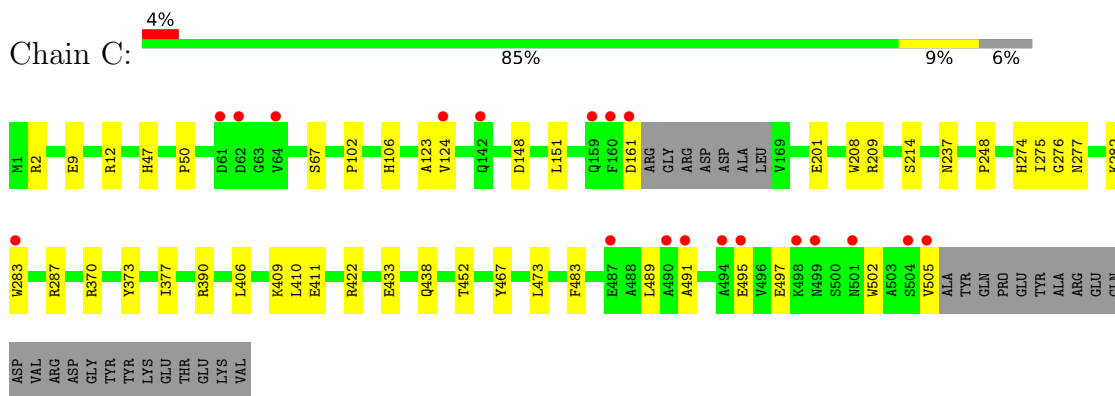
Chain C:

- Molecule 1: 4-hydroxyphenylacetate 3-hydroxylase

Chain A:

- Molecule 1: 4-hydroxyphenylacetate 3-hydroxylase

Chain B:
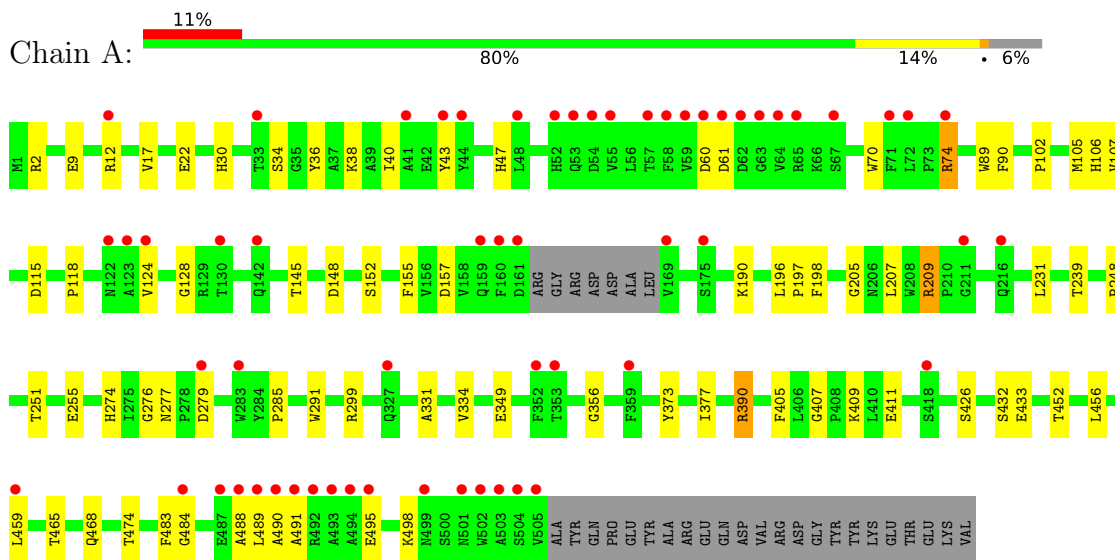
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.01Å 150.01Å 321.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.78 – 2.50 49.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (22.78-2.50) 99.9 (49.41-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.242 , 0.291 0.241 , 0.289	Depositor DCC
R_{free} test set	3237 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.4	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11969	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.49 % 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 4.3305e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.42	0/4068	0.56	0/5540
1	B	0.41	0/4068	0.55	0/5540
1	C	0.48	0/4068	0.64	0/5540
All	All	0.44	0/12204	0.58	0/16620

There are no bond length outliers.

There are no bond angle outliers.

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	3965	0	3815	49	0
1	B	3965	0	3815	44	0
1	C	3965	0	3815	35	0
2	A	12	0	0	0	0
2	B	10	0	0	0	0
2	C	52	0	0	0	0
All	All	11969	0	11445	120	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 5.

All (120) 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:349:GLU:HG3	1:B:349:GLU:HG3	1.51	0.92
1:C:406:LEU:O	1:C:410:LEU:HD22	1.72	0.90
1:B:159:GLN:HA	1:B:209:ARG:HH12	1.37	0.89
1:B:488:ALA:O	1:B:492:ARG:HG3	1.79	0.81
1:C:406:LEU:O	1:C:410:LEU:CD2	2.30	0.80
1:A:331:ALA:HA	1:B:462:MET:HE2	1.67	0.77
1:B:406:LEU:O	1:B:410:LEU:CD2	2.33	0.76
1:B:60:ASP:OD2	1:B:66:LYS:HE3	1.86	0.76
1:B:467:TYR:HD1	1:B:473:LEU:HD22	1.54	0.73
1:A:17:VAL:HG22	1:A:231:LEU:HD12	1.73	0.70
1:C:124:VAL:HB	1:C:276:GLY:HA3	1.74	0.69
1:B:406:LEU:O	1:B:410:LEU:HD22	1.93	0.69
1:C:9:GLU:OE2	1:C:12:ARG:NH1	2.27	0.68
1:B:406:LEU:O	1:B:410:LEU:HD23	1.95	0.65
1:C:248:PRO:HD2	1:C:433:GLU:HG3	1.79	0.65
1:A:465:THR:HA	1:A:468:GLN:HG2	1.79	0.64
1:B:2:ARG:HG3	1:B:148:ASP:HB3	1.79	0.63
1:B:207:LEU:CD1	1:B:285:PRO:HB2	2.30	0.62
1:B:207:LEU:HD13	1:B:285:PRO:HB2	1.81	0.62
1:C:283:TRP:CD1	1:C:287:ARG:HD2	2.35	0.61
1:B:179:GLN:HG2	1:B:184:ILE:HG22	1.83	0.61
1:B:452:THR:HG23	1:B:456:LEU:HD23	1.81	0.61
1:C:502:TRP:HB2	1:C:505:VAL:HG12	1.83	0.60
1:A:248:PRO:HD2	1:A:433:GLU:HG3	1.83	0.59
1:C:467:TYR:CD1	1:C:473:LEU:HD22	2.38	0.59
1:A:124:VAL:HB	1:A:276:GLY:HA3	1.85	0.59
1:C:497:GLU:HG3	1:C:502:TRP:HZ3	1.68	0.58
1:B:159:GLN:HA	1:B:209:ARG:NH1	2.15	0.58
1:C:124:VAL:HB	1:C:276:GLY:CA	2.33	0.58
1:B:208:TRP:CG	1:B:282:LYS:HG2	2.40	0.57
1:A:331:ALA:HA	1:B:462:MET:CE	2.35	0.56
1:B:47:HIS:CD2	1:B:67:SER:HB3	2.41	0.55
1:A:197:PRO:HG2	1:A:198:PHE:CE2	2.43	0.53
1:C:283:TRP:HE1	1:C:287:ARG:CZ	2.20	0.53
1:A:390:ARG:HG2	1:A:390:ARG:HH21	1.72	0.53
1:A:274:HIS:HE1	1:A:277:ASN:H	1.56	0.53
1:C:248:PRO:HD2	1:C:433:GLU:CG	2.38	0.53
1:C:467:TYR:HD1	1:C:473:LEU:HD22	1.73	0.53
1:C:2:ARG:HG3	1:C:148:ASP:HB3	1.89	0.52
1:A:2:ARG:HG3	1:A:148:ASP:HB3	1.90	0.52
1:B:132:SER:HB2	1:B:135:ASP:HB2	1.91	0.52
1:B:371:ALA:HB2	1:B:457:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:TRP:HD1	1:B:287:ARG:HH11	1.58	0.52
1:C:373:TYR:CE2	1:C:377:ILE:HD13	2.44	0.52
1:C:274:HIS:HE1	1:C:277:ASN:H	1.58	0.52
1:B:151:LEU:HD22	1:B:221:ILE:HD11	1.91	0.51
1:A:407:GLY:O	1:A:411:GLU:HG3	2.11	0.51
1:C:411:GLU:OE1	1:C:422:ARG:HD2	2.11	0.51
1:C:124:VAL:N	1:C:275:ILE:O	2.41	0.50
1:A:34:SER:O	1:A:38:LYS:HG2	2.10	0.50
1:A:70:TRP:CD2	1:A:145:THR:HG22	2.46	0.50
1:B:248:PRO:HD2	1:B:433:GLU:HG3	1.94	0.50
1:A:207:LEU:HD13	1:A:285:PRO:HB2	1.92	0.50
1:B:107:VAL:HB	1:B:291:TRP:HB3	1.93	0.50
1:A:107:VAL:HB	1:A:291:TRP:HB3	1.94	0.49
1:A:274:HIS:CE1	1:A:277:ASN:H	2.31	0.49
1:A:334:VAL:HG21	1:B:462:MET:HE1	1.95	0.49
1:C:370:ARG:NH1	1:C:452:THR:O	2.37	0.49
1:A:22:GLU:OE2	1:A:30:HIS:NE2	2.38	0.49
1:B:467:TYR:CD1	1:B:473:LEU:HD22	2.41	0.49
1:B:160:PHE:CD1	1:B:171:THR:HG22	2.48	0.49
1:B:1:MET:HE1	1:B:48:LEU:HD23	1.95	0.48
1:C:47:HIS:CD2	1:C:67:SER:HB3	2.48	0.48
1:C:50:PRO:HG3	1:A:61:ASP:CG	2.33	0.48
1:C:124:VAL:HG23	1:C:277:ASN:HB2	1.93	0.48
1:A:405:PHE:CE1	1:A:409:LYS:NZ	2.72	0.48
1:A:373:TYR:CE2	1:A:377:ILE:HD13	2.48	0.48
1:A:9:GLU:OE2	1:A:12:ARG:NH1	2.46	0.48
1:B:50:PRO:HA	1:B:53:GLN:HG3	1.96	0.48
1:C:124:VAL:HB	1:C:276:GLY:C	2.34	0.47
1:A:155:PHE:HB3	1:A:207:LEU:CD2	2.44	0.47
1:B:107:VAL:HG12	1:B:110:TYR:CE2	2.49	0.47
1:A:483:PHE:CD2	1:A:489:LEU:HD11	2.49	0.47
1:A:452:THR:HG23	1:A:456:LEU:HD23	1.96	0.47
1:C:283:TRP:CD1	1:C:287:ARG:NH1	2.83	0.47
1:A:483:PHE:CD1	1:A:489:LEU:HD21	2.49	0.47
1:A:484:GLY:HA3	1:A:488:ALA:HB3	1.96	0.47
1:A:157:ASP:OD1	1:A:190:LYS:NZ	2.47	0.47
1:B:483:PHE:CD2	1:B:489:LEU:HD21	2.49	0.47
1:A:491:ALA:O	1:A:495:GLU:HG2	2.15	0.46
1:B:102:PRO:HB3	1:B:106:HIS:CE1	2.49	0.46
1:C:406:LEU:O	1:C:410:LEU:HD23	2.13	0.46
1:A:190:LYS:HD2	1:A:190:LYS:HA	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HB3	1:A:106:HIS:CE1	2.50	0.46
1:A:105:MET:SD	1:A:152:SER:HB2	2.56	0.46
1:A:115:ASP:O	1:A:118:PRO:HD2	2.16	0.45
1:C:123:ALA:HA	1:C:274:HIS:CD2	2.52	0.45
1:C:237:ASN:OD1	1:C:438:GLN:NE2	2.50	0.45
1:C:102:PRO:HB3	1:C:106:HIS:CE1	2.52	0.44
1:A:74:ARG:NH2	1:A:356:GLY:O	2.43	0.44
1:A:196:LEU:HB3	1:A:231:LEU:HD13	1.99	0.44
1:A:209:ARG:HB2	1:A:209:ARG:NH1	2.33	0.44
1:A:490:ALA:HA	1:B:418:SER:O	2.17	0.44
1:B:112:GLN:HG2	1:B:119:TRP:CE2	2.53	0.44
1:C:422:ARG:NH2	1:A:128:GLY:HA3	2.33	0.44
1:B:158:VAL:O	1:B:209:ARG:NH2	2.50	0.44
1:C:151:LEU:HD12	1:C:201:GLU:HB2	1.99	0.44
1:C:214:SER:O	1:C:276:GLY:HA2	2.17	0.44
1:A:40:ILE:O	1:A:43:TYR:HB3	2.17	0.43
1:A:155:PHE:HA	1:A:205:GLY:O	2.18	0.43
1:C:208:TRP:CE2	1:C:282:LYS:HE2	2.53	0.43
1:B:60:ASP:OD2	1:B:64:VAL:HB	2.19	0.43
1:A:155:PHE:HB3	1:A:207:LEU:HD22	2.01	0.43
1:B:105:MET:SD	1:B:152:SER:HB2	2.58	0.43
1:A:239:THR:O	1:A:251:THR:HG22	2.19	0.42
1:A:390:ARG:HG2	1:A:390:ARG:NH2	2.34	0.42
1:B:190:LYS:HA	1:B:190:LYS:HD2	1.79	0.42
1:C:497:GLU:HG3	1:C:502:TRP:CZ3	2.52	0.42
1:A:90:PHE:CZ	1:A:299:ARG:HB2	2.55	0.42
1:B:160:PHE:CE1	1:B:171:THR:HG22	2.55	0.41
1:B:208:TRP:CB	1:B:282:LYS:HG2	2.50	0.41
1:B:498:LYS:HD3	1:B:498:LYS:HA	1.82	0.41
1:B:155:PHE:HB3	1:B:207:LEU:HD22	2.01	0.41
1:C:483:PHE:CD1	1:C:489:LEU:HD21	2.55	0.41
1:A:36:TYR:CZ	1:A:255:GLU:HG3	2.56	0.41
1:B:312:LEU:HD23	1:B:330:LEU:HD22	2.03	0.41
1:A:456:LEU:HD12	1:A:459:LEU:HD12	2.04	0.40
1:C:491:ALA:O	1:C:495:GLU:HG2	2.22	0.40
1:A:47:HIS:CE1	1:A:89:TRP:HZ2	2.40	0.40
1:A:474:THR:HG22	1:B:309:GLY:HA2	2.03	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	494/528 (94%)	487 (99%)	6 (1%)	1 (0%)	47	68
1	B	494/528 (94%)	481 (97%)	13 (3%)	0	100	100
1	C	494/528 (94%)	488 (99%)	6 (1%)	0	100	100
All	All	1482/1584 (94%)	1456 (98%)	25 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP

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	420/445 (94%)	413 (98%)	7 (2%)	60	82
1	B	420/445 (94%)	417 (99%)	3 (1%)	84	94
1	C	420/445 (94%)	416 (99%)	4 (1%)	76	90
All	All	1260/1335 (94%)	1246 (99%)	14 (1%)	73	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	161	ASP
1	C	209	ARG

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Mol	Chain	Res	Type
1	C	390	ARG
1	C	409	LYS
1	A	74	ARG
1	A	209	ARG
1	A	279	ASP
1	A	390	ARG
1	A	426	SER
1	A	432	SER
1	A	498	LYS
1	B	62	ASP
1	B	283	TRP
1	B	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	237	ASN
1	C	274	HIS
1	C	438	GLN
1	A	142	GLN
1	B	293	HIS

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	498/528 (94%)	0.59	59 (11%)	4	4	31, 42, 69, 110	0
1	B	498/528 (94%)	0.54	60 (12%)	4	4	30, 43, 74, 104	0
1	C	498/528 (94%)	0.16	19 (3%)	40	43	16, 25, 53, 85	0
All	All	1494/1584 (94%)	0.43	138 (9%)	9	9	16, 39, 67, 110	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	11.0
1	B	503	ALA	10.9
1	A	169	VAL	9.0
1	B	504	SER	8.7
1	B	283	TRP	7.8
1	A	505	VAL	6.7
1	A	64	VAL	6.3
1	A	59	VAL	6.3
1	B	124	VAL	6.2
1	A	160	PHE	5.6
1	B	50	PRO	5.5
1	A	65	ARG	5.5
1	C	124	VAL	5.4
1	B	502	TRP	5.3
1	B	487	GLU	5.3
1	B	505	VAL	5.3
1	A	504	SER	5.2
1	B	499	ASN	5.1
1	C	283	TRP	4.9
1	C	505	VAL	4.8
1	B	123	ALA	4.8
1	B	494	ALA	4.8
1	A	502	TRP	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	494	ALA	4.7
1	A	487	GLU	4.6
1	B	161	ASP	4.6
1	A	501	ASN	4.5
1	A	161	ASP	4.5
1	A	489	LEU	4.3
1	A	63	GLY	4.3
1	A	283	TRP	4.2
1	B	122	ASN	4.2
1	A	123	ALA	4.1
1	B	63	GLY	4.1
1	C	62	ASP	4.1
1	B	132	SER	4.0
1	B	495	GLU	4.0
1	A	352	PHE	3.9
1	B	498	LYS	3.8
1	A	503	ALA	3.8
1	B	486	THR	3.8
1	B	500	SER	3.7
1	A	122	ASN	3.7
1	B	497	GLU	3.7
1	A	493	ALA	3.7
1	B	488	ALA	3.7
1	B	159	GLN	3.6
1	B	65	ARG	3.6
1	A	61	ASP	3.6
1	A	353	THR	3.6
1	B	352	PHE	3.5
1	C	498	LYS	3.5
1	C	161	ASP	3.5
1	B	113	ILE	3.4
1	C	501	ASN	3.4
1	A	488	ALA	3.4
1	A	74	ARG	3.4
1	A	211	GLY	3.4
1	A	72	LEU	3.3
1	C	495	GLU	3.2
1	A	490	ALA	3.2
1	B	491	ALA	3.2
1	A	60	ASP	3.1
1	B	64	VAL	3.1
1	B	484	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	61	ASP	3.1
1	A	495	GLU	3.0
1	B	501	ASN	3.0
1	B	142	GLN	3.0
1	A	48	LEU	3.0
1	A	327	GLN	2.9
1	A	494	ALA	2.9
1	A	359	PHE	2.9
1	B	492	ARG	2.8
1	C	491	ALA	2.8
1	C	504	SER	2.8
1	B	470	ASP	2.8
1	A	62	ASP	2.7
1	A	279	ASP	2.7
1	A	491	ALA	2.7
1	B	61	ASP	2.7
1	B	145	THR	2.7
1	A	55	VAL	2.7
1	A	492	ARG	2.7
1	A	459	LEU	2.6
1	C	487	GLU	2.6
1	B	489	LEU	2.6
1	B	133	PHE	2.5
1	B	485	ASP	2.5
1	A	67	SER	2.5
1	C	64	VAL	2.4
1	A	124	VAL	2.4
1	A	484	GLY	2.4
1	B	66	LYS	2.4
1	C	490	ALA	2.4
1	A	418	SER	2.4
1	A	159	GLN	2.4
1	B	58	PHE	2.4
1	A	499	ASN	2.4
1	B	208	TRP	2.4
1	B	217	THR	2.4
1	A	53	GLN	2.4
1	A	58	PHE	2.4
1	A	41	ALA	2.4
1	C	160	PHE	2.3
1	B	120	GLY	2.3
1	B	134	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	67	SER	2.3
1	A	52	HIS	2.3
1	B	62	ASP	2.3
1	B	128	GLY	2.3
1	B	59	VAL	2.3
1	C	499	ASN	2.3
1	B	490	ALA	2.3
1	A	130	THR	2.3
1	B	353	THR	2.3
1	A	71	PHE	2.3
1	B	25	ASP	2.3
1	A	33	THR	2.3
1	A	216	GLN	2.2
1	B	6	GLN	2.2
1	B	356	GLY	2.2
1	A	54	ASP	2.2
1	B	71	PHE	2.2
1	A	44	TYR	2.2
1	C	159	GLN	2.1
1	B	34	SER	2.1
1	B	493	ALA	2.1
1	A	57	THR	2.1
1	A	12	ARG	2.1
1	B	125	VAL	2.1
1	B	496	VAL	2.1
1	B	421	ALA	2.1
1	A	175	SER	2.1
1	C	142	GLN	2.1
1	B	127	GLY	2.0
1	A	142	GLN	2.0
1	A	43	TYR	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.