



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 PM UTC

PDB ID : 4ZXD / pdb_00004zxd
Title : Crystal Structure of hydroquinone 1,2-dioxygenase PnpCD
Authors : Liu, S.; Su, T.; Zhang, C.; Gu, L.
Deposited on : 2015-05-20
Resolution : 3.05 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

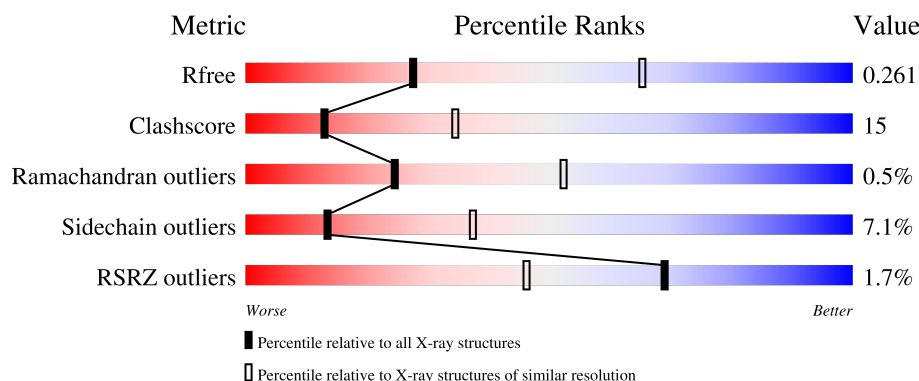
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	168	
1	B	168	
2	W	339	
2	X	339	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7678 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 Hydroquinone dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1240	796	213	227	4			
1	B	160	Total	C	N	O	S	0	0	0
			1240	796	213	227	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP C1I210
A	-2	PRO	-	expression tag	UNP C1I210
A	-1	GLY	-	expression tag	UNP C1I210
A	0	SER	-	expression tag	UNP C1I210
B	-3	GLY	-	expression tag	UNP C1I210
B	-2	PRO	-	expression tag	UNP C1I210
B	-1	GLY	-	expression tag	UNP C1I210
B	0	SER	-	expression tag	UNP C1I210

- Molecule 2 is a protein called Hydroquinone dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	324	Total	C	N	O	S	0	0	0
			2601	1657	444	487	13			
2	X	321	Total	C	N	O	S	0	0	0
			2578	1644	441	480	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		

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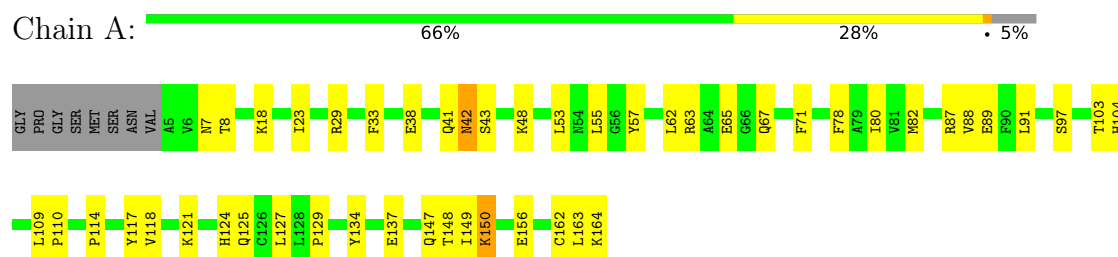
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	W	9	Total	O	0	0
			9	9		
3	X	3	Total	O	0	0
			3	3		

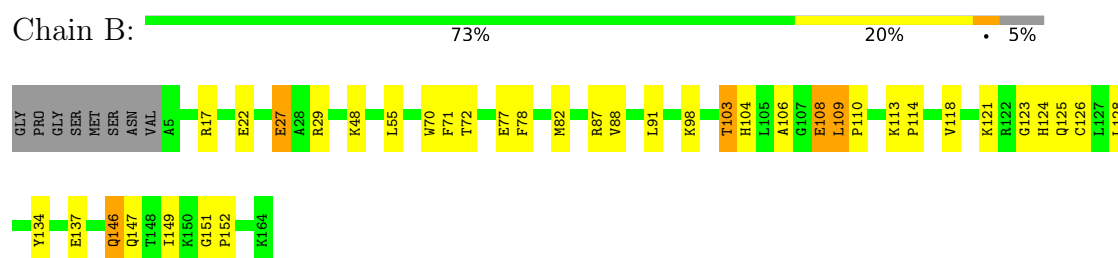
3 Residue-property plots

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.

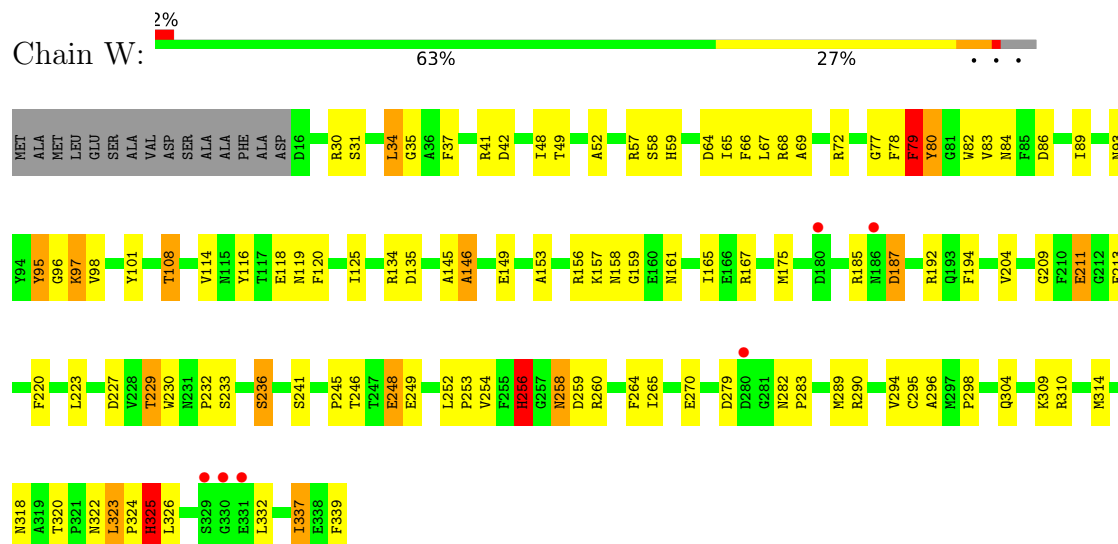
• Molecule 1: Hydroquinone dioxygenase small subunit



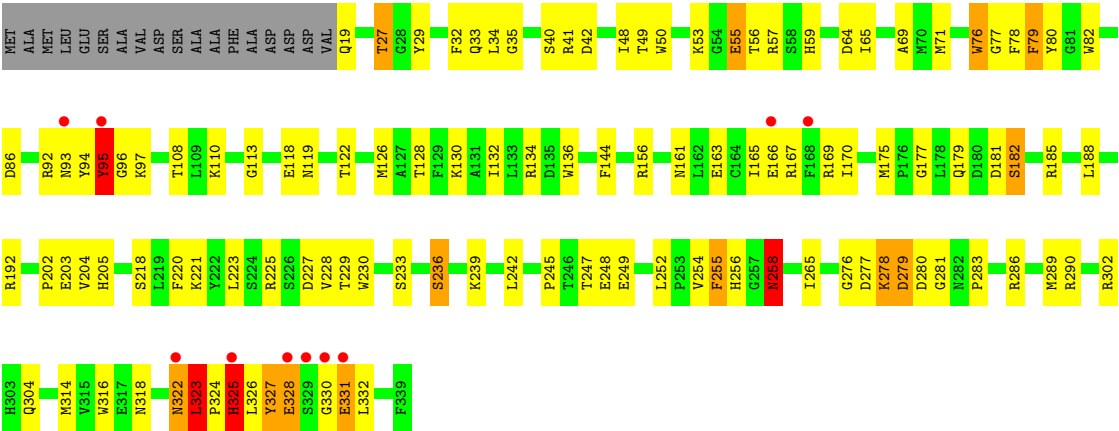
• Molecule 1: Hydroquinone dioxygenase small subunit



• Molecule 2: Hydroquinone dioxygenase large subunit



• Molecule 2: Hydroquinone dioxygenase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.20Å 114.01Å 158.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.69 – 3.05 38.69 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.69-3.05) 99.3 (38.69-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.253 0.210 , 0.261	Depositor DCC
R_{free} test set	1130 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	1.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.3	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	0.92	EDS
Total number of atoms	7678	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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	0.60	1/1269 (0.1%)	0.92	0/1717
1	B	0.57	0/1269	0.98	4/1717 (0.2%)
2	W	0.70	3/2678 (0.1%)	1.00	7/3639 (0.2%)
2	X	0.77	4/2655 (0.2%)	1.11	20/3607 (0.6%)
All	All	0.69	8/7871 (0.1%)	1.02	31/10680 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	205	HIS	CD2-NE2	-9.32	1.27	1.37
2	X	205	HIS	CG-CD2	7.85	1.44	1.35
1	A	104	HIS	CE1-NE2	6.80	1.39	1.32
2	X	76	TRP	NE1-CE2	-6.76	1.30	1.37
2	W	325	HIS	CE1-NE2	6.67	1.39	1.32
2	X	205	HIS	CE1-NE2	6.65	1.39	1.32
2	W	256	HIS	CA-C	-5.60	1.45	1.53
2	W	325	HIS	CG-ND1	5.36	1.44	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	327	TYR	CA-C-N	8.02	131.34	120.44
2	X	327	TYR	C-N-CA	8.02	131.34	120.44
2	X	325	HIS	N-CA-C	-7.79	101.98	112.26
2	X	258	ASN	N-CA-C	-6.97	100.72	110.35
2	X	323	LEU	CA-CB-CG	6.57	139.31	116.30
2	X	327	TYR	N-CA-C	-6.52	105.33	113.28
2	X	323	LEU	CA-C-N	-6.51	112.89	120.12
2	X	323	LEU	C-N-CA	-6.51	112.89	120.12
2	X	255	PHE	N-CA-CB	6.47	120.67	110.84
2	W	209	GLY	N-CA-C	-6.45	105.61	114.64
2	W	323	LEU	CA-C-N	-6.38	112.26	119.28
2	W	323	LEU	C-N-CA	-6.38	112.26	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	122	THR	CA-C-N	-6.27	113.23	119.56
2	X	122	THR	C-N-CA	-6.27	113.23	119.56
2	X	205	HIS	ND1-CG-CD2	-5.86	100.25	106.10
1	B	128	LEU	CA-C-N	5.84	125.77	119.76
1	B	128	LEU	C-N-CA	5.84	125.77	119.76
1	B	151	GLY	CA-C-N	5.82	125.53	119.82
1	B	151	GLY	C-N-CA	5.82	125.53	119.82
2	W	80	TYR	N-CA-C	-5.49	100.73	109.07
2	X	76	TRP	CD2-CE2-CZ2	-5.34	117.06	122.40
2	W	79	PHE	CB-CA-C	-5.20	110.56	116.54
2	W	270	GLU	N-CA-C	5.16	116.69	108.79
2	X	182	SER	CA-C-N	5.16	125.13	120.03
2	X	182	SER	C-N-CA	5.16	125.13	120.03
2	W	146	ALA	N-CA-C	-5.15	103.46	110.36
2	X	50	TRP	N-CA-C	5.12	112.73	108.13
2	X	79	PHE	CB-CA-C	-5.08	110.70	116.54
2	X	276	GLY	N-CA-C	5.06	118.64	110.90
2	X	330	GLY	CA-C-N	5.03	127.33	120.54
2	X	330	GLY	C-N-CA	5.03	127.33	120.54

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	1240	0	1239	36	0
1	B	1240	0	1239	29	0
2	W	2601	0	2461	90	0
2	X	2578	0	2444	95	0
3	A	4	0	0	0	0
3	B	3	0	0	2	0
3	W	9	0	0	0	0
3	X	3	0	0	1	0
All	All	7678	0	7383	225	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 15.

All (225) 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)
2:W:82:TRP:O	2:W:256:HIS:HB2	1.64	0.97
1:A:42:ASN:HD22	1:A:42:ASN:N	1.70	0.88
2:W:41:ARG:NH1	2:W:42:ASP:O	2.07	0.86
2:W:258:ASN:HD22	2:W:258:ASN:H	1.23	0.86
2:W:229:THR:HG23	2:W:230:TRP:HD1	1.44	0.82
1:A:125:GLN:HE21	2:W:175:MET:HE2	1.46	0.80
2:X:177:GLY:O	3:X:401:HOH:O	1.99	0.79
2:W:260:ARG:HH21	2:W:324:PRO:HG3	1.47	0.79
2:W:41:ARG:NH2	2:W:153:ALA:O	2.17	0.77
2:W:78:PHE:O	2:W:93:ASN:ND2	2.18	0.76
1:B:87:ARG:HB3	1:B:137:GLU:HB2	1.68	0.76
1:A:53:LEU:HB3	2:W:337:ILE:HD11	1.70	0.74
1:A:67:GLN:NE2	1:A:137:GLU:OE1	2.22	0.73
2:X:258:ASN:ND2	2:X:258:ASN:H	1.84	0.73
2:X:322:ASN:O	2:X:326:LEU:HG	1.88	0.73
2:X:59:HIS:NE2	2:X:86:ASP:OD2	2.23	0.72
2:W:229:THR:HG23	2:W:230:TRP:CD1	2.25	0.72
2:X:323:LEU:HB2	2:X:324:PRO:HD3	1.71	0.71
2:W:192:ARG:NH2	2:W:249:GLU:OE2	2.26	0.69
2:X:281:GLY:HA2	2:X:302:ARG:HH22	1.60	0.66
1:B:22:GLU:HG2	2:X:286:ARG:HB3	1.76	0.66
2:W:258:ASN:HD22	2:W:258:ASN:N	1.93	0.65
2:W:161:ASN:O	2:W:165:ILE:HG12	1.96	0.65
2:X:169:ARG:HH22	2:X:228:VAL:HG11	1.61	0.65
2:W:258:ASN:N	2:W:258:ASN:ND2	2.40	0.64
1:B:103:THR:O	1:B:152:PRO:HD2	1.96	0.64
2:W:258:ASN:H	2:W:258:ASN:ND2	1.91	0.64
2:X:41:ARG:NH1	2:X:42:ASP:O	2.31	0.64
2:W:95:TYR:CG	2:W:96:GLY:N	2.65	0.63
2:X:326:LEU:HD22	2:X:331:GLU:OE2	1.99	0.62
2:X:325:HIS:O	2:X:325:HIS:ND1	2.33	0.62
2:X:161:ASN:O	2:X:165:ILE:HG12	2.01	0.61
2:X:281:GLY:HA2	2:X:302:ARG:HH12	1.65	0.61
2:W:57:ARG:HG3	2:W:114:VAL:HG13	1.82	0.61
1:A:42:ASN:N	1:A:42:ASN:ND2	2.45	0.61
2:W:145:ALA:HB1	2:W:149:GLU:HB2	1.83	0.61
2:X:258:ASN:H	2:X:258:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:97:LYS:HE3	2:W:119:ASN:CG	2.26	0.60
1:A:82:MET:HE1	2:W:220:PHE:CZ	2.36	0.60
2:X:318:ASN:O	2:X:323:LEU:HD11	2.01	0.60
1:A:87:ARG:HH21	1:A:89:GLU:HG2	1.66	0.59
1:A:55:LEU:HD11	2:W:332:LEU:HD11	1.84	0.59
2:W:260:ARG:NH1	2:W:318:ASN:O	2.35	0.59
2:X:229:THR:HG23	2:X:230:TRP:HD1	1.67	0.59
2:X:77:GLY:O	2:X:78:PHE:HB2	2.02	0.59
1:A:41:GLN:C	1:A:42:ASN:HD22	2.11	0.59
3:B:201:HOH:O	2:X:290:ARG:NH1	2.34	0.58
2:W:233:SER:O	2:W:245:PRO:HD2	2.03	0.58
2:W:248:GLU:O	2:W:310:ARG:HA	2.04	0.58
2:W:320:THR:HB	2:W:323:LEU:CD1	2.34	0.58
2:W:134:ARG:HG2	2:W:165:ILE:HD12	1.85	0.58
2:X:245:PRO:HG3	2:X:314:MET:HE1	1.86	0.58
2:W:156:ARG:HG3	2:W:156:ARG:HH11	1.68	0.57
2:X:281:GLY:CA	2:X:302:ARG:HH22	2.17	0.57
2:X:328:GLU:CD	2:X:328:GLU:H	2.12	0.57
2:W:77:GLY:C	2:W:79:PHE:H	2.12	0.57
2:W:283:PRO:HD2	2:X:108:THR:OG1	2.04	0.57
2:X:185:ARG:HD3	2:X:188:LEU:HD12	1.85	0.57
2:X:94:TYR:O	2:X:95:TYR:HB2	2.04	0.57
2:W:64:ASP:O	2:W:68:ARG:HG3	2.06	0.56
2:W:59:HIS:NE2	2:W:86:ASP:OD2	2.38	0.56
2:X:27:THR:HG21	2:X:42:ASP:HA	1.88	0.56
1:A:48:LYS:HE2	1:A:103:THR:HG21	1.88	0.55
2:X:80:TYR:HA	2:X:93:ASN:O	2.06	0.55
1:A:82:MET:HA	1:A:82:MET:HE2	1.88	0.55
2:W:68:ARG:HB3	2:W:253:PRO:HB3	1.89	0.55
2:X:277:ASP:O	2:X:302:ARG:NH2	2.39	0.55
2:W:192:ARG:HG2	2:W:192:ARG:HH11	1.70	0.55
2:W:41:ARG:HG2	2:W:41:ARG:HH11	1.71	0.54
1:A:8:THR:HA	2:W:309:LYS:HE3	1.90	0.54
2:W:322:ASN:O	2:W:326:LEU:HG	2.07	0.54
2:X:41:ARG:HH11	2:X:41:ARG:HG3	1.72	0.54
2:X:229:THR:HG23	2:X:230:TRP:CD1	2.43	0.54
2:X:328:GLU:CD	2:X:328:GLU:N	2.65	0.54
1:B:17:ARG:NH1	3:B:201:HOH:O	2.31	0.54
1:A:18:LYS:O	2:W:290:ARG:NH1	2.41	0.54
1:B:91:LEU:HD23	1:B:114:PRO:HA	1.90	0.54
2:X:278:LYS:HD3	2:X:302:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:157:LYS:NZ	2:W:159:GLY:O	2.30	0.53
2:W:325:HIS:CG	2:W:325:HIS:O	2.61	0.53
2:W:194:PHE:CE2	2:W:310:ARG:HD3	2.43	0.53
1:A:63:ARG:NH2	1:A:65:GLU:OE1	2.41	0.53
1:A:29:ARG:HD3	1:A:164:LYS:NZ	2.24	0.53
2:X:34:LEU:HD22	2:X:128:THR:HG21	1.91	0.52
2:X:41:ARG:HD3	2:X:136:TRP:CG	2.44	0.52
1:B:27:GLU:OE2	1:B:29:ARG:NH2	2.41	0.52
1:B:55:LEU:HD11	2:X:332:LEU:HD21	1.91	0.52
2:X:281:GLY:N	2:X:302:ARG:HH22	2.08	0.52
2:W:116:TYR:OH	2:W:118:GLU:OE1	2.23	0.52
2:X:82:TRP:CD2	2:X:92:ARG:HD3	2.45	0.52
2:X:323:LEU:CB	2:X:324:PRO:HD3	2.39	0.52
1:A:78:PHE:CD1	2:W:175:MET:HE3	2.45	0.52
2:W:260:ARG:NH2	2:W:324:PRO:HG3	2.21	0.52
2:W:108:THR:HG21	2:X:283:PRO:HD2	1.92	0.51
2:X:192:ARG:HH22	2:X:249:GLU:CD	2.18	0.51
2:W:84:ASN:OD1	2:W:101:TYR:OH	2.27	0.51
2:X:326:LEU:HB3	2:X:331:GLU:OE1	2.11	0.51
1:A:33:PHE:O	1:A:162:CYS:HA	2.10	0.51
2:X:82:TRP:CG	2:X:278:LYS:HE3	2.46	0.50
1:A:57:TYR:CD1	2:W:241:SER:HB2	2.47	0.50
1:B:48:LYS:HZ2	1:B:146:GLN:HE21	1.59	0.50
2:W:52:ALA:O	2:W:57:ARG:NH1	2.44	0.50
2:W:289:MET:HE2	2:W:295:CYS:HB3	1.93	0.50
1:B:149:ILE:HD11	2:X:239:LYS:HD2	1.93	0.50
1:B:78:PHE:CE1	2:X:175:MET:HE3	2.47	0.50
1:A:38:GLU:O	1:A:42:ASN:ND2	2.45	0.49
2:W:66:PHE:HD1	2:W:67:LEU:HD23	1.77	0.49
1:B:118:VAL:HG22	2:X:204:VAL:HG22	1.95	0.49
2:W:192:ARG:HH22	2:W:249:GLU:CD	2.18	0.49
2:W:245:PRO:HG3	2:W:314:MET:HE1	1.94	0.49
1:B:70:TRP:HB3	1:B:106:ALA:HB3	1.94	0.49
2:X:77:GLY:HA2	2:X:126:MET:HE1	1.95	0.49
2:X:258:ASN:ND2	2:X:258:ASN:N	2.55	0.49
1:B:78:PHE:CD1	2:X:175:MET:HE3	2.47	0.49
2:X:19:GLN:CB	2:X:33:GLN:HB2	2.43	0.49
2:X:130:LYS:O	2:X:134:ARG:HG3	2.13	0.49
2:W:232:PRO:HA	2:W:246:THR:HB	1.95	0.48
2:X:233:SER:O	2:X:245:PRO:HD2	2.13	0.48
2:X:255:PHE:HD1	2:X:302:ARG:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:264:PHE:HB2	2:W:289:MET:HE1	1.95	0.48
2:X:192:ARG:HG2	2:X:192:ARG:HH11	1.79	0.48
2:X:245:PRO:HG3	2:X:314:MET:CE	2.43	0.48
2:W:289:MET:CE	2:W:295:CYS:HB3	2.44	0.48
2:W:97:LYS:HE3	2:W:120:PHE:N	2.28	0.48
2:W:265:ILE:HG23	2:W:294:VAL:HG22	1.95	0.48
2:X:223:LEU:HD21	2:X:245:PRO:HB2	1.95	0.48
2:X:325:HIS:O	2:X:325:HIS:CG	2.66	0.48
2:W:296:ALA:O	2:W:298:PRO:HD3	2.14	0.48
2:X:327:TYR:N	2:X:328:GLU:OE2	2.37	0.47
1:A:127:LEU:O	1:A:129:PRO:HD3	2.14	0.47
1:B:147:GLN:OE1	2:X:236:SER:HB2	2.13	0.47
2:W:35:GLY:HA3	2:W:118:GLU:OE2	2.14	0.47
2:W:34:LEU:HD21	2:W:125:ILE:HG13	1.96	0.47
2:X:252:LEU:O	2:X:304:GLN:NE2	2.42	0.47
2:W:97:LYS:CE	2:W:119:ASN:CG	2.88	0.47
2:X:35:GLY:HA3	2:X:118:GLU:OE2	2.14	0.47
1:B:48:LYS:NZ	1:B:146:GLN:HE21	2.12	0.47
1:B:103:THR:O	1:B:104:HIS:HD2	1.98	0.47
2:X:144:PHE:CD2	2:X:228:VAL:HB	2.50	0.47
1:B:123:GLY:HA3	2:X:220:PHE:CD2	2.50	0.47
2:W:282:ASN:HA	2:X:108:THR:HG21	1.95	0.47
2:X:19:GLN:HB3	2:X:33:GLN:HB2	1.96	0.47
2:X:110:LYS:O	2:X:113:GLY:N	2.48	0.47
1:A:150:LYS:NZ	1:A:156:GLU:OE1	2.36	0.47
1:B:77:GLU:OE2	1:B:103:THR:HG23	2.15	0.46
2:X:55:GLU:HB2	2:X:57:ARG:NH1	2.30	0.46
1:B:124:HIS:HD2	2:X:218:SER:HA	1.80	0.46
1:B:17:ARG:HD2	2:X:290:ARG:NH1	2.31	0.46
2:X:71:MET:HE3	2:X:71:MET:HA	1.97	0.46
1:A:82:MET:HE1	2:W:220:PHE:HZ	1.81	0.46
1:B:72:THR:O	1:B:104:HIS:HB2	2.15	0.46
2:W:252:LEU:HD23	2:W:304:GLN:HA	1.98	0.45
2:X:252:LEU:HB3	2:X:304:GLN:HG3	1.98	0.45
2:X:218:SER:HB3	2:X:221:LYS:HB3	1.99	0.45
1:B:48:LYS:NZ	1:B:146:GLN:NE2	2.64	0.45
1:B:82:MET:HE2	1:B:82:MET:HA	1.97	0.45
2:W:149:GLU:CD	2:W:310:ARG:HH12	2.25	0.45
1:A:147:GLN:OE1	2:W:236:SER:HB2	2.16	0.45
1:B:71:PHE:HB2	1:B:134:TYR:CE2	2.52	0.45
2:X:29:TYR:CD2	2:X:41:ARG:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:O	2:W:309:LYS:HE3	2.17	0.45
2:X:110:LYS:O	2:X:110:LYS:HD2	2.16	0.44
1:A:29:ARG:HD3	1:A:164:LYS:HZ3	1.82	0.44
2:W:314:MET:HE2	2:W:314:MET:HB2	1.85	0.44
2:X:167:ARG:NH1	2:X:227:ASP:OD2	2.51	0.44
1:A:48:LYS:NZ	1:A:62:LEU:HD21	2.32	0.44
1:A:87:ARG:HG3	1:A:117:TYR:HD2	1.81	0.44
1:A:91:LEU:HD23	1:A:114:PRO:HA	1.98	0.44
2:W:227:ASP:OD1	2:W:227:ASP:N	2.50	0.44
2:W:79:PHE:HB3	2:W:80:TYR:H	1.47	0.44
2:W:30:ARG:HG3	2:W:135:ASP:CG	2.43	0.44
1:A:43:SER:O	1:A:63:ARG:HD3	2.18	0.43
1:A:109:LEU:HA	1:A:110:PRO:HD3	1.68	0.43
2:W:337:ILE:HG22	2:W:339:PHE:HD2	1.82	0.43
2:X:221:LYS:O	2:X:225:ARG:HG3	2.18	0.43
2:W:34:LEU:O	2:W:37:PHE:HB2	2.18	0.43
2:X:32:PHE:CD1	2:X:132:ILE:HG12	2.53	0.43
2:X:281:GLY:HA2	2:X:302:ARG:NH1	2.32	0.43
1:A:71:PHE:HB2	1:A:134:TYR:CE2	2.53	0.43
2:W:97:LYS:HE2	2:W:98:VAL:H	1.83	0.43
2:X:181:ASP:OD1	2:X:182:SER:N	2.48	0.43
2:X:79:PHE:HD2	2:X:80:TYR:H	1.67	0.43
2:X:279:ASP:HB2	2:X:280:ASP:H	1.59	0.43
2:W:252:LEU:HA	2:W:253:PRO:HD3	1.84	0.43
2:X:78:PHE:O	2:X:79:PHE:C	2.62	0.43
2:W:185:ARG:C	2:W:187:ASP:H	2.26	0.42
2:X:95:TYR:HB3	2:X:96:GLY:H	1.52	0.42
2:X:281:GLY:HA2	2:X:302:ARG:NH2	2.29	0.42
1:A:121:LYS:HB2	1:A:124:HIS:CE1	2.54	0.42
2:W:97:LYS:HE2	2:W:98:VAL:N	2.34	0.42
2:X:64:ASP:OD1	2:X:65:ILE:N	2.53	0.42
1:A:33:PHE:HB3	1:A:163:LEU:HB2	2.01	0.42
2:X:76:TRP:C	2:X:78:PHE:H	2.27	0.42
2:X:278:LYS:C	2:X:278:LYS:HD2	2.44	0.42
1:B:121:LYS:HG3	1:B:124:HIS:CE1	2.54	0.42
2:W:72:ARG:CZ	2:W:253:PRO:HG2	2.50	0.42
2:X:230:TRP:HA	2:X:248:GLU:OE1	2.19	0.42
1:B:108:GLU:H	1:B:108:GLU:HG2	1.51	0.42
2:W:69:ALA:HB1	2:W:254:VAL:HG12	2.02	0.42
2:W:82:TRP:HZ3	2:W:259:ASP:OD1	2.02	0.42
2:X:192:ARG:HH11	2:X:192:ARG:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:223:LEU:HD21	2:W:245:PRO:HB2	2.02	0.41
2:X:242:LEU:O	2:X:316:TRP:HD1	2.03	0.41
2:W:65:ILE:HD13	2:W:65:ILE:HA	1.88	0.41
2:W:167:ARG:HD3	2:W:227:ASP:OD2	2.19	0.41
2:W:118:GLU:HG2	2:W:120:PHE:CZ	2.54	0.41
1:A:148:THR:OG1	1:A:149:ILE:N	2.54	0.41
2:X:69:ALA:HB1	2:X:254:VAL:HG12	2.03	0.41
2:X:331:GLU:HG3	2:X:332:LEU:H	1.85	0.41
1:A:80:ILE:HG21	1:A:82:MET:HE3	2.02	0.41
2:W:72:ARG:HA	2:W:72:ARG:HD3	1.75	0.41
2:X:229:THR:HA	2:X:247:THR:O	2.21	0.41
1:A:89:GLU:O	1:A:134:TYR:HA	2.19	0.41
2:W:146:ALA:HB2	2:W:249:GLU:HB3	2.03	0.40
2:W:246:THR:HG23	2:W:248:GLU:OE2	2.21	0.40
2:W:248:GLU:OE1	2:W:248:GLU:HA	2.21	0.40
2:X:97:LYS:HD3	2:X:119:ASN:HD21	1.86	0.40
2:X:163:GLU:HA	2:X:166:GLU:HB2	2.02	0.40
2:W:83:VAL:HA	2:W:256:HIS:CB	2.51	0.40
1:B:109:LEU:HA	1:B:110:PRO:HD3	1.82	0.40
2:W:157:LYS:HG3	2:W:158:ASN:N	2.36	0.40
2:W:230:TRP:HA	2:W:248:GLU:OE1	2.22	0.40
2:X:289:MET:HE2	2:X:289:MET:HB3	1.95	0.40
1:B:113:LYS:HA	1:B:114:PRO:HD3	1.89	0.40
1:B:124:HIS:CG	2:X:202:PRO:HG3	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	158/168 (94%)	148 (94%)	10 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	158/168 (94%)	151 (96%)	7 (4%)	0	100	100
2	W	322/339 (95%)	292 (91%)	28 (9%)	2 (1%)	21	48
2	X	319/339 (94%)	282 (88%)	34 (11%)	3 (1%)	14	39
All	All	957/1014 (94%)	873 (91%)	79 (8%)	5 (0%)	24	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	53	LYS
2	X	95	TYR
2	X	179	GLN
2	W	95	TYR
2	W	211	GLU

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	130/136 (96%)	124 (95%)	6 (5%)	24	52
1	B	130/136 (96%)	121 (93%)	9 (7%)	14	38
2	W	274/284 (96%)	253 (92%)	21 (8%)	12	35
2	X	271/284 (95%)	250 (92%)	21 (8%)	12	35
All	All	805/840 (96%)	748 (93%)	57 (7%)	13	37

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	42	ASN
1	A	88	VAL
1	A	97	SER
1	A	118	VAL
1	A	150	LYS

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Mol	Chain	Res	Type
1	B	27	GLU
1	B	88	VAL
1	B	98	LYS
1	B	103	THR
1	B	108	GLU
1	B	109	LEU
1	B	125	GLN
1	B	126	CYS
1	B	146	GLN
2	W	31	SER
2	W	34	LEU
2	W	48	ILE
2	W	49	THR
2	W	58	SER
2	W	79	PHE
2	W	89	ILE
2	W	97	LYS
2	W	108	THR
2	W	187	ASP
2	W	204	VAL
2	W	211	GLU
2	W	213	GLU
2	W	229	THR
2	W	236	SER
2	W	248	GLU
2	W	256	HIS
2	W	258	ASN
2	W	279	ASP
2	W	325	HIS
2	W	337	ILE
2	X	27	THR
2	X	40	SER
2	X	48	ILE
2	X	49	THR
2	X	55	GLU
2	X	56	THR
2	X	95	TYR
2	X	156	ARG
2	X	170	ILE
2	X	203	GLU
2	X	236	SER
2	X	256	HIS

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Mol	Chain	Res	Type
2	X	258	ASN
2	X	265	ILE
2	X	278	LYS
2	X	279	ASP
2	X	322	ASN
2	X	323	LEU
2	X	325	HIS
2	X	328	GLU
2	X	331	GLU

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	41	GLN
1	A	42	ASN
1	A	125	GLN
1	B	41	GLN
1	B	104	HIS
1	B	146	GLN
2	W	33	GLN
2	W	179	GLN
2	W	186	ASN
2	W	256	HIS
2	W	258	ASN
2	W	282	ASN
2	W	325	HIS
2	X	256	HIS
2	X	258	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

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 [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	160/168 (95%)	-0.11	0 100 100	31, 45, 69, 85	0
1	B	160/168 (95%)	0.06	0 100 100	33, 46, 66, 84	0
2	W	324/339 (95%)	0.00	6 (1%) 66 43	30, 40, 77, 107	0
2	X	321/339 (94%)	0.19	10 (3%) 51 29	31, 50, 84, 106	0
All	All	965/1014 (95%)	0.06	16 (1%) 69 46	30, 45, 77, 107	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	329	SER	5.2
2	X	331	GLU	4.8
2	W	330	GLY	3.4
2	X	330	GLY	3.3
2	X	322	ASN	3.1
2	X	325	HIS	2.8
2	X	168	PHE	2.8
2	W	180	ASP	2.7
2	W	186	ASN	2.7
2	W	329	SER	2.5
2	W	331	GLU	2.3
2	X	166	GLU	2.2
2	X	93	ASN	2.1
2	X	95	TYR	2.1
2	X	328	GLU	2.1
2	W	280	ASP	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.