Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 10:10 AM JST

PDB ID	:	4ZXD
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 (i) 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 (1)) were used in the production of this report:

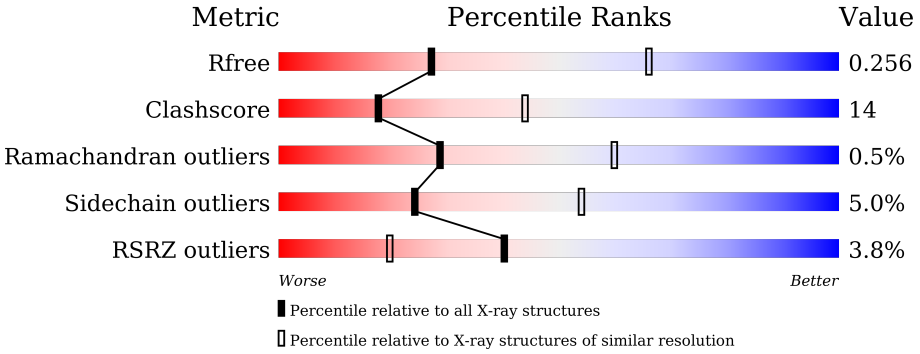
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (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 <=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	4% 70% 24% • 5%
1	B	168	.% 76% 17% • 5%
2	W	339	3% 66% 26% • •
2	X	339	6% 64% 27% • • 5%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	160	1240	796	213	227	4	0	0	0
1	B	160	1240	796	213	227	4	0	0	0

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
			Total	C	N	O	S			
2	W	324	2601	1657	444	487	13	0	0	0
2	X	321	2578	1644	441	480	13	0	0	0

- Molecule 3 is water.

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

Continued on next page...

Continued from previous page...

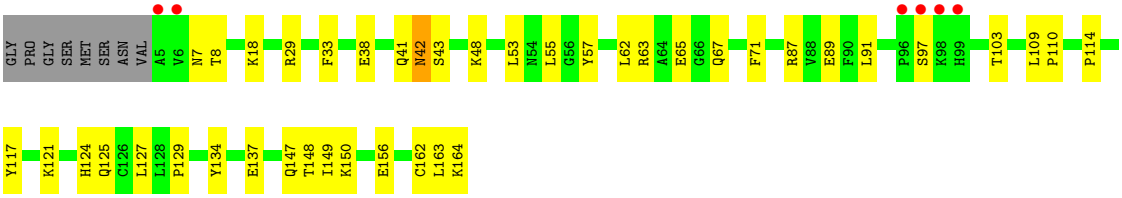
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	W	9	9	9	0	0
			Total	O		
3	X	3	3	3	0	0

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: Hydroquinone dioxygenase small subunit

Chain A:

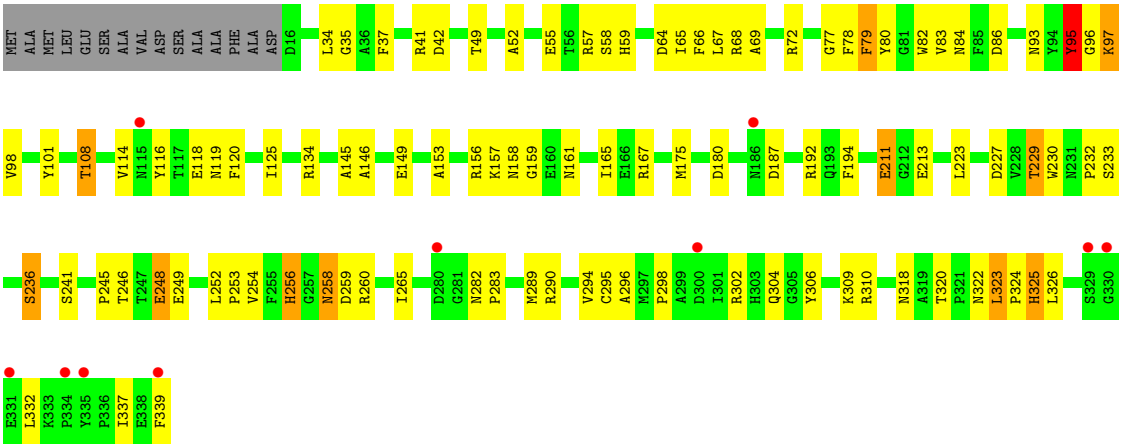


• Molecule 1: Hydroquinone dioxygenase small subunit

Chain B:

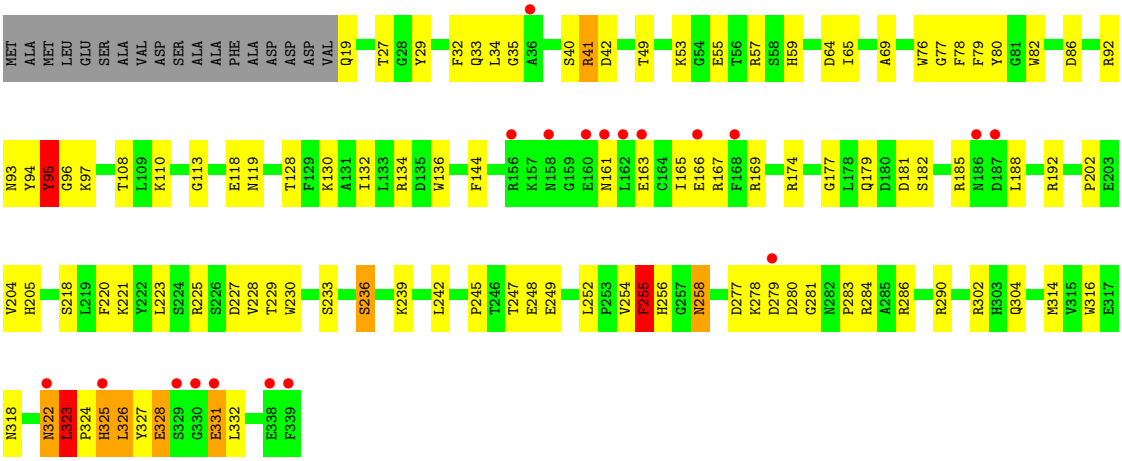
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain W:



• Molecule 2: Hydroquinone dioxygenase large subunit

Chain X:



4 Data and refinement statistics (i)

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) 99.4 (38.69-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.253 0.207 , 0.256	Depositor DCC
R_{free} test set	1130 reflections (5.15%)	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)	0.39 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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 (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	0.48	0/1269	0.63	0/1717
1	B	0.47	0/1269	0.67	0/1717
2	W	0.54	0/2678	0.72	2/3639 (0.1%)
2	X	0.60	2/2655 (0.1%)	0.78	3/3607 (0.1%)
All	All	0.54	2/7871 (0.0%)	0.72	5/10680 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	76	TRP	NE1-CE2	-5.79	1.30	1.37
2	X	205	HIS	CG-CD2	5.14	1.44	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	323	LEU	CA-CB-CG	10.44	139.31	115.30
2	X	326	LEU	CA-CB-CG	6.65	130.60	115.30
2	X	255	PHE	N-CA-CB	5.59	120.67	110.60
2	W	323	LEU	CA-CB-CG	5.49	127.92	115.30
2	W	302	ARG	NE-CZ-NH1	-5.41	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1240	0	1239	31	0
1	B	1240	0	1239	26	0
2	W	2601	0	2461	82	0
2	X	2578	0	2444	86	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	205	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 14.

All (205) 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:N	1:A:42:ASN:HD22	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
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
2:X:258:ASN:ND2	2:X:258:ASN:H	1.84	0.75
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: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:W:258:ASN:ND2	2:W:258:ASN:N	2.40	0.68
2:W:258:ASN:H	2:W:258:ASN:ND2	1.91	0.67
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
1:B:103:THR:O	1:B:152:PRO:HD2	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND1	2:X:325:HIS:O	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
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
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:W:156:ARG:HH11	2:W:156:ARG:HG3	1.68	0.57
2:X:281:GLY:CA	2:X:302:ARG:HH22	2.17	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:W:97:LYS:HE3	2:W:119:ASN:CG	2.26	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
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:HH11	2:W:192:ARG:HG2	1.70	0.55
2:W:41:ARG:HH11	2:W:41:ARG:HG2	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
1:A:41:GLN:C	1:A:42:ASN:HD22	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:W:157:LYS:NZ	2:W:159:GLY:O	2.30	0.53
2:W:325:HIS:O	2:W:325:HIS:CG	2.61	0.53
2:W:77:GLY:C	2:W:79:PHE:H	2.12	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:328:GLU:H	2:X:328:GLU:CD	2.12	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: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
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: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
2:W:52:ALA:O	2:W:57:ARG:NH1	2.44	0.50
1:B:149:ILE:HD11	2:X:239:LYS:HD2	1.93	0.50
2:W:289:MET:HE1	2:W:295:CYS:HB3	1.93	0.50
1:A:38:GLU:O	1:A:42:ASN:ND2	2.45	0.49
2:X:328:GLU:CD	2:X:328:GLU:N	2.65	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
1:B:48:LYS:HZ2	1:B:146:GLN:HE21	1.61	0.49
1:B:70:TRP:HB3	1:B:106:ALA:HB3	1.94	0.49
2:X:258:ASN:ND2	2:X:258:ASN:N	2.55	0.49
2:X:19:GLN:CB	2:X:33:GLN:HB2	2.43	0.49
2:X:245:PRO:HG3	2:X:314:MET:CE	2.43	0.49
2:W:116:TYR:OH	2:W:118:GLU:OE1	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:255:PHE:HD1	2:X:302:ARG:HD2	1.77	0.48
2:X:192:ARG:HG2	2:X:192:ARG:HH11	1.79	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
1:A:150:LYS:NZ	1:A:156:GLU:OE1	2.36	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: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
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: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
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
2:X:192:ARG:HH22	2:X:249:GLU:CD	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:192:ARG:HH22	2:W:249:GLU:CD	2.18	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
1:A:125:GLN:HE21	2:W:175:MET:CE	2.31	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
1:A:29:ARG:HD3	1:A:164:LYS:HZ2	1.82	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
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:W:97:LYS:CE	2:W:119:ASN:CG	2.88	0.42
2:X:192:ARG:HH11	2:X:192:ARG:CG	2.32	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:72:ARG:HD3	2:W:72:ARG:HA	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
2:W:149:GLU:CD	2:W:310:ARG:HH12	2.25	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
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
1	B	158/168 (94%)	151 (96%)	7 (4%)	0	100	100
2	W	322/339 (95%)	292 (91%)	28 (9%)	2 (1%)	25	55
2	X	319/339 (94%)	282 (88%)	34 (11%)	3 (1%)	17	47
All	All	957/1014 (94%)	873 (91%)	79 (8%)	5 (0%)	29	60

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 (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	130/136 (96%)	128 (98%)	2 (2%)	65	83
1	B	130/136 (96%)	125 (96%)	5 (4%)	33	63
2	W	274/284 (96%)	256 (93%)	18 (7%)	16	43
2	X	271/284 (95%)	256 (94%)	15 (6%)	21	50
All	All	805/840 (96%)	765 (95%)	40 (5%)	24	54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	97	SER
1	B	27	GLU
1	B	103	THR
1	B	125	GLN
1	B	126	CYS
1	B	146	GLN
2	W	49	THR
2	W	55	GLU
2	W	58	SER
2	W	79	PHE
2	W	95	TYR
2	W	97	LYS
2	W	108	THR
2	W	180	ASP
2	W	187	ASP
2	W	211	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	306	TYR
2	W	325	HIS
2	X	40	SER
2	X	41	ARG
2	X	49	THR
2	X	95	TYR
2	X	174	ARG
2	X	236	SER
2	X	255	PHE
2	X	256	HIS
2	X	258	ASN
2	X	284	ARG
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	125	GLN
1	B	104	HIS
1	B	146	GLN
2	W	186	ASN
2	W	256	HIS
2	W	258	ASN
2	W	325	HIS
2	X	258	ASN

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 monosaccharides 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	160/168 (95%)	-0.06	6 (3%)	40	20	31, 45, 69, 85	0
1	B	160/168 (95%)	-0.12	2 (1%)	77	56	33, 46, 66, 84	0
2	W	324/339 (95%)	0.01	10 (3%)	49	25	30, 40, 77, 107	0
2	X	321/339 (94%)	0.28	19 (5%)	22	9	31, 50, 84, 106	0
All	All	965/1014 (95%)	0.07	37 (3%)	40	20	30, 45, 77, 107	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	331	GLU	7.6
2	X	330	GLY	7.0
2	W	330	GLY	5.7
2	X	329	SER	4.7
1	A	5	ALA	4.7
2	X	322	ASN	4.6
2	X	168	PHE	4.3
2	X	161	ASN	4.1
2	W	331	GLU	3.9
2	W	115	ASN	3.3
2	W	280	ASP	3.3
1	B	5	ALA	3.0
2	W	329	SER	2.9
2	X	166	GLU	2.7
2	X	338	GLU	2.7
1	A	99	HIS	2.7
2	X	36	ALA	2.7
1	A	97	SER	2.7
2	W	335	TYR	2.5
2	X	279	ASP	2.4
1	A	98	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	X	339	PHE	2.3
2	X	160	GLU	2.3
2	X	187	ASP	2.3
2	X	186	ASN	2.3
2	W	339	PHE	2.3
2	X	158	ASN	2.2
2	X	156	ARG	2.2
2	X	163	GLU	2.1
2	W	300	ASP	2.1
1	B	164	LYS	2.1
2	W	334	PRO	2.1
2	X	162	LEU	2.1
1	A	6	VAL	2.1
1	A	96	PRO	2.1
2	X	325	HIS	2.1
2	W	186	ASN	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.