Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 03:25 PM JST

PDB ID	:	4ZXA
Title	:	Crystal Structure of hydroquinone 1,2-dioxygenase PnpCD in complex with Cd2+ and 4-hydroxybenzonitrile
Authors	:	Liu, S.; Su, T.; Zhang, C.; Gu, L.
Deposited on	:	2015-05-20
Resolution	:	2.49 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:

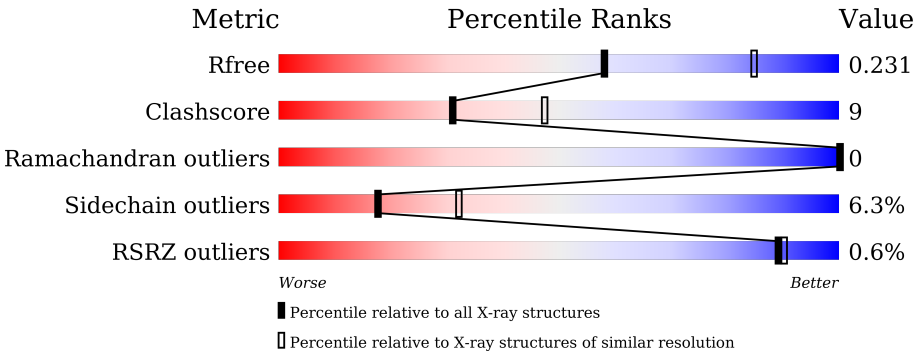
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.49 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	79% 17%
1	B	168	% 73% 21%
1	C	168	% 74% 21%
1	D	168	% 78% 18%
2	W	339	80% 14%
2	X	339	% 73% 20%

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Mol	Chain	Length	Quality of chain
2	Y	339	
2	Z	339	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16274 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	163	Total	C	N	O	S	0	1	0
			1269	812	219	234	4			
1	B	163	Total	C	N	O	S	0	0	0
			1261	808	217	232	4			
1	C	163	Total	C	N	O	S	0	1	0
			1272	814	221	233	4			
1	D	163	Total	C	N	O	S	0	0	0
			1261	808	217	232	4			

There are 16 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
C	-3	GLY	-	expression tag	UNP C1I210
C	-2	PRO	-	expression tag	UNP C1I210
C	-1	GLY	-	expression tag	UNP C1I210
C	0	SER	-	expression tag	UNP C1I210
D	-3	GLY	-	expression tag	UNP C1I210
D	-2	PRO	-	expression tag	UNP C1I210
D	-1	GLY	-	expression tag	UNP C1I210
D	0	SER	-	expression tag	UNP C1I210

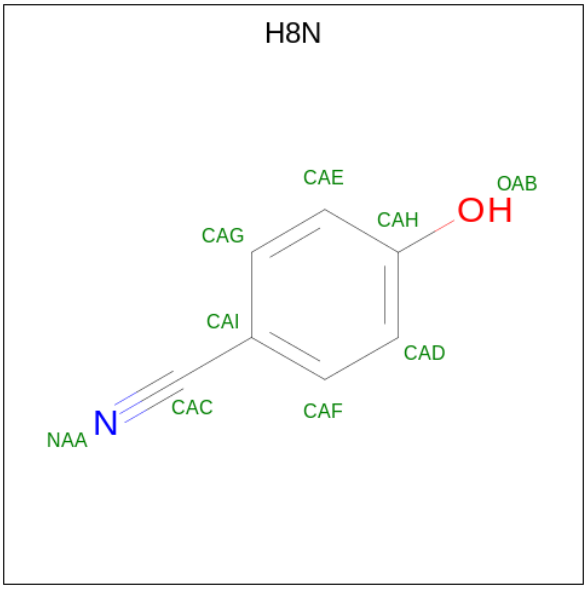
- Molecule 2 is a protein called Hydroquinone dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	324	Total	C	N	O	S	0	2	0
			2620	1668	448	491	13			
2	X	324	Total	C	N	O	S	0	1	0
			2611	1663	447	488	13			
2	Y	324	Total	C	N	O	S	0	1	0
			2611	1663	447	488	13			
2	Z	324	Total	C	N	O	S	0	1	0
			2610	1662	445	490	13			

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	W	1	Total	Cd	0	0
			1	1		
3	X	1	Total	Cd	0	0
			1	1		
3	Y	1	Total	Cd	0	0
			1	1		
3	Z	1	Total	Cd	0	0
			1	1		

- Molecule 4 is 4-hydroxybenzonitrile (three-letter code: H8N) (formula: C_7H_5NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	W	1	Total	C	N	O	0	0
			9	7	1	1		
4	X	1	Total	C	N	O	0	0
			9	7	1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total C N O 9 7 1 1	0	0
4	Z	1	Total C N O 9 7 1 1	0	0

- Molecule 5 is water.

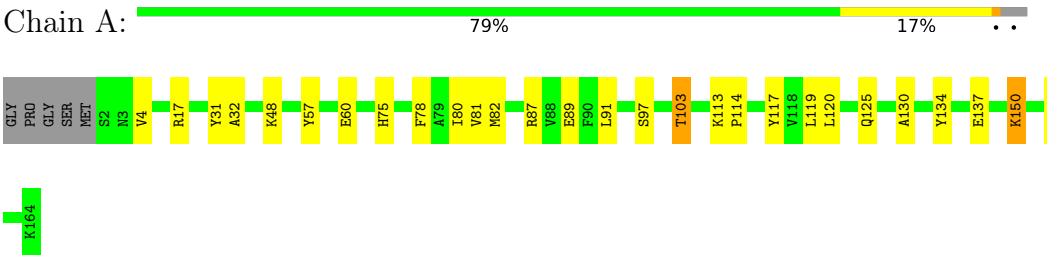
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	B	38	Total O 38 38	0	0
5	C	38	Total O 38 38	0	0
5	D	65	Total O 65 65	0	0
5	W	156	Total O 156 156	0	0
5	X	123	Total O 123 123	0	0
5	Y	117	Total O 117 117	0	0
5	Z	119	Total O 119 119	0	0

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.

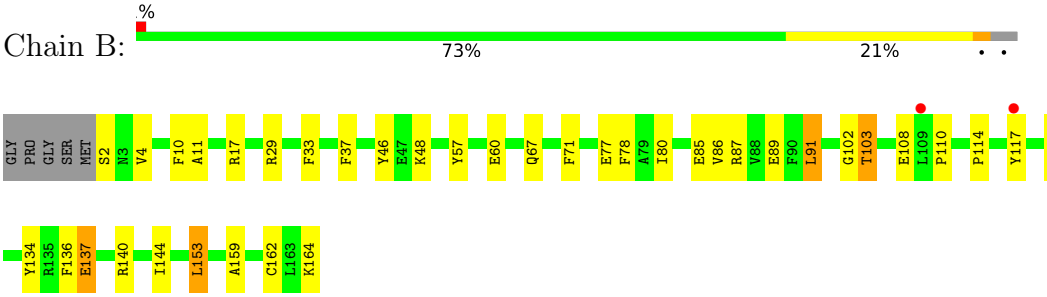
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain A:



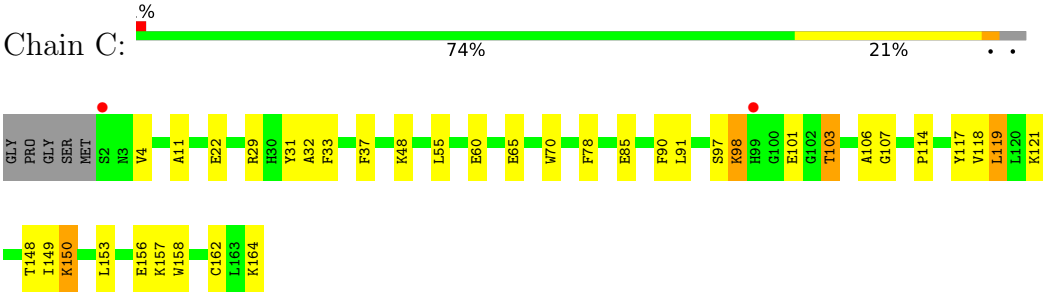
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain B:



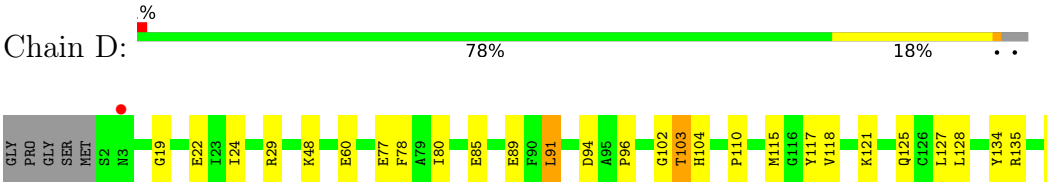
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain C:



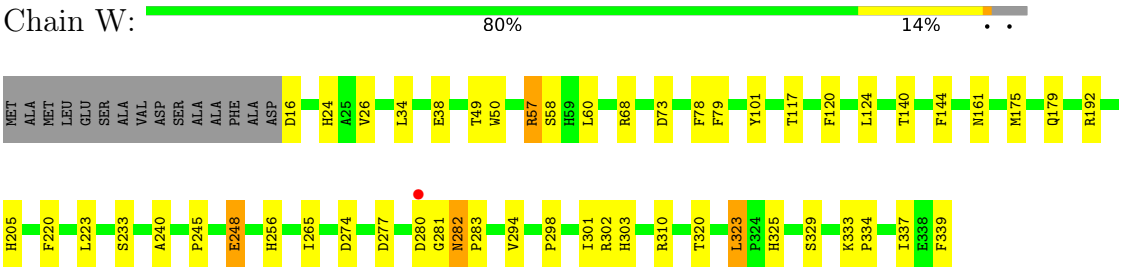
• Molecule 1: Hydroquinone dioxygenase small subunit

Chain D:



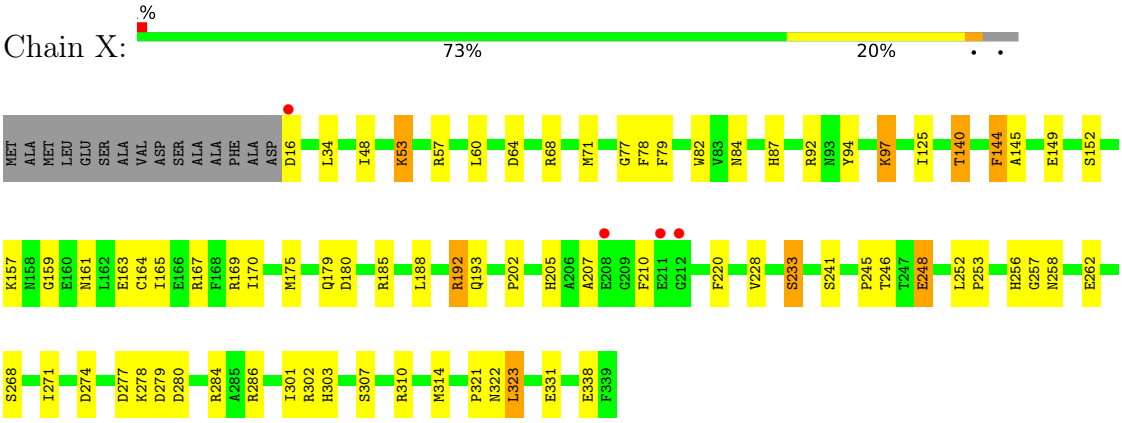
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain W:



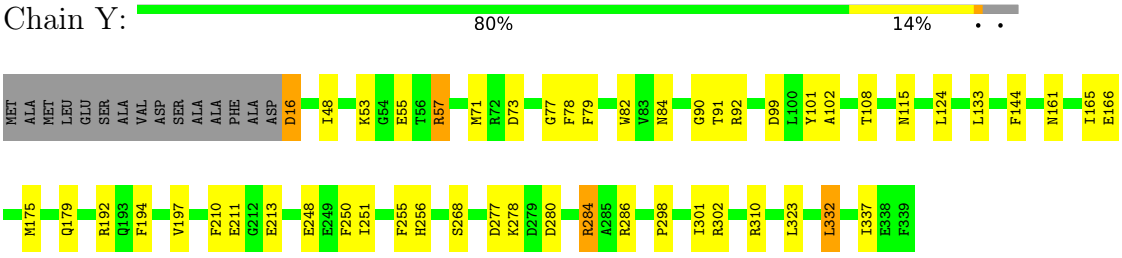
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain X:



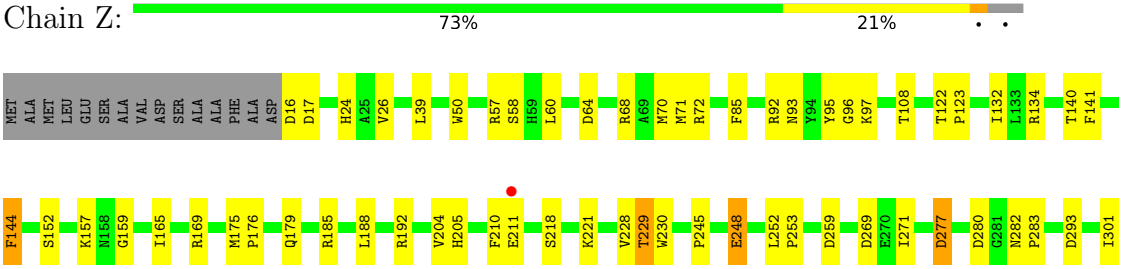
• Molecule 2: Hydroquinone dioxygenase large subunit

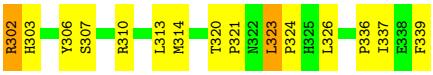
Chain Y:



• Molecule 2: Hydroquinone dioxygenase large subunit

Chain Z:




R302
H303
Y306
S307
R310
L313
M314
T320
P321
N322
L323
P324
H325
L326
P336
I337
E338
F339

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.02Å 181.05Å 186.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.73 – 2.49 40.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.73-2.49) 99.5 (40.73-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	6.23 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.186 , 0.237 0.182 , 0.231	Depositor DCC
R_{free} test set	4606 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16274	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H8N, CD

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	0.40	0/1298	0.55	0/1757
1	B	0.38	0/1290	0.52	0/1746
1	C	0.39	0/1301	0.52	0/1761
1	D	0.42	0/1290	0.56	0/1746
2	W	0.41	0/2698	0.57	0/3666
2	X	0.41	0/2689	0.55	0/3654
2	Y	0.42	0/2689	0.57	0/3654
2	Z	0.41	0/2687	0.57	0/3651
All	All	0.41	0/15942	0.55	0/21635

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	1269	0	1264	26	0
1	B	1261	0	1259	33	0
1	C	1272	0	1272	28	0
1	D	1261	0	1259	32	0
2	W	2620	0	2472	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	2611	0	2467	64	0
2	Y	2611	0	2467	36	0
2	Z	2610	0	2466	71	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	W	9	0	5	0	0
4	X	9	0	5	0	0
4	Y	9	0	5	0	0
4	Z	9	0	5	0	0
5	A	63	0	0	0	0
5	B	38	0	0	2	0
5	C	38	0	0	3	0
5	D	65	0	0	2	0
5	W	156	0	0	2	0
5	X	123	0	0	6	0
5	Y	117	0	0	5	0
5	Z	119	0	0	4	0
All	All	16274	0	14946	279	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 9.

All (279) 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:48:LYS:HE2	1:B:103:THR:HG21	1.45	0.98
2:X:170:ILE:HD12	2:X:170:ILE:H	1.40	0.86
2:Z:229:THR:HG23	2:Z:230:TRP:CD1	2.13	0.83
1:A:87:ARG:HB3	1:A:137:GLU:HB2	1.61	0.83
1:C:65:GLU:OE2	5:C:201:HOH:O	1.96	0.83
2:X:277:ASP:HB2	2:X:284:ARG:NH2	1.95	0.82
1:A:48:LYS:HE2	1:A:103:THR:HG21	1.60	0.82
2:Z:72:ARG:HH21	2:Z:229:THR:HG22	1.46	0.80
1:C:48:LYS:HZ1	1:C:103:THR:HG21	1.46	0.79
1:B:48:LYS:HE2	1:B:103:THR:CG2	2.14	0.78
1:D:125:GLN:HE21	2:Z:175:MET:HE2	1.48	0.78
1:D:117:TYR:CE2	2:Z:205:HIS:HD2	2.02	0.76
2:X:71:MET:HE1	2:X:165:ILE:HA	1.69	0.74
1:C:48:LYS:NZ	1:C:103:THR:HG21	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:336:PRO:HB2	2:Z:337:ILE:HD12	1.71	0.73
1:D:80:ILE:HD13	1:D:125:GLN:HB2	1.70	0.73
1:A:48:LYS:HE2	1:A:103:THR:CG2	2.19	0.71
1:D:117:TYR:CZ	2:Z:205:HIS:HD2	2.07	0.71
1:D:117:TYR:CZ	2:Z:205:HIS:CD2	2.79	0.71
2:W:281:GLY:HA3	5:W:529:HOH:O	1.92	0.69
2:X:34:LEU:HD21	2:X:125:ILE:HG13	1.73	0.69
2:X:331:GLU:OE1	5:X:502:HOH:O	2.11	0.68
1:C:107:GLY:O	5:C:202:HOH:O	2.11	0.67
1:C:164:LYS:O	5:C:203:HOH:O	2.12	0.67
2:X:71:MET:CE	2:X:165:ILE:HA	2.24	0.67
2:X:170:ILE:HD12	2:X:170:ILE:N	2.10	0.67
2:X:277:ASP:HB3	2:X:280:ASP:HB2	1.76	0.66
2:Y:197:VAL:O	5:Y:501:HOH:O	2.13	0.66
2:Z:72:ARG:NH2	2:Z:229:THR:HG22	2.10	0.65
1:D:85:GLU:HG2	1:D:121:LYS:HG2	1.76	0.65
2:Z:269:ASP:O	5:Z:502:HOH:O	2.14	0.65
2:Y:16:ASP:N	5:Y:504:HOH:O	2.30	0.65
2:Z:93:ASN:OD1	5:Z:503:HOH:O	2.14	0.65
2:Z:185:ARG:HG2	2:Z:188:LEU:HD12	1.79	0.64
2:Y:277:ASP:CB	2:Y:280:ASP:HB2	2.27	0.64
2:Z:157:LYS:HE3	2:Z:159:GLY:O	1.98	0.64
2:X:164:CYS:HA	2:X:167:ARG:NH1	2.13	0.64
1:D:22:GLU:OE2	5:D:201:HOH:O	2.14	0.63
1:C:150:LYS:NZ	1:C:156:GLU:OE1	2.32	0.63
1:D:77:GLU:OE2	1:D:103:THR:HG22	2.00	0.62
1:B:89:GLU:O	1:B:134:TYR:HA	2.00	0.61
2:Z:277:ASP:O	2:Z:302:ARG:HD3	2.01	0.61
1:B:29:ARG:HH12	1:B:164:LYS:HB3	1.65	0.60
2:Y:55:GLU:HB2	2:Y:57:ARG:NH1	2.17	0.60
1:D:85:GLU:CG	1:D:121:LYS:HG2	2.32	0.60
2:X:170:ILE:H	2:X:170:ILE:CD1	2.11	0.60
2:Z:71:MET:CE	2:Z:165:ILE:HG22	2.32	0.59
2:Y:108:THR:CG2	2:Z:282:ASN:HA	2.31	0.59
2:W:58:SER:HB2	2:X:286:ARG:NH1	2.16	0.59
2:W:337:ILE:HG22	2:W:339:PHE:HD2	1.67	0.59
2:Y:277:ASP:OD1	2:Y:284:ARG:HD3	2.03	0.59
2:X:233:SER:OG	5:X:501:HOH:O	2.07	0.58
1:D:48:LYS:HE3	1:D:60:GLU:OE1	2.03	0.58
2:Y:108:THR:HG22	2:Z:283:PRO:HD2	1.85	0.58
1:B:48:LYS:HE3	1:B:60:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:229:THR:CG2	2:Z:230:TRP:CD1	2.86	0.58
2:Z:229:THR:CG2	2:Z:230:TRP:HD1	2.17	0.58
1:A:150:LYS:NZ	1:A:156:GLU:OE1	2.37	0.57
1:B:102:GLY:O	5:B:201:HOH:O	2.18	0.57
2:X:302:ARG:NH1	5:X:506:HOH:O	2.34	0.57
2:Z:337:ILE:HG22	2:Z:339:PHE:HD2	1.69	0.57
1:B:46:TYR:CE1	1:B:136:PHE:HB2	2.40	0.57
2:X:71:MET:HE2	2:X:144:PHE:CD1	2.40	0.57
2:X:87[B]:HIS:CD2	2:X:87[B]:HIS:H	2.21	0.56
1:D:94:ASP:O	1:D:96:PRO:HD3	2.05	0.56
1:B:78:PHE:HD1	2:X:175:MET:CE	2.17	0.56
2:X:68:ARG:NH2	5:X:504:HOH:O	2.28	0.56
2:Z:140:THR:CG2	2:Z:152:SER:H	2.18	0.56
2:W:265:ILE:HD13	2:W:294:VAL:HG22	1.87	0.56
1:A:4:VAL:HG12	1:A:4:VAL:O	2.05	0.56
1:A:91:LEU:HD23	1:A:114:PRO:HA	1.88	0.56
2:X:164:CYS:HA	2:X:167:ARG:HH11	1.70	0.56
2:X:277:ASP:HB2	2:X:284:ARG:CZ	2.35	0.56
2:Z:70:MET:HE1	2:Z:132:ILE:CG2	2.35	0.56
2:X:256:HIS:CD2	2:X:257:GLY:N	2.73	0.56
1:B:71:PHE:HB2	1:B:134:TYR:CE2	2.41	0.56
2:Z:71:MET:HE1	2:Z:165:ILE:HG22	1.86	0.56
1:B:80:ILE:HD13	1:B:125:GLN:HB2	1.87	0.56
1:B:117:TYR:CE2	2:X:205:HIS:HD2	2.25	0.55
1:D:29:ARG:HD3	1:D:164:LYS:HE3	1.88	0.55
1:D:48:LYS:HE2	1:D:103:THR:CG2	2.36	0.55
1:B:121:LYS:HB2	1:B:124:HIS:CE1	2.41	0.55
1:C:55:LEU:HD21	2:Y:332:LEU:HD11	1.89	0.55
2:X:140:THR:HG22	2:X:152:SER:O	2.06	0.55
1:C:48:LYS:NZ	1:C:103:THR:CG2	2.70	0.55
1:B:159:ALA:O	1:B:164:LYS:HE2	2.08	0.54
1:B:78:PHE:CD1	2:X:175:MET:CE	2.91	0.54
1:C:11:ALA:HB3	1:C:37:PHE:CE2	2.43	0.54
2:Y:286:ARG:NH2	5:Y:510:HOH:O	2.40	0.53
2:Y:165:ILE:HG13	2:Y:166:GLU:HG3	1.89	0.53
2:Z:71:MET:HE1	2:Z:165:ILE:CB	2.38	0.53
2:X:53:LYS:HB3	2:X:57:ARG:HH21	1.73	0.53
1:A:48:LYS:CE	1:A:103:THR:HG21	2.35	0.53
1:B:48:LYS:CE	1:B:103:THR:HG21	2.31	0.53
2:Y:57:ARG:HD2	2:Y:57:ARG:N	2.22	0.53
2:X:248:GLU:O	2:X:310:ARG:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:336:PRO:C	2:Z:337:ILE:HD12	2.29	0.53
2:W:16:ASP:HB2	2:W:124:LEU:HA	1.91	0.52
2:Y:277:ASP:HB2	2:Y:280:ASP:HB2	1.91	0.52
2:Z:218:SER:HB3	2:Z:221:LYS:HB3	1.90	0.52
1:C:117:TYR:HE2	1:C:119:LEU:HD12	1.75	0.52
1:B:67:GLN:HG3	1:B:137:GLU:OE2	2.10	0.52
2:W:223:LEU:HD21	2:W:245:PRO:HB2	1.93	0.51
2:X:277:ASP:CG	2:X:284:ARG:HH21	2.13	0.51
2:Y:277:ASP:HB3	2:Y:280:ASP:HB2	1.91	0.51
2:Z:95:TYR:OH	2:Z:259:ASP:OD2	2.28	0.51
2:X:78:PHE:CZ	2:X:125:ILE:HG23	2.46	0.51
2:X:94:TYR:HB2	2:X:97:LYS:O	2.11	0.51
2:Y:53:LYS:HB2	2:Y:57:ARG:HH12	1.76	0.51
1:C:78:PHE:CD1	2:Y:175:MET:CE	2.94	0.51
2:X:68:ARG:NE	5:X:504:HOH:O	2.32	0.51
2:X:277:ASP:CB	2:X:284:ARG:NH2	2.70	0.51
1:B:11:ALA:HB3	1:B:37:PHE:CE2	2.47	0.50
1:D:115:MET:HA	2:Z:210:PHE:CD1	2.46	0.50
2:W:265:ILE:CD1	2:W:294:VAL:HG22	2.42	0.50
1:B:85:GLU:HG2	1:B:121:LYS:HG2	1.94	0.50
1:D:29:ARG:HD2	2:Z:339:PHE:O	2.10	0.50
2:X:84:ASN:ND2	5:X:507:HOH:O	2.35	0.50
2:X:256:HIS:HD2	2:X:257:GLY:N	2.09	0.49
2:Y:55:GLU:OE2	2:Y:55:GLU:HA	2.10	0.49
2:Z:71:MET:CE	2:Z:165:ILE:HA	2.42	0.49
1:C:78:PHE:HD1	2:Y:175:MET:CE	2.25	0.49
2:X:157:LYS:HE3	2:X:159:GLY:O	2.12	0.49
1:C:4:VAL:HG12	1:C:4:VAL:O	2.11	0.49
2:Z:39:LEU:HD12	2:Z:39:LEU:N	2.27	0.49
2:W:325:HIS:CE1	2:W:329:SER:OG	2.65	0.49
2:X:82:TRP:O	2:X:256:HIS:HD2	1.95	0.49
1:A:87:ARG:HH11	1:A:137:GLU:HG3	1.78	0.49
2:X:164:CYS:O	2:X:167:ARG:NH1	2.45	0.49
2:Z:301:ILE:C	2:Z:301:ILE:HD12	2.33	0.49
1:B:77:GLU:OE2	1:B:103:THR:HB	2.13	0.48
1:B:125:GLN:HE21	2:X:175:MET:CE	2.26	0.48
1:D:117:TYR:OH	2:Z:205:HIS:CD2	2.66	0.48
2:Y:71:MET:HA	2:Y:133:LEU:HD11	1.94	0.48
1:A:82:MET:HE1	2:W:220:PHE:CZ	2.48	0.48
1:D:48:LYS:HE2	1:D:103:THR:HG21	1.96	0.48
2:Z:336:PRO:CB	2:Z:337:ILE:HD12	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HH12	1:A:89:GLU:CD	2.17	0.48
2:W:233:SER:O	2:W:245:PRO:HD2	2.14	0.48
2:Z:323:LEU:HD12	2:Z:326:LEU:HD12	1.95	0.48
2:Z:248:GLU:OE2	2:Z:313:LEU:HD23	2.14	0.48
1:B:124:HIS:HB3	2:X:202:PRO:HG3	1.96	0.47
2:Z:229:THR:HG21	5:Z:568:HOH:O	2.14	0.47
1:B:86:VAL:HG21	1:B:144:ILE:HD11	1.96	0.47
1:B:153:LEU:HB2	5:B:204:HOH:O	2.14	0.47
1:B:33:PHE:O	1:B:162:CYS:HA	2.15	0.47
1:B:91:LEU:HD22	1:B:114:PRO:HA	1.96	0.47
1:B:108:GLU:O	1:B:110:PRO:HD3	2.14	0.47
2:X:164:CYS:CA	2:X:167:ARG:NH1	2.76	0.47
2:X:245:PRO:HG3	2:X:314:MET:CE	2.45	0.47
1:C:90:PHE:HE2	1:C:118:VAL:HG22	1.79	0.47
2:Y:298:PRO:O	2:Y:301:ILE:HG13	2.15	0.47
2:Z:70:MET:HE1	2:Z:132:ILE:HG21	1.97	0.47
2:W:34:LEU:HG	2:W:120:PHE:CZ	2.50	0.47
2:W:101:TYR:HB3	2:W:117:THR:HG23	1.97	0.47
2:W:320:THR:O	2:W:323:LEU:HD22	2.15	0.47
2:Z:320:THR:HA	2:Z:321:PRO:HD3	1.80	0.47
2:Z:337:ILE:HG22	2:Z:339:PHE:CD2	2.49	0.46
1:C:70:TRP:HB3	1:C:106:ALA:HB3	1.98	0.46
1:D:91:LEU:HD13	1:D:110:PRO:HB2	1.97	0.46
2:W:73:ASP:OD1	2:W:78:PHE:HA	2.15	0.46
2:X:145:ALA:HB1	2:X:149:GLU:HB2	1.97	0.46
2:Y:77:GLY:O	2:Y:78:PHE:HB2	2.15	0.46
2:Y:90:GLY:HA3	2:Y:101:TYR:CZ	2.51	0.46
2:Y:194:PHE:CE2	2:Y:310:ARG:HD3	2.51	0.46
2:Z:144:PHE:CD2	2:Z:228:VAL:HB	2.51	0.46
2:Z:337:ILE:HD12	2:Z:337:ILE:N	2.30	0.46
1:A:78:PHE:CD1	2:W:175:MET:CE	2.99	0.46
1:C:148:THR:OG1	1:C:149:ILE:N	2.49	0.46
2:X:144:PHE:HB3	2:X:228:VAL:HG12	1.98	0.46
1:D:19:GLY:HA3	2:Z:293:ASP:OD2	2.16	0.46
2:Y:108:THR:HG21	2:Z:282:ASN:HA	1.96	0.45
1:A:78:PHE:HD1	2:W:175:MET:CE	2.29	0.45
2:Z:71:MET:HE1	2:Z:165:ILE:CG2	2.47	0.45
2:Z:71:MET:HE1	2:Z:165:ILE:HA	1.97	0.45
2:X:192:ARG:NH1	2:X:193:GLN:HG3	2.32	0.45
1:D:29:ARG:HG3	5:D:227:HOH:O	2.15	0.45
2:W:333:LYS:HB3	2:W:334:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:271:ILE:HG12	2:X:307:SER:HB2	1.97	0.45
2:Z:245:PRO:HD3	2:Z:314:MET:SD	2.55	0.45
1:D:125:GLN:HG2	2:Z:175:MET:HE1	1.99	0.45
2:X:82:TRP:O	2:X:256:HIS:CD2	2.69	0.45
2:Z:141:PHE:HB2	2:Z:152:SER:O	2.16	0.45
2:Z:140:THR:HG22	2:Z:152:SER:N	2.31	0.45
1:D:91:LEU:CD1	1:D:110:PRO:HB2	2.46	0.44
2:X:321:PRO:O	2:X:322:ASN:HB2	2.17	0.44
2:Z:336:PRO:HB2	2:Z:337:ILE:CD1	2.43	0.44
1:B:117:TYR:CE2	2:X:205:HIS:CD2	3.03	0.44
1:C:91:LEU:HD12	1:C:114:PRO:HA	1.98	0.44
2:Y:102:ALA:O	2:Y:115:ASN:HA	2.17	0.44
1:A:78:PHE:HD1	2:W:175:MET:HE3	1.82	0.44
2:X:179:GLN:O	2:X:180:ASP:HB2	2.18	0.44
1:B:4:VAL:HG12	1:B:4:VAL:O	2.18	0.44
1:C:70:TRP:CE2	1:C:135:ARG:HD3	2.52	0.44
2:W:49:THR:HA	2:W:57:ARG:O	2.18	0.44
2:Z:271:ILE:HG12	2:Z:307:SER:HB2	1.99	0.44
1:A:48:LYS:HE3	1:A:60:GLU:OE1	2.18	0.44
1:A:87:ARG:NH1	1:A:89:GLU:OE2	2.51	0.44
1:C:33:PHE:O	1:C:162:CYS:HA	2.16	0.44
1:D:118:VAL:HG22	2:Z:204:VAL:HA	1.99	0.44
1:A:4:VAL:O	1:A:4:VAL:CG1	2.66	0.44
1:A:78:PHE:CD1	2:W:175:MET:HE3	2.52	0.44
1:B:10:PHE:CE1	2:X:220:PHE:CE2	3.06	0.44
2:Y:90:GLY:HA3	2:Y:101:TYR:CE2	2.52	0.44
1:A:125:GLN:HE21	2:W:175:MET:CE	2.31	0.43
1:B:29:ARG:NH1	1:B:164:LYS:HB3	2.32	0.43
2:X:258:ASN:O	2:X:278:LYS:HD2	2.18	0.43
1:A:89:GLU:O	1:A:134:TYR:HA	2.18	0.43
1:C:31:TYR:O	1:C:32:ALA:C	2.56	0.43
1:D:89:GLU:O	1:D:134:TYR:HA	2.18	0.43
2:X:274:ASP:O	2:X:303:HIS:HA	2.18	0.43
2:X:82:TRP:N	2:X:82:TRP:CE3	2.86	0.43
2:X:185:ARG:HG2	2:X:188:LEU:HD12	2.01	0.43
1:C:158:TRP:CD2	2:Y:337:ILE:HD13	2.53	0.43
2:X:207:ALA:O	2:X:210:PHE:HB2	2.19	0.43
2:Y:278:LYS:HA	2:Y:302:ARG:HD2	2.01	0.43
2:Z:252:LEU:HA	2:Z:253:PRO:HD3	1.87	0.43
1:D:127:LEU:N	2:Z:175:MET:HE3	2.33	0.43
1:D:24:ILE:HG21	2:Z:283:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:230:TRP:HA	2:Z:248:GLU:OE1	2.18	0.43
2:Z:64:ASP:O	2:Z:68:ARG:HG3	2.19	0.43
2:Z:169:ARG:NE	5:Z:518:HOH:O	2.52	0.43
2:Z:175:MET:HG2	2:Z:176:PRO:HD2	2.01	0.43
2:X:82:TRP:CE2	2:X:92:ARG:HG3	2.54	0.43
2:X:323:LEU:HA	2:X:323:LEU:HD12	1.80	0.43
1:B:57:TYR:CD1	2:X:241:SER:HB2	2.54	0.42
2:Y:250:PHE:CG	2:Y:251:ILE:N	2.86	0.42
1:D:78:PHE:HD1	2:Z:175:MET:CE	2.32	0.42
2:W:282:ASN:HA	2:W:283:PRO:HD3	1.88	0.42
2:X:77:GLY:O	2:X:78:PHE:HB2	2.18	0.42
2:Y:84:ASN:ND2	5:Y:509:HOH:O	2.40	0.42
2:Z:248:GLU:O	2:Z:310:ARG:HA	2.19	0.42
1:B:117:TYR:CZ	2:X:205:HIS:CD2	3.07	0.42
1:D:117:TYR:CE2	2:Z:205:HIS:CD2	2.93	0.42
2:Y:82:TRP:O	2:Y:256:HIS:HD2	2.03	0.42
1:C:48:LYS:NZ	1:C:60:GLU:OE1	2.53	0.42
2:X:64:ASP:O	2:X:68:ARG:HG3	2.20	0.42
1:A:75:HIS:C	1:A:130:ALA:HB2	2.40	0.42
2:W:50:TRP:CE2	2:W:57:ARG:HB2	2.54	0.42
2:W:298:PRO:HD2	2:W:301:ILE:HG12	2.02	0.42
2:Y:16:ASP:HB3	2:Y:124:LEU:HD13	2.01	0.42
2:X:233:SER:O	2:X:245:PRO:HD2	2.19	0.42
1:A:81:VAL:HG21	1:A:120:LEU:HB2	2.01	0.42
2:W:68:ARG:NH2	5:W:507:HOH:O	2.36	0.42
1:A:57:TYR:CZ	2:W:240:ALA:HB3	2.55	0.41
1:C:48:LYS:HZ2	1:C:103:THR:CG2	2.31	0.41
2:W:248:GLU:O	2:W:310:ARG:HA	2.20	0.41
2:W:256:HIS:O	2:W:302:ARG:HA	2.20	0.41
2:X:252:LEU:HA	2:X:253:PRO:HD3	1.91	0.41
2:X:256:HIS:HD2	2:X:257:GLY:H	1.67	0.41
2:W:24:HIS:CE1	2:W:26:VAL:H	2.38	0.41
2:X:87[B]:HIS:H	2:X:87[B]:HIS:HD2	1.66	0.41
2:Y:91:THR:HA	2:Y:99:ASP:O	2.19	0.41
2:Z:122:THR:HB	2:Z:123:PRO:HD3	2.03	0.41
2:Z:50:TRP:CE2	2:Z:57:ARG:HB2	2.55	0.41
2:Z:24:HIS:CE1	2:Z:26:VAL:H	2.37	0.41
1:C:101:GLU:HG2	1:C:149:ILE:HD12	2.01	0.41
1:C:158:TRP:CD1	2:Y:337:ILE:HG21	2.55	0.41
1:D:158:TRP:CG	2:Z:337:ILE:HG21	2.55	0.41
2:Z:323:LEU:N	2:Z:324:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:O	1:A:32:ALA:C	2.59	0.41
2:Z:96:GLY:O	2:Z:97:LYS:HG3	2.21	0.41
1:A:80:ILE:HG22	1:A:82:MET:HE2	2.03	0.41
1:C:29:ARG:HG2	5:Y:511:HOH:O	2.21	0.41
1:D:102:GLY:O	1:D:104:HIS:CD2	2.74	0.41
2:Y:301:ILE:HD12	2:Y:301:ILE:C	2.42	0.41
2:Z:85:PHE:N	2:Z:85:PHE:CD1	2.88	0.41
2:Z:175:MET:HG2	2:Z:176:PRO:CD	2.50	0.41
1:C:98:LYS:NZ	1:C:98:LYS:HB3	2.35	0.41
2:Z:306:TYR:N	2:Z:306:TYR:CD1	2.89	0.41
2:X:301:ILE:HD12	2:X:301:ILE:C	2.41	0.40
2:Y:210:PHE:HD2	2:Y:213:GLU:HG3	1.86	0.40
1:C:55:LEU:CD2	2:Y:332:LEU:HD11	2.50	0.40
1:D:127:LEU:HD12	1:D:128:LEU:N	2.36	0.40
1:B:162:CYS:O	1:B:164:LYS:HE3	2.22	0.40
1:D:91:LEU:HA	1:D:91:LEU:HD23	1.90	0.40
2:W:280:ASP:N	2:W:280:ASP:OD2	2.53	0.40
1:A:81:VAL:HG21	1:A:120:LEU:CB	2.52	0.40
1:A:117:TYR:CE2	2:W:205:HIS:HD2	2.39	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	162/168 (96%)	158 (98%)	4 (2%)	0	100	100
1	B	161/168 (96%)	157 (98%)	4 (2%)	0	100	100
1	C	162/168 (96%)	157 (97%)	5 (3%)	0	100	100
1	D	161/168 (96%)	156 (97%)	5 (3%)	0	100	100
2	W	324/339 (96%)	307 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	323/339 (95%)	304 (94%)	19 (6%)	0	100	100
2	Y	323/339 (95%)	306 (95%)	17 (5%)	0	100	100
2	Z	323/339 (95%)	305 (94%)	18 (6%)	0	100	100
All	All	1939/2028 (96%)	1850 (95%)	89 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	134/136 (98%)	126 (94%)	8 (6%)	19	34
1	B	133/136 (98%)	125 (94%)	8 (6%)	19	34
1	C	134/136 (98%)	123 (92%)	11 (8%)	11	20
1	D	133/136 (98%)	127 (96%)	6 (4%)	27	48
2	W	276/284 (97%)	261 (95%)	15 (5%)	22	40
2	X	275/284 (97%)	255 (93%)	20 (7%)	14	25
2	Y	275/284 (97%)	258 (94%)	17 (6%)	18	33
2	Z	275/284 (97%)	257 (94%)	18 (6%)	17	31
All	All	1635/1680 (97%)	1532 (94%)	103 (6%)	18	32

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	97	SER
1	A	103	THR
1	A	113	LYS
1	A	119	LEU
1	A	150	LYS
1	A	153	LEU
1	A	157	LYS

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Mol	Chain	Res	Type
1	B	2	SER
1	B	17	ARG
1	B	87	ARG
1	B	91	LEU
1	B	103	THR
1	B	137	GLU
1	B	140	ARG
1	B	153	LEU
1	C	22	GLU
1	C	85	GLU
1	C	97	SER
1	C	98	LYS
1	C	103	THR
1	C	119	LEU
1	C	121	LYS
1	C	137	GLU
1	C	150	LYS
1	C	153	LEU
1	C	157	LYS
1	D	91	LEU
1	D	103	THR
1	D	135	ARG
1	D	139	SER
1	D	153	LEU
1	D	157	LYS
2	W	38	GLU
2	W	57	ARG
2	W	60	LEU
2	W	79	PHE
2	W	140	THR
2	W	144	PHE
2	W	161	ASN
2	W	179	GLN
2	W	192	ARG
2	W	248	GLU
2	W	274	ASP
2	W	277	ASP
2	W	282	ASN
2	W	303	HIS
2	W	323	LEU
2	X	16	ASP
2	X	48	ILE

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Mol	Chain	Res	Type
2	X	53	LYS
2	X	60	LEU
2	X	79	PHE
2	X	97	LYS
2	X	140	THR
2	X	144	PHE
2	X	161	ASN
2	X	163	GLU
2	X	169	ARG
2	X	192	ARG
2	X	233	SER
2	X	246	THR
2	X	248	GLU
2	X	262	GLU
2	X	268	SER
2	X	279	ASP
2	X	323	LEU
2	X	338	GLU
2	Y	16	ASP
2	Y	48	ILE
2	Y	57	ARG
2	Y	73	ASP
2	Y	79	PHE
2	Y	92	ARG
2	Y	144	PHE
2	Y	161	ASN
2	Y	179	GLN
2	Y	192	ARG
2	Y	211	GLU
2	Y	248	GLU
2	Y	255	PHE
2	Y	268	SER
2	Y	284	ARG
2	Y	323	LEU
2	Y	332	LEU
2	Z	16	ASP
2	Z	17	ASP
2	Z	58	SER
2	Z	60	LEU
2	Z	92	ARG
2	Z	108	THR
2	Z	134	ARG

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Mol	Chain	Res	Type
2	Z	144	PHE
2	Z	179	GLN
2	Z	192	ARG
2	Z	211	GLU
2	Z	229	THR
2	Z	248	GLU
2	Z	277	ASP
2	Z	280	ASP
2	Z	302	ARG
2	Z	303	HIS
2	Z	323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	42	ASN
1	B	41	GLN
1	B	125	GLN
1	C	41	GLN
1	C	42	ASN
1	C	67	GLN
1	C	125	GLN
1	D	104	HIS
1	D	125	GLN
2	W	19	GLN
2	W	84	ASN
2	W	161	ASN
2	W	205	HIS
2	W	325	HIS
2	X	84	ASN
2	X	161	ASN
2	X	205	HIS
2	X	322	ASN
2	Y	84	ASN
2	Y	161	ASN
2	Z	84	ASN
2	Z	119	ASN
2	Z	179	GLN
2	Z	205	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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	H8N	X	402	3	9,9,9	1.02	1 (11%)	11,11,11	0.87	0
4	H8N	W	402	3	9,9,9	0.80	1 (11%)	11,11,11	0.90	0
4	H8N	Y	402	3	9,9,9	0.86	1 (11%)	11,11,11	1.02	0
4	H8N	Z	402	3	9,9,9	0.82	1 (11%)	11,11,11	1.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H8N	X	402	3	-	0/2/2/2	0/1/1/1
4	H8N	W	402	3	-	0/2/2/2	0/1/1/1
4	H8N	Y	402	3	-	0/2/2/2	0/1/1/1
4	H8N	Z	402	3	-	0/2/2/2	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	402	H8N	CAI-CAC	2.50	1.50	1.44
4	Z	402	H8N	CAI-CAC	2.36	1.49	1.44
4	W	402	H8N	CAI-CAC	2.30	1.49	1.44
4	Y	402	H8N	CAI-CAC	2.11	1.49	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	163/168 (97%)	-0.62	0 100 100	21, 31, 46, 61	0
1	B	163/168 (97%)	-0.34	2 (1%) 79 80	25, 40, 58, 70	0
1	C	163/168 (97%)	-0.36	2 (1%) 79 80	24, 38, 63, 87	0
1	D	163/168 (97%)	-0.59	1 (0%) 89 90	22, 32, 50, 70	0
2	W	324/339 (95%)	-0.51	1 (0%) 94 94	18, 28, 48, 72	0
2	X	324/339 (95%)	-0.36	4 (1%) 79 80	18, 30, 58, 90	0
2	Y	324/339 (95%)	-0.37	0 100 100	17, 29, 51, 74	0
2	Z	324/339 (95%)	-0.50	1 (0%) 94 94	20, 30, 52, 74	0
All	All	1948/2028 (96%)	-0.45	11 (0%) 89 90	17, 31, 54, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	5.6
2	X	16	ASP	4.2
2	X	208	GLU	3.4
2	W	280	ASP	3.1
1	C	99	HIS	2.8
1	D	3	ASN	2.2
2	Z	211	GLU	2.2
1	B	117	TYR	2.1
1	B	109	LEU	2.1
2	X	211	GLU	2.1
2	X	212	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	H8N	Z	402	9/9	0.96	0.12	26,28,32,33	0
4	H8N	X	402	9/9	0.97	0.15	17,29,32,33	0
4	H8N	Y	402	9/9	0.97	0.18	13,24,31,36	0
3	CD	Y	401	1/1	0.97	0.09	55,55,55,55	0
3	CD	X	401	1/1	0.99	0.07	49,49,49,49	0
3	CD	Z	401	1/1	0.99	0.08	31,31,31,31	0
4	H8N	W	402	9/9	0.99	0.12	21,23,26,26	0
3	CD	W	401	1/1	1.00	0.07	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.