



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:39 PM UTC

PDB ID : 4ZXA / pdb_00004zxa
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

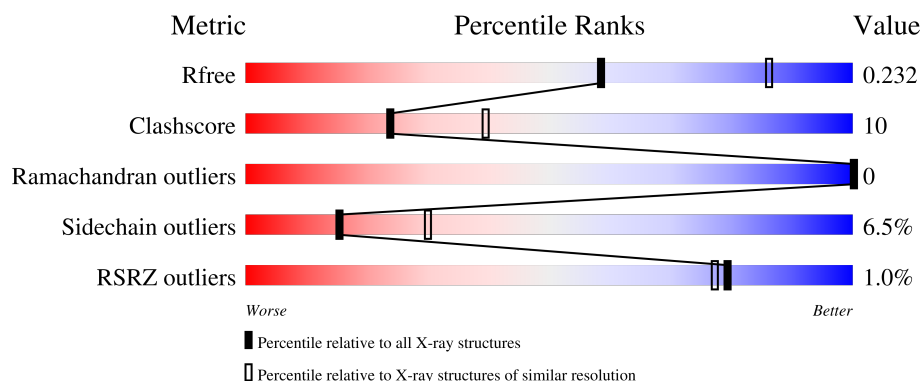
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 $\leq 5\%$. 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	% 79% 16% ..
1	B	168	% 73% 21% ..
1	C	168	2% 71% 23% ..
1	D	168	% 74% 20% ..
2	W	339	% 78% 15% ..

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Mol	Chain	Length	Quality of chain
2	X	339	% 71%22%••
2	Y	339	% 80%13%••
2	Z	339	% 73%20%••

2 Entry composition

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

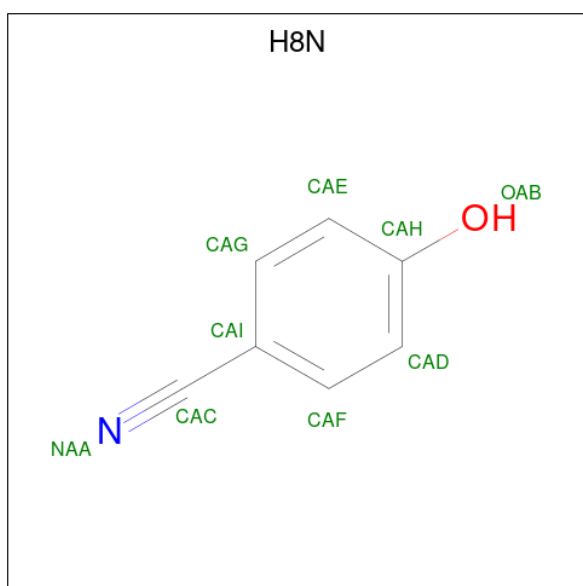
- Molecule 2 is a protein called Hydroquinone dioxygenase large subunit.

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 (CCD ID: 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 (CCD ID: H8N) (formula: C₇H₅NO).



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	0	0
			9	7	1	1		
4	Z	1	Total	C	N	O	0	0
			9	7	1	1		

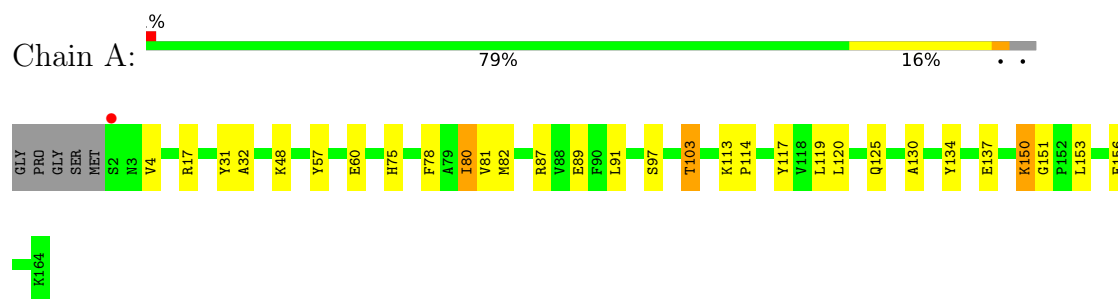
- Molecule 5 is water.

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

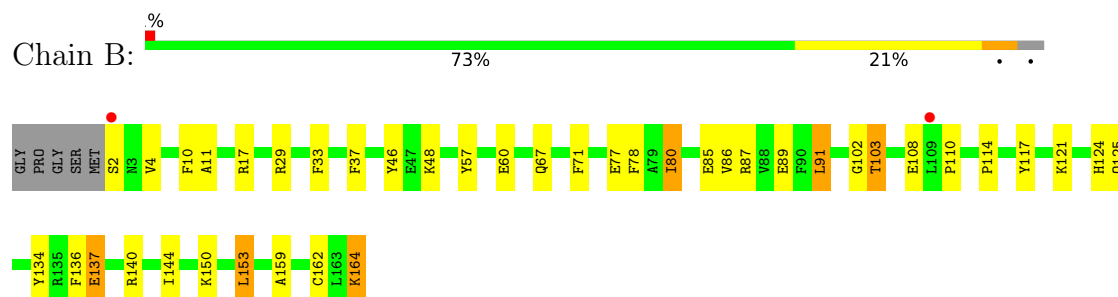
3 Residue-property plots [i](#)

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.

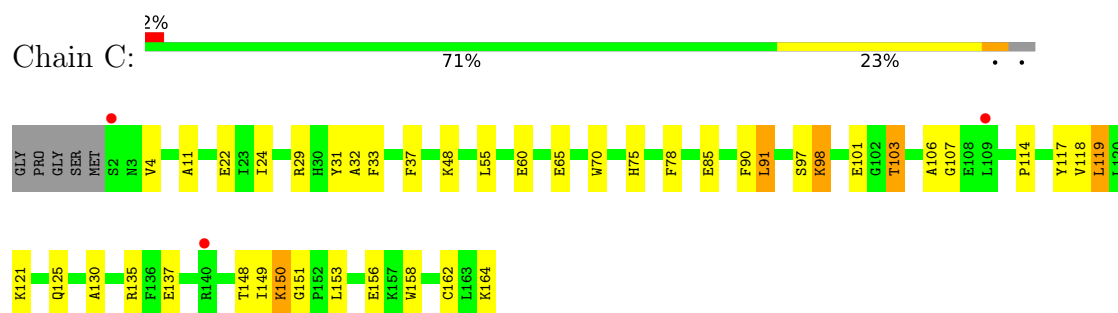
- Molecule 1: Hydroquinone dioxygenase small subunit



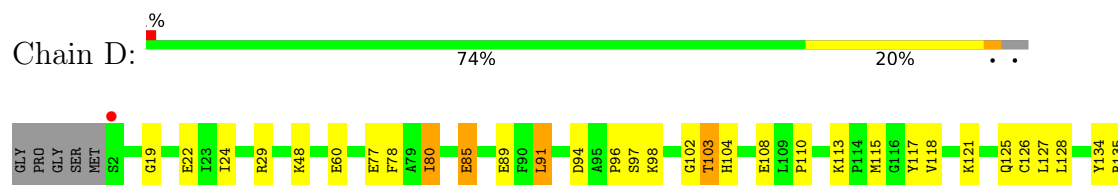
- Molecule 1: Hydroquinone dioxygenase small subunit



- Molecule 1: Hydroquinone dioxygenase small subunit

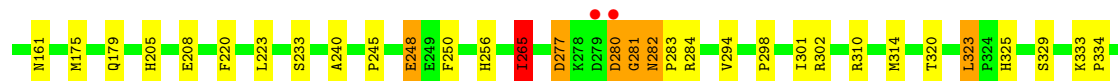
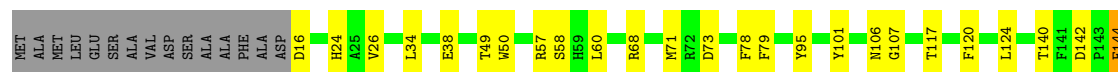
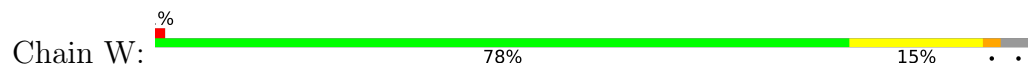


- Molecule 1: Hydroquinone dioxygenase small subunit





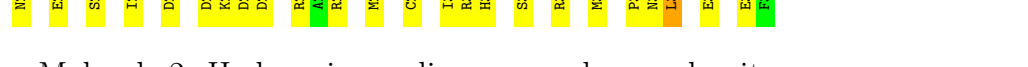
• Molecule 2: Hydroquinone dioxygenase large subunit



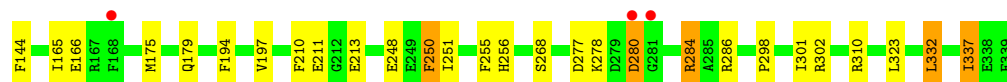
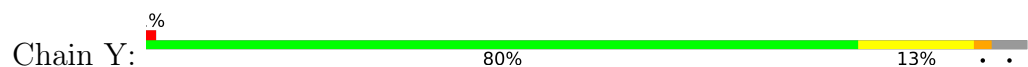
• Molecule 2: Hydroquinone dioxygenase large subunit



• Molecule 2: Hydroquinone dioxygenase large subunit

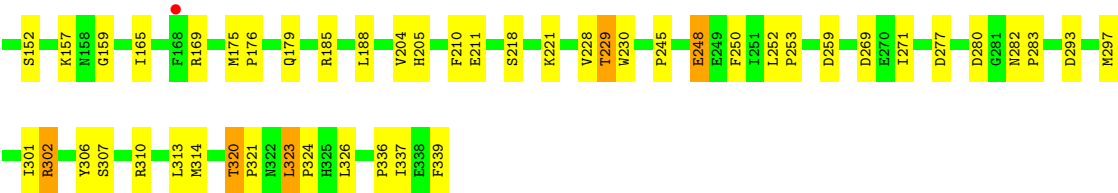


• Molecule 2: Hydroquinone dioxygenase large subunit



• 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	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) 99.4 (40.73-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.186 , 0.237 0.182 , 0.232	Depositor DCC
R_{free} test set	4607 reflections (4.98%)	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 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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 ⓘ

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	0.49	0/1298	0.85	2/1757 (0.1%)
1	B	0.45	0/1290	0.80	0/1746
1	C	0.47	0/1301	0.82	3/1761 (0.2%)
1	D	0.49	0/1290	0.83	0/1746
2	W	0.50	0/2698	0.87	7/3666 (0.2%)
2	X	0.49	0/2689	0.82	2/3654 (0.1%)
2	Y	0.50	0/2689	0.88	3/3654 (0.1%)
2	Z	0.49	0/2687	0.89	6/3651 (0.2%)
All	All	0.49	0/15942	0.85	23/21635 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	280	ASP	N-CA-C	8.79	120.94	111.36
2	Y	79	PHE	CB-CA-C	-6.66	108.90	116.63
2	W	142	ASP	CA-C-N	6.58	126.27	119.82
2	W	142	ASP	C-N-CA	6.58	126.27	119.82
2	Z	95	TYR	N-CA-C	6.47	120.58	111.52
1	C	151	GLY	CA-C-N	6.45	126.03	119.19
1	C	151	GLY	C-N-CA	6.45	126.03	119.19
2	Z	250	PHE	CB-CA-C	-5.85	109.84	116.63
2	W	281	GLY	N-CA-C	-5.82	107.29	115.32
1	C	24	ILE	N-CA-C	-5.64	106.31	111.67
2	X	79	PHE	CB-CA-C	-5.61	108.49	116.34
2	W	250	PHE	CB-CA-C	-5.50	110.25	116.63
2	Y	250	PHE	CB-CA-C	-5.39	110.38	116.63
2	W	95	TYR	N-CA-C	5.25	118.87	111.52
1	A	151	GLY	CA-C-N	5.17	124.97	119.28
1	A	151	GLY	C-N-CA	5.17	124.97	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	320	THR	CA-C-N	5.17	124.97	119.28
2	Z	320	THR	C-N-CA	5.17	124.97	119.28
2	X	250	PHE	CB-CA-C	-5.14	110.67	116.63
2	W	265	ILE	CB-CA-C	-5.10	104.36	110.99
2	Z	297	MET	CA-C-N	5.09	126.20	119.84
2	Z	297	MET	C-N-CA	5.09	126.20	119.84
2	W	337	ILE	N-CA-C	5.08	115.43	108.12

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	29	0
1	B	1261	0	1259	37	0
1	C	1272	0	1272	33	0
1	D	1261	0	1259	38	0
2	W	2620	0	2472	36	0
2	X	2611	0	2467	72	0
2	Y	2611	0	2467	41	0
2	Z	2610	0	2466	75	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	117	0	0	5	0
5	Z	119	0	0	4	0
All	All	16274	0	14946	308	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 10.

All (308) 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:X:71:MET:HE1	2:X:165:ILE:HA	1.31	1.11
1:B:48:LYS:HE2	1:B:103:THR:HG21	1.45	0.98
1:B:125:GLN:HE21	2:X:175:MET:HE2	1.30	0.97
1:A:125:GLN:HE21	2:W:175:MET:HE2	1.35	0.91
2:X:170:ILE:HD12	2:X:170:ILE:H	1.40	0.86
1:D:125:GLN:HE21	2:Z:175:MET:HE2	1.42	0.84
2:Z:229:THR:HG23	2:Z:230:TRP:CD1	2.13	0.83
2:Z:71:MET:HE1	2:Z:165:ILE:HA	1.59	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:X:71:MET:HE3	2:X:144:PHE:CD1	2.16	0.80
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:117:TYR:CE2	2:Z:205:HIS:HD2	2.02	0.76
1:D:78:PHE:CD1	2:Z:175:MET:HE3	2.20	0.76
1:C:48:LYS:NZ	1:C:103:THR:HG21	2.02	0.74
1:C:125:GLN:HE21	2:Y:175:MET:HE2	1.53	0.73
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:78:PHE:HD1	2:Z:175:MET:HE3	1.56	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
1:D:127:LEU:N	2:Z:175:MET:HE1	2.08	0.68
1:A:82:MET:HA	1:A:82:MET:HE2	1.74	0.68
1:A:82:MET:HE1	2:W:220:PHE:CZ	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:331:GLU:OE1	5:X:502:HOH:O	2.11	0.68
2:Z:70:MET:HE1	2:Z:132:ILE:CG2	2.24	0.68
1:B:78:PHE:CE1	2:X:175:MET:HE3	2.29	0.67
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: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
1:D:126:CYS:C	2:Z:175:MET:HE1	2.22	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
2:Z:71:MET:HE1	2:Z:165:ILE:CA	2.29	0.63
1:A:78:PHE:CE1	2:W:175:MET:HE3	2.34	0.62
1:B:78:PHE:CD1	2:X:175:MET:HE3	2.35	0.62
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
1:A:78:PHE:CD1	2:W:175:MET:HE3	2.37	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
2:X:245:PRO:HG3	2:X:314:MET:HE1	1.85	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:336:PRO:C	2:Z:337:ILE:HD12	2.29	0.57
2:Z:337:ILE:HG22	2:Z:339:PHE:HD2	1.69	0.57
1:C:78:PHE:CE1	2:Y:175:MET:HE3	2.40	0.57
1:B:46:TYR:CE1	1:B:136:PHE:HB2	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:X:256:HIS:CD2	2:X:257:GLY:N	2.73	0.56
2:X:277:ASP:CG	2:X:284:ARG:HH21	2.13	0.56
1:B:71:PHE:HB2	1:B:134:TYR:CE2	2.41	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:Z:301:ILE:C	2:Z:301:ILE:HD12	2.33	0.53
2:Y:165:ILE:HG13	2:Y:166:GLU:HG3	1.89	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)
1:A:87:ARG:HH12	1:A:89:GLU:CD	2.17	0.52
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:Y:66:PHE:CE1	2:Y:70:MET:HE2	2.45	0.52
2:W:223:LEU:HD21	2:W:245:PRO:HB2	1.93	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:Z:71:MET:HE1	2:Z:165:ILE:CB	2.40	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
1:C:78:PHE:HE1	2:Y:175:MET:HE3	1.76	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:C:70:TRP:NE1	1:C:135:ARG:HH11	2.09	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
1:C:78:PHE:HD1	2:Y:175:MET:CE	2.25	0.49
1:D:78:PHE:CE1	2:Z:175:MET:HE3	2.47	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
1:D:125:GLN:NE2	2:Z:175:MET:HE2	2.21	0.49
2:X:164:CYS:O	2:X:167:ARG:NH1	2.45	0.49
2:Z:70:MET:HE1	2:Z:132:ILE:HG21	1.92	0.49
1:A:80:ILE:HG22	1:A:82:MET:HE3	1.96	0.48
1:B:77:GLU:OE2	1:B:103:THR:HB	2.13	0.48
1:C:31:TYR:O	1:C:32:ALA:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:ILE:CG2	1:A:82:MET:HE3	2.42	0.48
1:D:48:LYS:HE2	1:D:103:THR:HG21	1.96	0.48
1:A:82:MET:HE1	2:W:220:PHE:CE1	2.48	0.48
2:Z:336:PRO:CB	2:Z:337:ILE:HD12	2.42	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:A:75:HIS:C	1:A:130:ALA:HB2	2.40	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: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: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:A:31:TYR:O	1:A:32:ALA:C	2.59	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
2:Y:301:ILE:HD12	2:Y:301:ILE:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PHE:CD1	2:W:175:MET:CE	2.99	0.45
1:A:78:PHE:HD1	2:W:175:MET:CE	2.29	0.45
2:X:192:ARG:NH1	2:X:193:GLN:HG3	2.32	0.45
2:X:71:MET:HE3	2:X:144:PHE:HD1	1.76	0.45
2:X:301:ILE:C	2:X:301:ILE:HD12	2.41	0.45
1:B:78:PHE:HE1	2:X:175:MET:HE3	1.76	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
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
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
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:W:71:MET:HE2	2:W:144:PHE:CE1	2.53	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:C:75:HIS:C	1:C:130:ALA:HB2	2.43	0.44
1:A:4:VAL:O	1:A:4:VAL:CG1	2.66	0.44
1:B:10:PHE:CE1	2:X:220:PHE:CE2	3.06	0.44
2:X:207:ALA:O	2:X:208:GLU:C	2.61	0.44
2:Y:90:GLY:HA3	2:Y:101:TYR:CE2	2.52	0.44
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
2:Y:70:MET:HE3	2:Y:132:ILE:CG2	2.48	0.43
1:A:89:GLU:O	1:A:134:TYR:HA	2.18	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
1:D:94:ASP:C	1:D:96:PRO:HD3	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:138:ASN:C	2:X:140:THR:H	2.25	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:24:ILE:HG21	2:Z:283:PRO:HB2	2.01	0.43
2:Z:71:MET:CE	2:Z:165:ILE:HA	2.42	0.43
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:W:106:ASN:O	2:W:107:GLY:C	2.61	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
2:Z:71:MET:HE1	2:Z:165:ILE:HG22	2.01	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
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
2:X:71:MET:CE	2:X:165:ILE:HA	2.24	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:W:277:ASP:CG	2:W:284:ARG:NH1	2.77	0.41
2:X:252:LEU:HA	2:X:253:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:256:HIS:HD2	2:X:257:GLY:H	1.67	0.41
2:X:289:MET:HE3	2:X:295:CYS:HB2	2.01	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
2:Z:96:GLY:O	2:Z:97:LYS:HG3	2.21	0.41
1:B:108:GLU:C	1:B:110:PRO:HD3	2.46	0.41
1:C:29:ARG:HG2	5:Y:511:HOH:O	2.21	0.41
1:D:91:LEU:HD23	1:D:113:LYS:C	2.46	0.41
1:D:102:GLY:O	1:D:104:HIS:CD2	2.74	0.41
1:D:125:GLN:HG2	2:Z:175:MET:HE2	2.02	0.41
2:W:245:PRO:HG3	2:W:314:MET:HE1	2.03	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: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:HD23	1:D:91:LEU:HA	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 ⓘ

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	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
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 ⓘ

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%)	17	33
1	B	133/136 (98%)	122 (92%)	11 (8%)	10	20
1	C	134/136 (98%)	123 (92%)	11 (8%)	10	21
1	D	133/136 (98%)	121 (91%)	12 (9%)	9	17
2	W	276/284 (97%)	262 (95%)	14 (5%)	21	40
2	X	275/284 (97%)	255 (93%)	20 (7%)	13	25
2	Y	275/284 (97%)	259 (94%)	16 (6%)	18	35
2	Z	275/284 (97%)	261 (95%)	14 (5%)	21	40
All	All	1635/1680 (97%)	1529 (94%)	106 (6%)	15	30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	80	ILE
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	B	2	SER
1	B	17	ARG
1	B	80	ILE
1	B	87	ARG
1	B	91	LEU
1	B	103	THR
1	B	137	GLU
1	B	140	ARG
1	B	150	LYS
1	B	153	LEU
1	B	164	LYS
1	C	22	GLU
1	C	85	GLU
1	C	91	LEU
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	D	80	ILE
1	D	85	GLU
1	D	91	LEU
1	D	97	SER
1	D	98	LYS
1	D	103	THR
1	D	108	GLU
1	D	135	ARG
1	D	139	SER
1	D	150	LYS
1	D	153	LEU
1	D	157	LYS
2	W	38	GLU

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Mol	Chain	Res	Type
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	208	GLU
2	W	248	GLU
2	W	265	ILE
2	W	277	ASP
2	W	280	ASP
2	W	282	ASN
2	W	323	LEU
2	X	16	ASP
2	X	48	ILE
2	X	53	LYS
2	X	60	LEU
2	X	79	PHE
2	X	92	ARG
2	X	97	LYS
2	X	140	THR
2	X	144	PHE
2	X	161	ASN
2	X	163	GLU
2	X	221	LYS
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	79	PHE
2	Y	92	ARG
2	Y	130	LYS
2	Y	144	PHE
2	Y	179	GLN
2	Y	211	GLU

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Mol	Chain	Res	Type
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	Y	337	ILE
2	Z	16	ASP
2	Z	17	ASP
2	Z	58	SER
2	Z	60	LEU
2	Z	108	THR
2	Z	134	ARG
2	Z	144	PHE
2	Z	179	GLN
2	Z	211	GLU
2	Z	229	THR
2	Z	248	GLU
2	Z	280	ASP
2	Z	302	ARG
2	Z	323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	C	125	GLN
1	D	42	ASN
1	D	99	HIS
1	D	104	HIS
2	W	84	ASN
2	W	161	ASN
2	W	205	HIS
2	W	215	HIS
2	W	325	HIS
2	X	84	ASN
2	X	161	ASN
2	X	205	HIS
2	X	256	HIS
2	X	322	ASN
2	X	325	HIS
2	Y	84	ASN

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Mol	Chain	Res	Type
2	Y	119	ASN
2	Y	161	ASN
2	Y	179	GLN
2	Y	325	HIS
2	Z	84	ASN
2	Z	87	HIS
2	Z	119	ASN
2	Z	158	ASN
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 oligosaccharides 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	W	402	3	9,9,9	0.84	1 (11%)	11,11,11	0.94	0
4	H8N	Z	402	3	9,9,9	0.86	1 (11%)	11,11,11	1.19	1 (9%)
4	H8N	X	402	3	9,9,9	1.06	1 (11%)	11,11,11	0.91	0
4	H8N	Y	402	3	9,9,9	0.91	1 (11%)	11,11,11	1.06	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	W	402	3	-	0/2/2/2	0/1/1/1
4	H8N	Z	402	3	-	0/2/2/2	0/1/1/1
4	H8N	X	402	3	-	0/2/2/2	0/1/1/1
4	H8N	Y	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	2.63	1.50	1.44
4	Z	402	H8N	CAI-CAC	2.48	1.49	1.44
4	W	402	H8N	CAI-CAC	2.42	1.49	1.44
4	Y	402	H8N	CAI-CAC	2.21	1.49	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	402	H8N	CAG-CAI-CAF	2.01	122.42	118.96

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	163/168 (97%)	-0.34	1 (0%) 85 83	14, 31, 46, 61	1 (0%)
1	B	163/168 (97%)	-0.09	2 (1%) 76 74	25, 40, 58, 70	0
1	C	163/168 (97%)	-0.02	3 (1%) 67 65	22, 37, 63, 87	1 (0%)
1	D	163/168 (97%)	-0.28	1 (0%) 85 83	22, 32, 50, 70	0
2	W	324/339 (95%)	-0.53	2 (0%) 85 83	12, 28, 48, 72	2 (0%)
2	X	324/339 (95%)	-0.38	5 (1%) 72 69	13, 30, 58, 90	1 (0%)
2	Y	324/339 (95%)	-0.41	4 (1%) 76 74	14, 29, 51, 74	1 (0%)
2	Z	324/339 (95%)	-0.38	2 (0%) 85 83	13, 30, 52, 74	1 (0%)
All	All	1948/2028 (96%)	-0.34	20 (1%) 79 77	12, 31, 54, 90	7 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	168	PHE	3.5
2	Y	87[A]	HIS	3.1
2	W	280	ASP	3.0
1	C	140[A]	ARG	2.9
2	X	16	ASP	2.8
1	A	2	SER	2.8
1	C	2	SER	2.7
1	D	2	SER	2.6
2	X	94	TYR	2.5
2	Y	280	ASP	2.5
2	X	168	PHE	2.4
2	Z	16	ASP	2.3
1	B	2	SER	2.3
2	W	279	ASP	2.2
2	X	280	ASP	2.2
1	C	109	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	Z	168	PHE	2.1
1	B	109	LEU	2.0
2	Y	281	GLY	2.0
2	X	95	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 oligosaccharides 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, 95th 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	X	402	9/9	0.95	0.12	17,29,32,33	0
4	H8N	Y	402	9/9	0.95	0.11	13,24,31,36	0
4	H8N	W	402	9/9	0.97	0.07	21,23,26,26	0
4	H8N	Z	402	9/9	0.97	0.09	26,28,32,33	0
3	CD	Y	401	1/1	0.99	0.02	55,55,55,55	0
3	CD	Z	401	1/1	0.99	0.02	31,31,31,31	0
3	CD	X	401	1/1	0.99	0.02	49,49,49,49	0
3	CD	W	401	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.