Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:29 PM GMT

PDB ID	:	4ZXC
Title	:	Crystal Structure of hydroquinone 1,2-dioxygenase PnpCD in complex with Fe3+
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

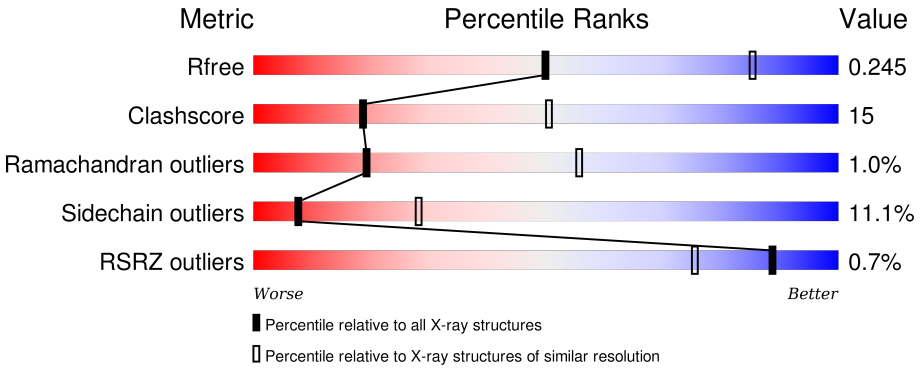
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	69% 24%
1	B	168	% 57% 33% 7%
1	C	168	% 74% 18% 5%
1	D	168	64% 30%
2	W	339	71% 21%

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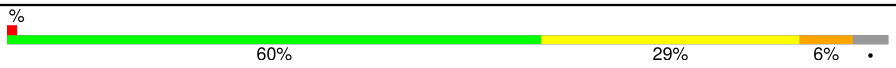
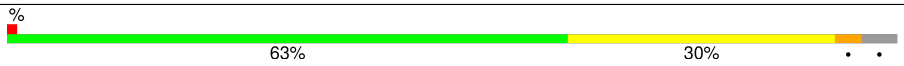
Mol	Chain	Length	Quality of chain
2	X	339	
2	Y	339	
2	Z	339	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15554 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	0	0
			1261	808	217	232	4			
1	D	163	Total	C	N	O	S	0	0	0
			1261	808	217	232	4			
1	C	163	Total	C	N	O	S	0	0	0
			1261	808	217	232	4			
1	B	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	0	0
			2601	1657	444	487	13			
2	Z	324	Total	C	N	O	S	0	0	0
			2601	1657	444	487	13			
2	Y	324	Total	C	N	O	S	0	0	0
			2601	1657	444	487	13			
2	X	324	Total	C	N	O	S	0	0	0
			2601	1657	444	487	13			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	W	1	Total	Fe	0	0
			1	1		
3	Z	1	Total	Fe	0	0
			1	1		

- Molecule 4 is water.

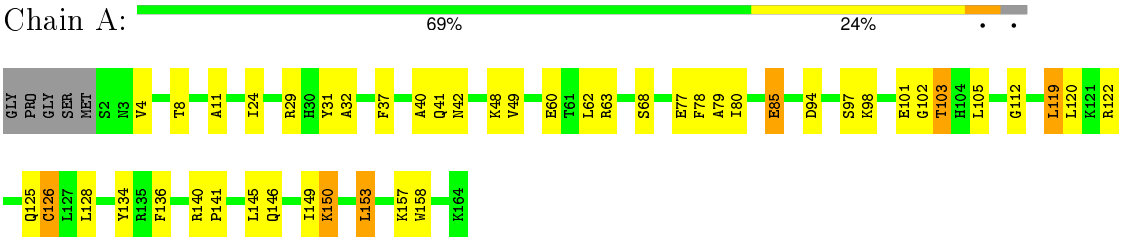
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	D	9	Total	O	0	0
			9	9		
4	C	9	Total	O	0	0
			9	9		
4	B	1	Total	O	0	0
			1	1		
4	W	20	Total	O	0	0
			20	20		
4	Z	16	Total	O	0	0
			16	16		
4	Y	18	Total	O	0	0
			18	18		
4	X	23	Total	O	0	0
			23	23		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

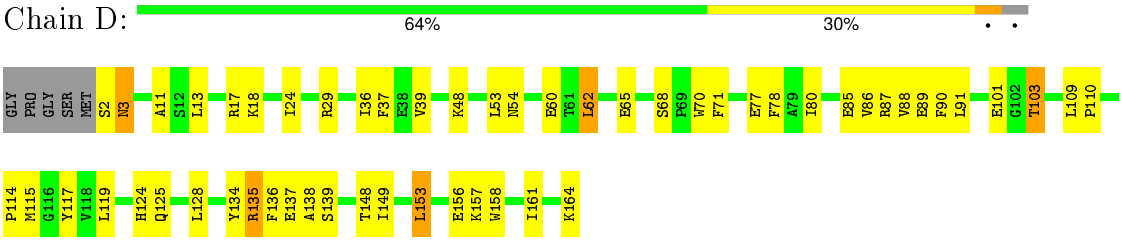
- Molecule 1: Hydroquinone dioxygenase small subunit

Chain A:



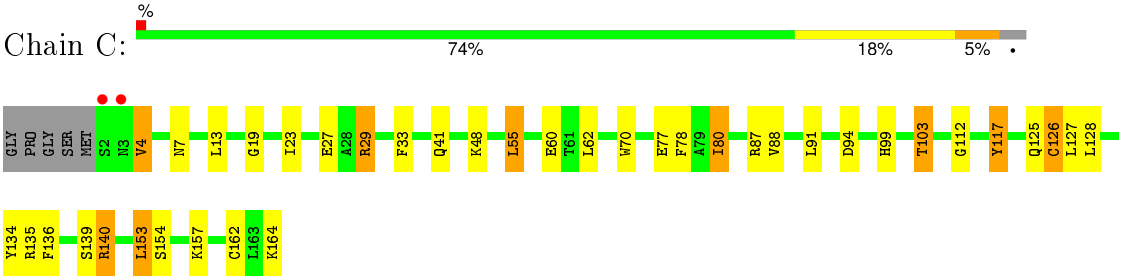
- Molecule 1: Hydroquinone dioxygenase small subunit

Chain D:



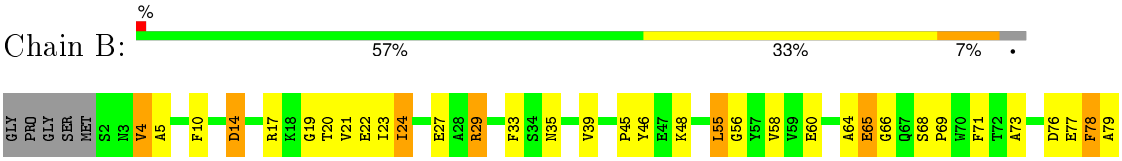
- Molecule 1: Hydroquinone dioxygenase small subunit

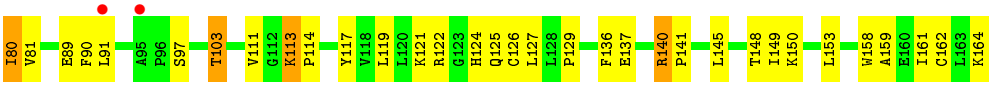
Chain C:



- Molecule 1: Hydroquinone dioxygenase small subunit

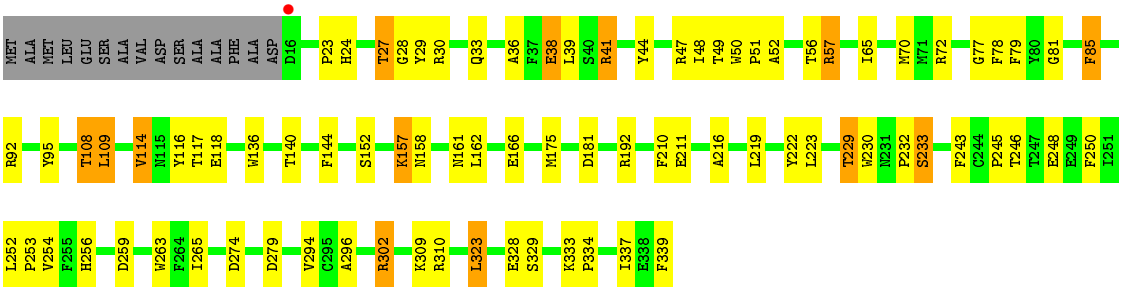
Chain B:





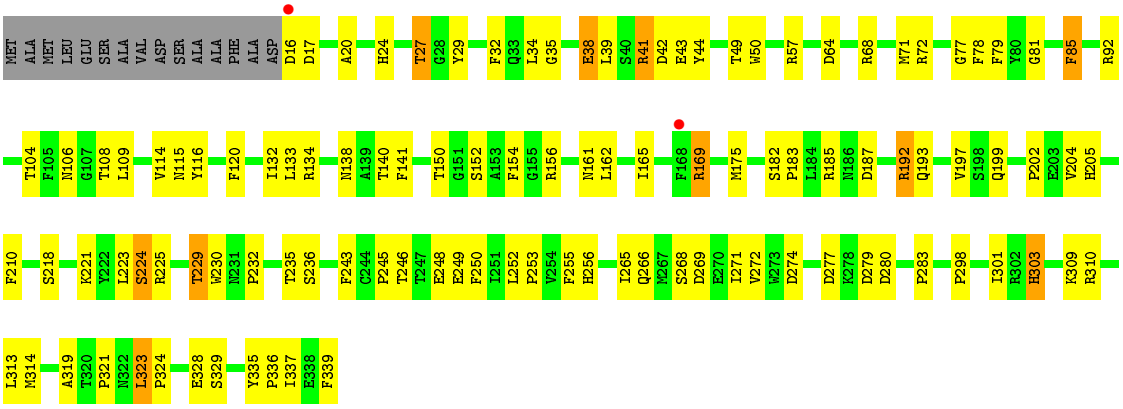
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain W:



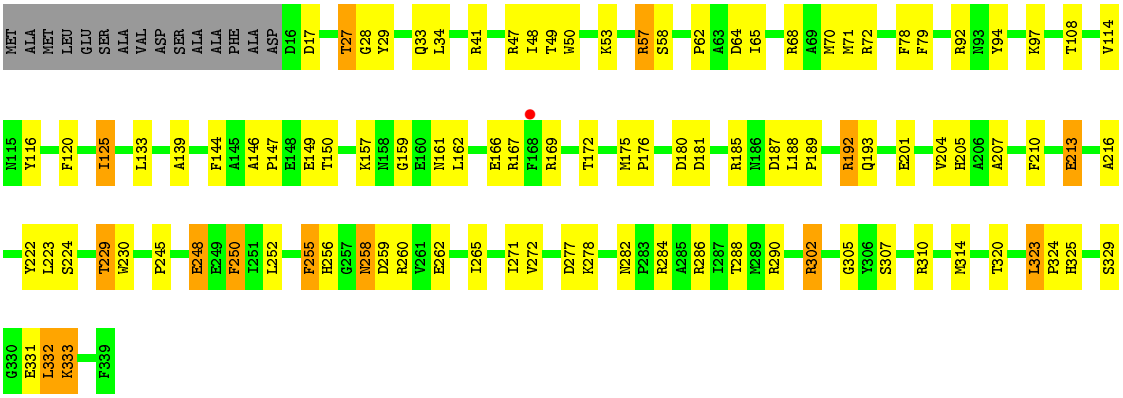
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain Z:



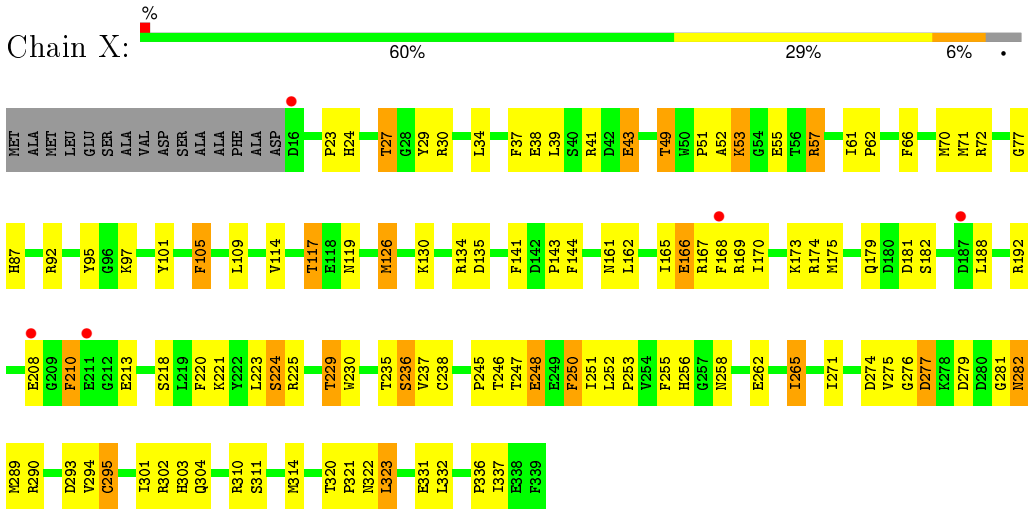
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain Y:



• Molecule 2: Hydroquinone dioxygenase large subunit

Chain X:


%
60%
29%
6%
MET ALA MET LEU GLU SER ALA VAL ASP SER ALA ALA PHE ALA ASP D16 P23 H24 T27 G28 Y29 R30 L34 F37 E38 L39 S40 R41 D42 E43 T49 W50 P51 A52 K53 G54 E55 T56 R57 I61 P62 F66 M70 M71 R72 G77 F78 F79 W82
H87 R92 Y95 G96 K97 Y101 F105 L109 V114 T117 E118 N119 M126 K130 R134 D135 F141 D142 P143 F144 N161 L162 I165 E166 R167 F168 R169 I170 K173 R174 M175 Q179 D180 D181 S182 D187 L188 R192 E201 P202 H205
E208 G209 F210 E211 G212 E213 S218 L219 F220 K221 Y222 L223 S224 R225 T229 W230 T235 S236 V237 C238 P245 T246 T247 E248 E249 F250 I251 L252 P253 V254 F255 H256 G257 N258 E262 I265 I271 D274 V275 G276 D277 K278 D279 D280 G281 N282 P283 R284 I287 T288
M289 R290 D293 V294 C295 I301 R302 H303 Q304 R310 S311 M314 T320 P321 N322 L323 E331 L332 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	76.84Å 181.74Å 186.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.12 – 3.05 33.12 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.12-3.05) 98.8 (33.12-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	7.44 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.188 , 0.245 0.188 , 0.245	Depositor DCC
R_{free} test set	2563 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.1	EDS
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 50567 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15554	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FE

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	0.51	0/1290	0.62	0/1746
1	B	0.45	0/1290	0.57	0/1746
1	C	0.51	0/1290	0.60	0/1746
1	D	0.48	0/1290	0.62	0/1746
2	W	0.50	0/2678	0.62	0/3639
2	X	0.52	0/2678	0.65	0/3639
2	Y	0.51	0/2678	0.63	0/3639
2	Z	0.50	0/2678	0.64	0/3639
All	All	0.50	0/15872	0.63	0/21540

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	1261	0	1259	35	0
1	B	1261	0	1259	65	0
1	C	1261	0	1259	34	0
1	D	1261	0	1259	46	0
2	W	2601	0	2461	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	2601	0	2461	135	0
2	Y	2601	0	2461	63	0
2	Z	2601	0	2461	95	0
3	W	1	0	0	0	0
3	Z	1	0	0	0	0
4	A	8	0	0	1	0
4	B	1	0	0	0	0
4	C	9	0	0	2	0
4	D	9	0	0	0	0
4	W	20	0	0	0	0
4	X	23	0	0	0	0
4	Y	18	0	0	1	0
4	Z	16	0	0	1	0
All	All	15554	0	14880	467	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (467) 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:C:29:ARG:HD2	1:C:164:LYS:HE3	1.22	1.13
1:B:48:LYS:HE2	1:B:103:THR:HG21	1.40	1.02
2:X:289:MET:CE	2:X:295:CYS:HB3	1.95	0.95
2:W:27:THR:HG22	2:W:29:TYR:H	1.30	0.93
2:X:105:PHE:HZ	2:X:302:ARG:HD2	1.34	0.93
2:X:27:THR:HG22	2:X:29:TYR:H	1.33	0.91
2:X:275:VAL:HG13	2:X:301:ILE:HD13	1.54	0.90
2:X:105:PHE:CZ	2:X:302:ARG:HD2	2.09	0.87
2:X:258:ASN:OD1	2:X:303:HIS:HE1	1.57	0.87
2:X:289:MET:HE2	2:X:295:CYS:HB3	1.56	0.86
2:Y:27:THR:HG22	2:Y:29:TYR:H	1.37	0.86
1:C:7:ASN:OD1	4:C:201:HOH:O	1.94	0.86
2:X:277:ASP:OD1	2:X:284:ARG:HD3	1.78	0.84
1:A:77:GLU:OE2	1:A:103:THR:HB	1.77	0.84
1:B:117:TYR:CZ	2:X:205:HIS:HD2	1.97	0.82
2:X:52:ALA:O	2:X:53:LYS:HB2	1.78	0.82
1:D:80:ILE:HD13	1:D:125:GLN:HB2	1.61	0.81
1:C:80:ILE:HD13	1:C:125:GLN:HG3	1.61	0.81
2:X:229:THR:HG23	2:X:230:TRP:CD1	2.16	0.81
1:C:29:ARG:CD	1:C:164:LYS:HE3	2.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:229:THR:HG23	2:Z:230:TRP:HD1	1.46	0.80
2:Z:252:LEU:HD12	2:Z:253:PRO:HD2	1.62	0.80
2:Z:229:THR:HG23	2:Z:230:TRP:CD1	2.17	0.80
1:A:48:LYS:HE2	1:A:103:THR:HG21	1.63	0.78
2:Y:27:THR:CG2	2:Y:29:TYR:H	1.97	0.77
2:Z:169:ARG:CG	2:Z:169:ARG:HH11	1.98	0.77
2:X:101:TYR:HB3	2:X:117:THR:HG23	1.65	0.76
2:Z:72:ARG:HH21	2:Z:229:THR:HG22	1.51	0.76
2:Z:27:THR:HG23	2:Z:29:TYR:CD2	2.21	0.75
2:X:82:TRP:CZ3	2:X:105:PHE:HB2	2.22	0.75
2:X:52:ALA:O	2:X:57:ARG:HD3	1.87	0.74
1:B:48:LYS:HE2	1:B:103:THR:CG2	2.16	0.74
2:X:27:THR:HG23	2:X:29:TYR:HD2	1.53	0.74
2:X:265:ILE:HG23	2:X:294:VAL:HG22	1.69	0.73
2:W:265:ILE:HD13	2:W:294:VAL:HG22	1.70	0.73
2:Y:333:LYS:N	2:Y:333:LYS:HD3	2.04	0.72
2:Z:218:SER:HB3	2:Z:221:LYS:HB3	1.70	0.71
1:A:11:ALA:HB3	1:A:37:PHE:CE2	2.25	0.71
2:X:27:THR:HG23	2:X:29:TYR:CD2	2.25	0.71
2:Z:29:TYR:CE2	2:Z:41:ARG:HD2	2.26	0.70
2:Z:337:ILE:HG22	2:Z:339:PHE:HD2	1.56	0.70
1:D:77:GLU:HG2	1:D:148:THR:HB	1.71	0.70
1:D:101:GLU:HB2	2:W:328:GLU:HG2	1.74	0.70
2:X:258:ASN:OD1	2:X:303:HIS:CE1	2.45	0.69
1:B:90:PHE:O	1:B:91:LEU:HD22	1.93	0.69
2:Y:229:THR:HG23	2:Y:230:TRP:HD1	1.58	0.68
1:D:48:LYS:HE3	1:D:60:GLU:OE1	1.92	0.68
2:Z:71:MET:HA	2:Z:71:MET:HE3	1.75	0.68
2:Y:223:LEU:HD21	2:Y:245:PRO:HB2	1.75	0.68
2:Y:210:PHE:O	2:Y:213:GLU:HB2	1.94	0.67
1:C:117:TYR:HE2	2:Y:205:HIS:CD2	2.11	0.67
2:X:97:LYS:HD3	2:X:119:ASN:OD1	1.94	0.67
1:C:140:ARG:HD2	4:C:202:HOH:O	1.95	0.67
1:B:117:TYR:OH	2:X:205:HIS:HD2	1.78	0.66
2:Z:27:THR:HG22	2:Z:29:TYR:H	1.60	0.66
1:C:117:TYR:HE2	2:Y:205:HIS:HD2	1.41	0.66
2:Z:169:ARG:HH11	2:Z:169:ARG:HG3	1.59	0.66
1:B:73:ALA:HB3	1:B:77:GLU:OE1	1.94	0.66
2:W:229:THR:HG23	2:W:230:TRP:CD1	2.30	0.66
2:W:252:LEU:HD12	2:W:253:PRO:HD2	1.77	0.66
2:X:245:PRO:HG3	2:X:314:MET:CE	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:HG22	1:D:138:ALA:HB2	1.76	0.66
1:D:2:SER:O	1:D:3:ASN:HB3	1.95	0.65
2:Z:248:GLU:O	2:Z:310:ARG:HA	1.96	0.65
1:D:117:TYR:CZ	2:Z:205:HIS:HD2	2.15	0.65
1:B:24:ILE:HG21	2:X:283:PRO:HB2	1.78	0.64
2:Z:81:GLY:O	4:Z:601:HOH:O	2.14	0.64
2:Z:134:ARG:HA	2:Z:165:ILE:CD1	2.26	0.64
2:Z:235:THR:HG21	2:Z:245:PRO:HG2	1.79	0.64
2:X:229:THR:HG23	2:X:230:TRP:HD1	1.62	0.64
2:W:27:THR:HG23	2:W:29:TYR:CD2	2.32	0.64
2:Y:62:PRO:HB2	2:Y:65:ILE:HG12	1.79	0.64
2:Z:283:PRO:HD3	2:Y:108:THR:CG2	2.28	0.64
1:A:158:TRP:CE2	2:W:337:ILE:HD13	2.33	0.64
2:X:262:GLU:OE1	2:X:303:HIS:CE1	2.51	0.63
1:A:48:LYS:HE3	1:A:60:GLU:OE1	1.98	0.63
1:B:117:TYR:CE2	2:X:205:HIS:CD2	2.87	0.63
1:D:29:ARG:HG2	1:D:164:LYS:HG3	1.80	0.63
2:X:290:ARG:HG3	2:X:290:ARG:HH11	1.63	0.63
1:B:80:ILE:HD13	1:B:125:GLN:HB2	1.81	0.63
2:X:250:PHE:CZ	2:X:251:ILE:HD12	2.34	0.62
2:X:282:ASN:O	2:X:284:ARG:N	2.32	0.62
2:Y:229:THR:HG23	2:Y:230:TRP:CD1	2.32	0.62
1:D:71:PHE:HB2	1:D:134:TYR:CE2	2.35	0.62
2:Z:27:THR:O	2:Z:156:ARG:HB3	2.00	0.62
2:W:114:VAL:O	2:W:114:VAL:HG13	2.00	0.62
1:A:48:LYS:HE2	1:A:103:THR:CG2	2.30	0.62
2:Z:27:THR:HG23	2:Z:29:TYR:HD2	1.61	0.62
2:X:235:THR:O	2:X:236:SER:HB3	2.00	0.61
2:Z:336:PRO:HB2	2:Z:337:ILE:HD12	1.81	0.61
2:X:105:PHE:C	2:X:105:PHE:CD1	2.73	0.61
1:B:48:LYS:HE3	1:B:60:GLU:OE1	1.99	0.61
1:B:127:LEU:HD21	2:X:174:ARG:NH2	2.15	0.61
2:X:105:PHE:HZ	2:X:302:ARG:CD	2.11	0.61
2:W:109:LEU:N	2:W:109:LEU:HD23	2.16	0.60
2:X:82:TRP:HZ3	2:X:105:PHE:HB2	1.66	0.60
2:Z:252:LEU:HD12	2:Z:253:PRO:CD	2.31	0.60
1:C:48:LYS:HE2	1:C:103:THR:HG21	1.83	0.60
1:C:55:LEU:HD11	2:Y:332:LEU:HD11	1.82	0.60
1:C:88:VAL:HG22	1:C:136:PHE:CD1	2.37	0.60
2:X:30:ARG:HG3	2:X:135:ASP:OD2	2.02	0.60
1:D:88:VAL:HG22	1:D:136:PHE:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLY:HA2	2:X:290:ARG:NH1	2.17	0.59
2:Z:72:ARG:HH11	2:Z:72:ARG:HG2	1.66	0.59
1:B:33:PHE:CD1	2:X:295:CYS:HB2	2.38	0.59
2:Z:108:THR:HG21	2:Y:282:ASN:HB3	1.84	0.59
1:A:41:GLN:C	1:A:42:ASN:HD22	2.05	0.59
1:D:156:GLU:HG2	1:D:158:TRP:NE1	2.17	0.59
2:Y:256:HIS:O	2:Y:302:ARG:HA	2.02	0.59
2:X:277:ASP:CG	2:X:282:ASN:HB2	2.23	0.59
1:D:70:TRP:CE2	1:D:135:ARG:HD3	2.38	0.59
1:A:94:ASP:OD1	1:A:112:GLY:HA2	2.02	0.58
2:W:109:LEU:CD2	2:X:283:PRO:HG2	2.33	0.58
1:D:125:GLN:HE21	2:Z:175:MET:HE2	1.68	0.58
1:B:127:LEU:O	1:B:129:PRO:HD3	2.03	0.58
2:X:201:GLU:HB3	2:X:202:PRO:HD2	1.85	0.58
2:Z:104:THR:HG23	2:Z:115:ASN:ND2	2.19	0.58
1:D:68:SER:HB3	1:D:136:PHE:HB2	1.86	0.58
1:B:35:ASN:O	1:B:39:VAL:HG23	2.04	0.58
2:Y:271:ILE:HG12	2:Y:307:SER:HB2	1.85	0.58
2:Y:157:LYS:HE3	2:Y:159:GLY:O	2.03	0.58
2:W:223:LEU:HD21	2:W:245:PRO:HB2	1.85	0.58
2:W:256:HIS:O	2:W:302:ARG:HA	2.04	0.57
1:A:105:LEU:HG	1:A:153:LEU:HD21	1.86	0.57
1:C:48:LYS:CE	1:C:103:THR:HG21	2.34	0.57
2:Z:265:ILE:HB	2:Z:314:MET:HB3	1.86	0.57
1:B:45:PRO:HG3	1:B:65:GLU:OE1	2.04	0.57
2:X:72:ARG:HH11	2:X:72:ARG:HG2	1.69	0.57
2:W:233:SER:O	2:W:245:PRO:HD2	2.04	0.57
1:C:127:LEU:HB2	2:Y:175:MET:CE	2.34	0.57
2:X:252:LEU:HD12	2:X:253:PRO:HD2	1.87	0.57
1:B:117:TYR:CE2	2:X:205:HIS:HD2	2.22	0.57
2:Z:35:GLY:HA3	2:Z:120:PHE:HZ	1.69	0.57
2:X:275:VAL:CG1	2:X:301:ILE:HD13	2.30	0.56
2:X:229:THR:CG2	2:X:230:TRP:HD1	2.18	0.56
1:B:14:ASP:OD1	1:B:14:ASP:N	2.37	0.56
1:D:91:LEU:HD12	1:D:110:PRO:HB2	1.86	0.56
2:X:55:GLU:HB2	2:X:57:ARG:NH1	2.21	0.56
2:Y:94:TYR:HB2	2:Y:97:LYS:O	2.06	0.56
1:B:71:PHE:HE1	1:B:153:LEU:HD23	1.71	0.56
1:B:39:VAL:HG22	1:B:161:ILE:HG22	1.86	0.55
2:Z:192:ARG:NH1	2:Z:193:GLN:HG3	2.21	0.55
2:X:114:VAL:CG1	2:X:114:VAL:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:229:THR:HG23	2:W:230:TRP:HD1	1.70	0.55
1:C:48:LYS:HE3	1:C:60:GLU:OE1	2.07	0.55
1:A:126:CYS:HB2	2:W:216:ALA:HB2	1.89	0.55
1:B:117:TYR:CZ	2:X:205:HIS:CD2	2.87	0.55
2:Y:207:ALA:O	2:Y:210:PHE:HB2	2.06	0.55
1:C:127:LEU:HB2	2:Y:175:MET:HE3	1.88	0.55
1:A:125:GLN:HG2	2:W:175:MET:HE1	1.89	0.55
1:C:117:TYR:CE2	2:Y:205:HIS:HB2	2.41	0.55
1:C:48:LYS:HE2	1:C:103:THR:CG2	2.35	0.55
1:B:68:SER:HB3	1:B:136:PHE:H	1.71	0.55
2:Z:41:ARG:HD3	2:Z:42:ASP:O	2.05	0.55
1:B:4:VAL:CG1	1:B:4:VAL:O	2.54	0.55
1:B:33:PHE:O	1:B:162:CYS:HA	2.07	0.55
2:W:108:THR:HG21	2:X:283:PRO:HD2	1.90	0.54
1:B:148:THR:OG1	1:B:149:ILE:N	2.39	0.54
2:Z:221:LYS:O	2:Z:224:SER:HB3	2.08	0.54
1:A:8:THR:HA	2:W:309:LYS:HE3	1.89	0.54
1:A:4:VAL:HG12	1:A:4:VAL:O	2.07	0.54
2:X:114:VAL:HG12	2:X:114:VAL:O	2.05	0.54
1:B:71:PHE:CE1	1:B:153:LEU:HD23	2.43	0.54
1:A:68:SER:HB3	1:A:136:PHE:HB2	1.89	0.54
2:Z:77:GLY:O	2:Z:78:PHE:HB2	2.08	0.54
2:W:49:THR:HG23	2:W:56:THR:HG23	1.90	0.54
2:Z:39:LEU:N	2:Z:39:LEU:HD12	2.22	0.53
1:B:78:PHE:HD1	2:X:175:MET:CE	2.22	0.53
1:C:55:LEU:HD11	2:Y:332:LEU:CD1	2.39	0.53
2:W:50:TRP:CD1	2:W:116:TYR:HB3	2.44	0.53
1:B:79:ALA:HA	1:B:145:LEU:O	2.09	0.53
2:X:24:HIS:HB3	2:X:27:THR:HB	1.89	0.53
1:C:91:LEU:HD21	1:C:112:GLY:O	2.09	0.53
1:D:24:ILE:HG21	2:Z:283:PRO:HG2	1.91	0.53
1:D:89:GLU:O	1:D:134:TYR:HA	2.09	0.53
2:Y:258:ASN:OD1	2:Y:258:ASN:N	2.41	0.53
2:Y:27:THR:HG23	2:Y:29:TYR:CD2	2.44	0.52
1:D:124:HIS:CG	2:Z:202:PRO:HG3	2.44	0.52
2:W:108:THR:CG2	2:X:283:PRO:HD2	2.40	0.52
2:X:71:MET:HA	2:X:71:MET:HE3	1.90	0.52
1:A:85:GLU:HB2	1:A:140:ARG:HD3	1.91	0.52
2:Z:85:PHE:N	2:Z:85:PHE:HD1	2.07	0.52
2:X:256:HIS:O	2:X:302:ARG:HA	2.10	0.52
1:B:121:LYS:HB2	1:B:124:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:42:ASP:HB2	2:Z:43:GLU:OE1	2.09	0.52
2:Z:29:TYR:CD2	2:Z:41:ARG:HD2	2.45	0.52
1:B:78:PHE:CZ	2:X:237:VAL:O	2.63	0.52
1:C:94:ASP:OD1	1:C:112:GLY:HA2	2.09	0.52
1:D:87:ARG:HB3	1:D:137:GLU:HB2	1.91	0.52
2:X:170:ILE:O	2:X:182:SER:HB3	2.09	0.52
1:B:78:PHE:CD1	2:X:175:MET:CE	2.93	0.51
1:B:73:ALA:CB	1:B:77:GLU:OE1	2.59	0.51
2:X:276:GLY:O	2:X:302:ARG:HG2	2.10	0.51
1:D:65:GLU:HG2	1:D:65:GLU:O	2.11	0.51
2:W:140:THR:HG23	2:W:152:SER:O	2.09	0.51
2:W:157:LYS:HG3	2:W:158:ASN:N	2.25	0.51
2:Z:72:ARG:HG2	2:Z:72:ARG:NH1	2.26	0.51
2:Y:258:ASN:HB2	2:Y:260:ARG:O	2.10	0.51
1:B:125:GLN:HE22	2:X:236:SER:HB3	1.75	0.51
2:W:41:ARG:HG2	2:W:136:TRP:CD2	2.45	0.51
2:W:117:THR:HG22	2:W:118:GLU:N	2.26	0.51
2:X:79:PHE:CE2	2:X:256:HIS:CE1	3.00	0.50
1:B:78:PHE:N	1:B:78:PHE:CD2	2.79	0.50
2:X:87:HIS:H	2:X:87:HIS:CD2	2.29	0.50
2:Z:64:ASP:O	2:Z:68:ARG:HG3	2.11	0.50
2:Y:70:MET:HG2	2:Y:133:LEU:HG	1.93	0.50
1:D:125:GLN:HE21	2:Z:175:MET:CE	2.24	0.50
1:D:117:TYR:OH	2:Z:205:HIS:HD2	1.95	0.50
1:D:62:LEU:N	1:D:62:LEU:HD12	2.27	0.50
1:B:78:PHE:HZ	2:X:237:VAL:O	1.94	0.50
2:Y:262:GLU:OE1	4:Y:401:HOH:O	2.19	0.50
2:Y:146:ALA:HB3	2:Y:149:GLU:HG3	1.93	0.50
2:Y:27:THR:HG22	2:Y:28:GLY:N	2.26	0.50
1:D:90:PHE:O	1:D:115:MET:HB2	2.11	0.50
2:X:210:PHE:O	2:X:213:GLU:HG2	2.12	0.50
1:A:101:GLU:HB2	2:Z:328:GLU:HG2	1.94	0.50
2:Z:85:PHE:CD1	2:Z:85:PHE:N	2.79	0.50
2:X:126:MET:HE3	2:X:126:MET:HA	1.93	0.50
1:C:41:GLN:HG2	1:C:41:GLN:O	2.10	0.50
2:Z:20:ALA:HB2	2:Z:32:PHE:CE2	2.46	0.49
2:X:248:GLU:O	2:X:310:ARG:HA	2.12	0.49
2:W:248:GLU:O	2:W:310:ARG:HA	2.12	0.49
2:Z:245:PRO:HG3	2:Z:314:MET:CE	2.42	0.49
1:D:148:THR:OG1	1:D:149:ILE:N	2.45	0.49
1:A:62:LEU:N	1:A:62:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:249:GLU:OE1	2:Z:310:ARG:HB2	2.12	0.49
2:X:290:ARG:HG3	2:X:290:ARG:NH1	2.27	0.49
2:W:27:THR:HG23	2:W:29:TYR:HD2	1.76	0.49
1:C:128:LEU:HD13	1:C:134:TYR:CZ	2.48	0.49
2:X:105:PHE:CZ	2:X:302:ARG:CD	2.89	0.49
1:A:49:VAL:O	1:A:60:GLU:HA	2.13	0.49
2:Z:24:HIS:HB3	2:Z:27:THR:HG22	1.95	0.49
2:Z:221:LYS:O	2:Z:225:ARG:HG3	2.12	0.49
2:W:248:GLU:OE1	2:W:248:GLU:HA	2.12	0.49
1:D:39:VAL:HG22	1:D:161:ILE:CG2	2.43	0.49
1:D:77:GLU:OE2	1:D:103:THR:HB	2.13	0.49
1:B:91:LEU:HD13	1:B:114:PRO:HA	1.95	0.49
2:W:248:GLU:CA	2:W:248:GLU:OE1	2.61	0.49
1:A:24:ILE:HG12	2:X:57:ARG:HH21	1.78	0.49
2:W:72:ARG:HH21	2:W:229:THR:HG22	1.76	0.49
2:W:24:HIS:ND1	2:W:27:THR:HB	2.28	0.48
2:X:275:VAL:HG21	2:X:287:ILE:HD12	1.95	0.48
2:Z:27:THR:CG2	2:Z:29:TYR:H	2.25	0.48
2:X:245:PRO:HG3	2:X:314:MET:HE2	1.95	0.48
2:Y:325:HIS:O	2:Y:329:SER:HB2	2.13	0.48
2:Z:38:GLU:C	2:Z:39:LEU:HD12	2.33	0.48
2:Y:185:ARG:HG3	2:Y:222:TYR:CE1	2.48	0.48
1:B:76:ASP:O	1:B:77:GLU:HG3	2.13	0.48
2:Z:283:PRO:HD3	2:Y:108:THR:HG22	1.96	0.48
2:W:265:ILE:CD1	2:W:294:VAL:HG22	2.41	0.48
1:D:91:LEU:HD23	1:D:114:PRO:HA	1.94	0.48
1:A:102:GLY:HA2	1:A:149:ILE:O	2.13	0.48
1:C:77:GLU:OE2	1:C:103:THR:HB	2.13	0.48
1:C:48:LYS:HD3	1:C:153:LEU:HB3	1.95	0.48
2:W:38:GLU:HB3	2:W:49:THR:HB	1.94	0.48
2:Z:298:PRO:HD2	2:Z:301:ILE:HG12	1.95	0.48
2:Y:252:LEU:HB3	2:Y:305:GLY:H	1.78	0.48
2:W:109:LEU:HD22	2:X:283:PRO:HG2	1.96	0.48
1:B:117:TYR:OH	2:X:205:HIS:CD2	2.62	0.48
2:W:52:ALA:O	2:W:57:ARG:NH1	2.46	0.48
2:W:108:THR:HG21	2:X:282:ASN:HA	1.95	0.48
1:D:115:MET:HA	2:Z:210:PHE:CD1	2.49	0.48
1:B:10:PHE:CE1	2:X:220:PHE:CE2	3.02	0.48
1:D:88:VAL:HG22	1:D:136:PHE:HD1	1.77	0.47
1:B:29:ARG:HD2	1:B:164:LYS:NZ	2.29	0.47
1:D:11:ALA:HB3	1:D:37:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:262:GLU:OE2	2:X:303:HIS:CE1	2.66	0.47
2:W:77:GLY:O	2:W:78:PHE:HB2	2.14	0.47
2:W:85:PHE:CD1	2:W:85:PHE:N	2.82	0.47
2:X:82:TRP:N	2:X:82:TRP:CD1	2.82	0.47
2:Z:223:LEU:HD21	2:Z:245:PRO:HB2	1.97	0.47
1:B:19:GLY:HA2	2:X:290:ARG:HH11	1.80	0.47
1:B:4:VAL:HG13	1:B:4:VAL:O	2.13	0.47
2:X:126:MET:O	2:X:130:LYS:HG3	2.13	0.47
2:Y:192:ARG:HG2	2:Y:193:GLN:N	2.30	0.47
2:W:23:PRO:HD3	2:W:30:ARG:NH1	2.29	0.47
2:X:277:ASP:HB2	2:X:282:ASN:HB2	1.96	0.47
2:X:277:ASP:O	2:X:302:ARG:HD3	2.14	0.47
2:Z:35:GLY:HA3	2:Z:120:PHE:CZ	2.47	0.47
2:Y:272:VAL:HG22	2:Y:288:THR:HG23	1.95	0.47
2:Y:188:LEU:HB3	2:Y:189:PRO:HD2	1.96	0.47
1:C:70:TRP:HE1	1:C:135:ARG:HH21	1.63	0.47
2:X:27:THR:CG2	2:X:29:TYR:HD2	2.23	0.47
2:Z:235:THR:HG23	2:Z:245:PRO:HD2	1.96	0.47
2:W:44:TYR:CD2	2:X:250:PHE:CD1	3.03	0.47
2:Z:34:LEU:HG	2:Z:120:PHE:CE2	2.50	0.47
2:Y:248:GLU:O	2:Y:310:ARG:HA	2.15	0.47
2:W:27:THR:HG22	2:W:28:GLY:N	2.29	0.47
1:B:124:HIS:HD2	2:X:218:SER:HA	1.79	0.47
2:X:126:MET:HA	2:X:126:MET:CE	2.44	0.47
1:C:4:VAL:O	1:C:4:VAL:HG13	2.15	0.47
2:Y:172:THR:HG21	2:Y:176:PRO:HD3	1.97	0.47
2:X:247:THR:HA	2:X:311:SER:O	2.15	0.47
2:W:232:PRO:HA	2:W:246:THR:HB	1.96	0.47
1:B:127:LEU:HD21	2:X:174:ARG:HH21	1.78	0.46
2:Y:68:ARG:O	2:Y:72:ARG:HG2	2.15	0.46
2:X:77:GLY:O	2:X:78:PHE:HB2	2.14	0.46
2:Z:197:VAL:O	2:Z:199:GLN:NE2	2.37	0.46
2:X:262:GLU:CD	2:X:303:HIS:CE1	2.88	0.46
1:A:158:TRP:CD2	2:W:337:ILE:HD13	2.49	0.46
2:X:23:PRO:HD3	2:X:30:ARG:NH2	2.30	0.46
1:D:88:VAL:HG22	1:D:136:PHE:CE1	2.51	0.46
1:D:156:GLU:HG2	1:D:158:TRP:HE1	1.80	0.46
2:X:332:LEU:HD23	2:X:332:LEU:HA	1.66	0.46
2:X:277:ASP:H	2:X:284:ARG:HG2	1.80	0.46
1:D:88:VAL:HG12	1:D:90:PHE:CE2	2.50	0.46
2:Y:278:LYS:HA	2:Y:302:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:252:LEU:HD12	2:W:253:PRO:CD	2.44	0.46
2:W:85:PHE:N	2:W:85:PHE:HD1	2.14	0.46
1:D:53:LEU:HD12	1:D:54:ASN:N	2.30	0.46
2:Z:335:TYR:HB2	2:Z:336:PRO:HD2	1.97	0.46
2:X:256:HIS:ND1	2:X:262:GLU:OE2	2.49	0.46
2:Z:106:ASN:OD1	2:Z:109:LEU:HG	2.16	0.46
1:C:126:CYS:HB2	2:Y:216:ALA:HB2	1.98	0.46
2:Y:50:TRP:CD1	2:Y:116:TYR:HB3	2.51	0.45
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.67	0.45
2:X:320:THR:HB	2:X:323:LEU:CD1	2.46	0.45
2:Z:114:VAL:O	2:Z:114:VAL:CG1	2.63	0.45
2:Y:57:ARG:HD2	2:Y:57:ARG:N	2.32	0.45
1:A:158:TRP:CZ2	2:W:337:ILE:CD1	3.00	0.45
2:X:250:PHE:CE2	2:X:251:ILE:HD12	2.51	0.45
1:D:91:LEU:CD1	1:D:110:PRO:HB2	2.45	0.45
2:Z:269:ASP:OD1	2:Z:309:LYS:HD3	2.16	0.45
2:X:66:PHE:CZ	2:X:70:MET:HE3	2.50	0.45
1:B:24:ILE:CG2	2:X:283:PRO:O	2.64	0.45
2:X:109:LEU:HA	2:X:109:LEU:HD23	1.64	0.45
1:A:150:LYS:HD2	2:Z:329:SER:O	2.16	0.45
1:A:40:ALA:O	1:A:63:ARG:HD2	2.16	0.45
1:C:99:HIS:N	1:C:99:HIS:CD2	2.85	0.45
2:W:162:LEU:HD22	2:W:166:GLU:OE1	2.16	0.45
1:B:39:VAL:HG22	1:B:161:ILE:CG2	2.45	0.45
2:Y:78:PHE:CZ	2:Y:125:ILE:HG12	2.51	0.45
1:D:48:LYS:HE2	1:D:103:THR:HG21	1.98	0.45
2:Y:245:PRO:HA	2:Y:314:MET:HA	1.99	0.45
2:W:72:ARG:NH2	2:W:229:THR:HG22	2.32	0.45
1:B:78:PHE:HD1	2:X:175:MET:HE1	1.80	0.45
2:X:265:ILE:HD13	2:X:294:VAL:HG22	1.99	0.45
1:B:46:TYR:CE1	1:B:136:PHE:HB2	2.51	0.45
1:B:24:ILE:HB	2:X:283:PRO:O	2.16	0.45
1:B:46:TYR:HE2	1:B:65:GLU:O	2.00	0.45
2:X:105:PHE:O	2:X:105:PHE:CD1	2.71	0.44
1:C:88:VAL:HG22	1:C:136:PHE:HD1	1.78	0.44
1:A:126:CYS:CB	2:W:216:ALA:HB2	2.47	0.44
2:Z:185:ARG:C	2:Z:187:ASP:H	2.20	0.44
2:Y:162:LEU:O	2:Y:166:GLU:HB2	2.17	0.44
1:D:48:LYS:HE2	1:D:103:THR:CG2	2.47	0.44
2:X:188:LEU:HA	2:X:188:LEU:HD23	1.83	0.44
2:Z:141:PHE:HB2	2:Z:152:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:134:ARG:HG3	2:Z:162:LEU:HD21	1.99	0.44
1:A:79:ALA:HA	1:A:145:LEU:O	2.17	0.44
2:Z:268:SER:O	2:Z:269:ASP:HB2	2.18	0.44
1:C:13:LEU:HD23	1:C:13:LEU:HA	1.67	0.44
2:X:218:SER:HB3	2:X:221:LYS:HB3	2.00	0.44
2:X:255:PHE:HB3	2:X:304:GLN:HB2	2.00	0.44
1:D:2:SER:O	1:D:3:ASN:CB	2.63	0.44
2:Z:271:ILE:HG22	2:Z:272:VAL:N	2.33	0.44
1:A:128:LEU:HD13	1:A:134:TYR:CE2	2.53	0.44
1:C:33:PHE:O	1:C:162:CYS:HA	2.17	0.44
2:Y:175:MET:HG2	2:Y:176:PRO:O	2.18	0.43
2:X:61:ILE:O	2:X:62:PRO:C	2.55	0.43
1:C:78:PHE:CD1	2:Y:175:MET:HE2	2.54	0.43
2:Z:323:LEU:N	2:Z:324:PRO:CD	2.81	0.43
2:X:223:LEU:HD21	2:X:245:PRO:HB2	2.00	0.43
1:B:140:ARG:H	1:B:140:ARG:HG2	1.71	0.43
2:Y:259:ASP:HB3	2:Y:324:PRO:HG3	2.00	0.43
2:Z:236:SER:OG	2:Z:243:PHE:HB2	2.19	0.43
1:B:33:PHE:HD1	2:X:295:CYS:HB2	1.80	0.43
2:Z:199:GLN:OE1	2:Z:225:ARG:NH2	2.49	0.43
2:Y:64:ASP:O	2:Y:65:ILE:C	2.55	0.43
1:D:128:LEU:HD13	1:D:134:TYR:CZ	2.54	0.43
1:D:114:PRO:O	2:Z:210:PHE:CE1	2.72	0.43
2:Z:323:LEU:N	2:Z:324:PRO:HD2	2.34	0.43
2:Y:147:PRO:HG2	2:Y:250:PHE:CD2	2.53	0.43
2:Z:274:ASP:O	2:Z:303:HIS:HA	2.19	0.43
2:Y:320:THR:HB	2:Y:323:LEU:HD22	2.01	0.43
2:Y:27:THR:HG22	2:Y:29:TYR:N	2.19	0.43
2:Z:32:PHE:CD1	2:Z:132:ILE:HG12	2.54	0.43
2:X:248:GLU:HG3	2:X:271:ILE:HD11	2.00	0.43
1:A:125:GLN:HE21	2:W:175:MET:CE	2.32	0.43
2:Z:301:ILE:HD12	2:Z:301:ILE:C	2.39	0.43
2:Z:44:TYR:HA	2:Z:154:PHE:CD1	2.54	0.43
2:X:277:ASP:OD1	2:X:284:ARG:NH1	2.50	0.43
2:X:27:THR:CG2	2:X:29:TYR:CD2	2.98	0.43
1:A:31:TYR:O	1:A:32:ALA:C	2.56	0.42
1:C:62:LEU:HD12	1:C:62:LEU:N	2.34	0.42
1:B:81:VAL:HG12	1:B:122:ARG:HA	2.00	0.42
2:X:277:ASP:CB	2:X:282:ASN:HB2	2.48	0.42
2:X:144:PHE:O	2:X:229:THR:HB	2.18	0.42
1:D:77:GLU:C	1:D:78:PHE:CD2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:252:LEU:HA	2:Z:253:PRO:HD3	1.71	0.42
1:B:149:ILE:HG22	1:B:150:LYS:N	2.34	0.42
2:W:210:PHE:O	2:W:211:GLU:C	2.58	0.42
2:W:333:LYS:HB3	2:W:334:PRO:HD2	2.00	0.42
2:Y:277:ASP:O	2:Y:302:ARG:HD3	2.19	0.42
2:W:39:LEU:HD23	2:W:48:ILE:CD1	2.49	0.42
2:Z:232:PRO:HA	2:Z:246:THR:HB	2.02	0.42
1:A:158:TRP:CZ2	2:W:337:ILE:HD13	2.54	0.42
2:X:320:THR:HA	2:X:321:PRO:HD3	1.62	0.42
2:Z:182:SER:HA	2:Z:183:PRO:HD3	1.81	0.42
2:X:141:PHE:O	2:X:143:PRO:HD3	2.19	0.42
2:Z:71:MET:HA	2:Z:133:LEU:HD11	2.01	0.42
2:Z:235:THR:HG23	2:Z:245:PRO:CD	2.50	0.42
2:X:320:THR:HB	2:X:323:LEU:HD13	2.01	0.42
1:B:158:TRP:CH2	2:X:337:ILE:HD11	2.54	0.42
2:W:65:ILE:HD13	2:W:65:ILE:N	2.34	0.42
2:Z:138:ASN:C	2:Z:140:THR:H	2.22	0.42
2:W:36:ALA:HB1	2:W:51:PRO:HD3	2.01	0.42
2:W:252:LEU:HG	2:W:254:VAL:O	2.20	0.42
2:Z:104:THR:HG23	2:Z:115:ASN:HD22	1.85	0.42
2:X:281:GLY:HA2	2:X:302:ARG:NH2	2.35	0.42
1:B:22:GLU:O	1:B:22:GLU:HG3	2.19	0.42
2:W:323:LEU:HD12	2:W:323:LEU:HA	1.80	0.42
1:B:55:LEU:HA	1:B:55:LEU:HD12	1.67	0.42
2:X:282:ASN:O	2:X:283:PRO:C	2.57	0.41
1:A:85:GLU:OE1	1:A:119:LEU:HD22	2.20	0.41
2:W:109:LEU:N	2:W:109:LEU:CD2	2.83	0.41
2:W:337:ILE:HG22	2:W:339:PHE:HD2	1.85	0.41
2:Z:50:TRP:CD1	2:Z:116:TYR:HB3	2.56	0.41
1:C:78:PHE:CD1	2:Y:175:MET:CE	3.03	0.41
1:B:158:TRP:CE3	2:X:337:ILE:HD13	2.55	0.41
1:B:64:ALA:O	1:B:141:PRO:HA	2.19	0.41
1:B:66:GLY:O	1:B:137:GLU:HA	2.20	0.41
1:B:33:PHE:CZ	2:X:293:ASP:OD2	2.73	0.41
2:X:265:ILE:HG23	2:X:294:VAL:CG2	2.43	0.41
1:B:90:PHE:C	1:B:91:LEU:HD22	2.39	0.41
2:Y:277:ASP:OD2	2:Y:284:ARG:HD3	2.21	0.41
2:Y:185:ARG:HG3	2:Y:222:TYR:CD1	2.55	0.41
2:X:43:GLU:H	2:X:43:GLU:HG2	1.49	0.41
1:B:21:VAL:HG22	2:X:287:ILE:HG23	2.01	0.41
2:Z:72:ARG:NH2	2:Z:229:THR:HG22	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:72:ARG:NH1	2:X:72:ARG:HG2	2.34	0.41
2:Y:162:LEU:HD23	2:Y:162:LEU:HA	1.60	0.41
1:C:19:GLY:HA2	2:Y:290:ARG:NH1	2.35	0.41
1:B:56:GLY:O	1:B:58:VAL:HG13	2.21	0.41
2:Z:256:HIS:HB3	2:Z:303:HIS:CD2	2.55	0.41
2:X:34:LEU:HA	2:X:34:LEU:HD12	1.84	0.41
2:Y:71:MET:HA	2:Y:71:MET:HE3	2.02	0.41
2:Z:169:ARG:HH11	2:Z:169:ARG:HG2	1.81	0.41
2:X:221:LYS:O	2:X:224:SER:HB3	2.21	0.41
2:Y:34:LEU:HG	2:Y:120:PHE:CE1	2.56	0.41
2:X:281:GLY:O	2:X:282:ASN:C	2.59	0.41
1:D:114:PRO:O	2:Z:210:PHE:HE1	2.04	0.41
2:Y:255:PHE:CD2	2:Y:302:ARG:HG3	2.56	0.41
1:A:94:ASP:N	4:A:201:HOH:O	2.53	0.41
1:D:153:LEU:HD12	1:D:153:LEU:HA	1.91	0.41
2:Z:169:ARG:NH1	2:Z:169:ARG:HG3	2.33	0.41
2:Y:72:ARG:HH21	2:Y:229:THR:HG22	1.85	0.41
2:X:223:LEU:C	2:X:225:ARG:N	2.74	0.41
2:W:70:MET:HB2	2:W:70:MET:HE3	1.92	0.41
2:X:162:LEU:O	2:X:166:GLU:HB2	2.21	0.41
2:Z:266:GLN:OE1	2:Z:313:LEU:HD13	2.21	0.41
2:W:263:TRP:CZ3	2:W:296:ALA:HB2	2.56	0.41
2:X:223:LEU:C	2:X:225:ARG:H	2.24	0.40
2:Z:138:ASN:C	2:Z:140:THR:N	2.74	0.40
2:X:39:LEU:HD12	2:X:39:LEU:N	2.36	0.40
2:W:219:LEU:O	2:W:222:TYR:HB3	2.21	0.40
2:X:282:ASN:O	2:X:284:ARG:HG2	2.21	0.40
2:W:81:GLY:CA	2:W:259:ASP:HB2	2.52	0.40
2:Z:319:ALA:O	2:Z:321:PRO:HD3	2.22	0.40
1:A:78:PHE:O	1:A:146:GLN:HA	2.21	0.40
1:D:88:VAL:HA	1:D:135:ARG:O	2.20	0.40
1:A:120:LEU:HD21	1:A:126:CYS:HB3	2.03	0.40
2:X:134:ARG:HA	2:X:165:ILE:HD11	2.02	0.40
1:B:113:LYS:HG3	1:B:113:LYS:H	1.55	0.40
2:X:37:PHE:HA	2:X:49:THR:O	2.22	0.40
1:D:117:TYR:CZ	2:Z:205:HIS:CD2	3.04	0.40
2:X:210:PHE:HA	2:X:210:PHE:HD2	1.77	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	161/168 (96%)	156 (97%)	5 (3%)	0	100	100
1	B	161/168 (96%)	152 (94%)	6 (4%)	3 (2%)	10	38
1	C	161/168 (96%)	150 (93%)	11 (7%)	0	100	100
1	D	161/168 (96%)	153 (95%)	7 (4%)	1 (1%)	30	66
2	W	322/339 (95%)	299 (93%)	21 (6%)	2 (1%)	30	66
2	X	322/339 (95%)	290 (90%)	23 (7%)	9 (3%)	6	28
2	Y	322/339 (95%)	290 (90%)	30 (9%)	2 (1%)	30	66
2	Z	322/339 (95%)	291 (90%)	29 (9%)	2 (1%)	30	66
All	All	1932/2028 (95%)	1781 (92%)	132 (7%)	19 (1%)	19	56

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	W	95	TYR
2	W	250	PHE
2	Z	250	PHE
2	Y	139	ALA
2	Y	250	PHE
2	X	95	TYR
2	X	224	SER
2	X	277	ASP
1	D	3	ASN
1	B	159	ALA
2	Z	224	SER
2	X	236	SER
2	X	250	PHE
2	X	283	PRO
1	B	69	PRO
2	X	51	PRO
2	X	53	LYS

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Mol	Chain	Res	Type
1	B	5	ALA
2	X	336	PRO

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	133/136 (98%)	120 (90%)	13 (10%)	10 34
1	B	133/136 (98%)	113 (85%)	20 (15%)	3 14
1	C	133/136 (98%)	118 (89%)	15 (11%)	7 27
1	D	133/136 (98%)	120 (90%)	13 (10%)	10 34
2	W	274/284 (96%)	249 (91%)	25 (9%)	12 38
2	X	274/284 (96%)	240 (88%)	34 (12%)	6 22
2	Y	274/284 (96%)	236 (86%)	38 (14%)	4 18
2	Z	274/284 (96%)	252 (92%)	22 (8%)	15 46
All	All	1628/1680 (97%)	1448 (89%)	180 (11%)	8 28

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	80	ILE
1	A	85	GLU
1	A	97	SER
1	A	98	LYS
1	A	103	THR
1	A	119	LEU
1	A	122	ARG
1	A	126	CYS
1	A	141	PRO
1	A	150	LYS
1	A	153	LEU
1	A	157	LYS

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Mol	Chain	Res	Type
1	D	13	LEU
1	D	17	ARG
1	D	18	LYS
1	D	36	ILE
1	D	62	LEU
1	D	85	GLU
1	D	103	THR
1	D	109	LEU
1	D	119	LEU
1	D	135	ARG
1	D	139	SER
1	D	153	LEU
1	D	157	LYS
1	C	4	VAL
1	C	23	ILE
1	C	27	GLU
1	C	29	ARG
1	C	55	LEU
1	C	80	ILE
1	C	87	ARG
1	C	103	THR
1	C	117	TYR
1	C	126	CYS
1	C	139	SER
1	C	140	ARG
1	C	153	LEU
1	C	154	SER
1	C	157	LYS
1	B	4	VAL
1	B	14	ASP
1	B	17	ARG
1	B	20	THR
1	B	23	ILE
1	B	24	ILE
1	B	27	GLU
1	B	29	ARG
1	B	55	LEU
1	B	65	GLU
1	B	78	PHE
1	B	80	ILE
1	B	89	GLU
1	B	97	SER

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Mol	Chain	Res	Type
1	B	103	THR
1	B	111	VAL
1	B	113	LYS
1	B	119	LEU
1	B	126	CYS
1	B	140	ARG
2	W	27	THR
2	W	33	GLN
2	W	38	GLU
2	W	41	ARG
2	W	47	ARG
2	W	57	ARG
2	W	79	PHE
2	W	85	PHE
2	W	92	ARG
2	W	108	THR
2	W	109	LEU
2	W	114	VAL
2	W	144	PHE
2	W	157	LYS
2	W	161	ASN
2	W	181	ASP
2	W	192	ARG
2	W	229	THR
2	W	233	SER
2	W	243	PHE
2	W	274	ASP
2	W	279	ASP
2	W	302	ARG
2	W	323	LEU
2	W	329	SER
2	Z	16	ASP
2	Z	17	ASP
2	Z	27	THR
2	Z	38	GLU
2	Z	41	ARG
2	Z	49	THR
2	Z	57	ARG
2	Z	79	PHE
2	Z	85	PHE
2	Z	92	ARG
2	Z	150	THR

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Mol	Chain	Res	Type
2	Z	161	ASN
2	Z	169	ARG
2	Z	192	ARG
2	Z	204	VAL
2	Z	229	THR
2	Z	255	PHE
2	Z	277	ASP
2	Z	279	ASP
2	Z	280	ASP
2	Z	303	HIS
2	Z	323	LEU
2	Y	17	ASP
2	Y	27	THR
2	Y	33	GLN
2	Y	41	ARG
2	Y	47	ARG
2	Y	48	ILE
2	Y	49	THR
2	Y	53	LYS
2	Y	57	ARG
2	Y	58	SER
2	Y	79	PHE
2	Y	92	ARG
2	Y	114	VAL
2	Y	125	ILE
2	Y	144	PHE
2	Y	150	THR
2	Y	161	ASN
2	Y	167	ARG
2	Y	169	ARG
2	Y	180	ASP
2	Y	181	ASP
2	Y	187	ASP
2	Y	192	ARG
2	Y	201	GLU
2	Y	204	VAL
2	Y	213	GLU
2	Y	224	SER
2	Y	229	THR
2	Y	248	GLU
2	Y	255	PHE
2	Y	258	ASN

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Mol	Chain	Res	Type
2	Y	265	ILE
2	Y	286	ARG
2	Y	302	ARG
2	Y	323	LEU
2	Y	331	GLU
2	Y	332	LEU
2	Y	333	LYS
2	X	27	THR
2	X	38	GLU
2	X	41	ARG
2	X	43	GLU
2	X	49	THR
2	X	57	ARG
2	X	79	PHE
2	X	92	ARG
2	X	105	PHE
2	X	117	THR
2	X	126	MET
2	X	161	ASN
2	X	166	GLU
2	X	167	ARG
2	X	168	PHE
2	X	169	ARG
2	X	173	LYS
2	X	179	GLN
2	X	181	ASP
2	X	192	ARG
2	X	208	GLU
2	X	210	PHE
2	X	229	THR
2	X	238	CYS
2	X	246	THR
2	X	248	GLU
2	X	265	ILE
2	X	274	ASP
2	X	279	ASP
2	X	282	ASN
2	X	295	CYS
2	X	322	ASN
2	X	323	LEU
2	X	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	42	ASN
1	A	125	GLN
1	D	67	GLN
1	D	125	GLN
1	C	42	ASN
1	C	99	HIS
1	C	104	HIS
1	B	42	ASN
1	B	125	GLN
2	W	33	GLN
2	W	161	ASN
2	W	205	HIS
2	W	282	ASN
2	W	304	GLN
2	Z	33	GLN
2	Z	84	ASN
2	Z	115	ASN
2	Z	158	ASN
2	Z	161	ASN
2	Z	205	HIS
2	Z	303	HIS
2	Z	304	GLN
2	Y	33	GLN
2	Y	161	ASN
2	Y	205	HIS
2	Y	304	GLN
2	X	84	ASN
2	X	87	HIS
2	X	161	ASN
2	X	205	HIS
2	X	303	HIS
2	X	304	GLN
2	X	325	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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	17, 31, 49, 68	0
1	B	163/168 (97%)	-0.09	2 (1%) 81 61	39, 61, 80, 90	0
1	C	163/168 (97%)	-0.48	2 (1%) 81 61	22, 35, 62, 91	0
1	D	163/168 (97%)	-0.57	0 100 100	18, 36, 54, 80	0
2	W	324/339 (95%)	-0.58	1 (0%) 94 87	14, 29, 54, 79	0
2	X	324/339 (95%)	-0.37	5 (1%) 76 55	17, 40, 74, 100	0
2	Y	324/339 (95%)	-0.55	1 (0%) 94 87	18, 30, 60, 88	0
2	Z	324/339 (95%)	-0.53	2 (0%) 90 78	20, 33, 59, 88	0
All	All	1948/2028 (96%)	-0.48	13 (0%) 89 75	14, 34, 69, 100	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	16	ASP	4.3
2	Z	16	ASP	3.9
1	C	2	SER	3.8
2	X	16	ASP	3.4
2	X	208	GLU	3.0
2	Z	168	PHE	3.0
2	Y	168	PHE	2.7
2	X	187	ASP	2.5
1	B	91	LEU	2.2
2	X	211	GLU	2.1
1	B	95	ALA	2.1
1	C	3	ASN	2.1
2	X	168	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	FE	Z	500	1/1	0.98	0.13	-	25,25,25,25	0
3	FE	W	500	1/1	0.97	0.09	-	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.