



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 11:19 PM GMT

PDB ID : 1CD1  
Title : CD1(MOUSE) ANTIGEN PRESENTING MOLECULE  
Authors : Zeng, Z.H.; Segelke, B.W.; Wilson, I.A.  
Deposited on : 1997-04-02  
Resolution : 2.67 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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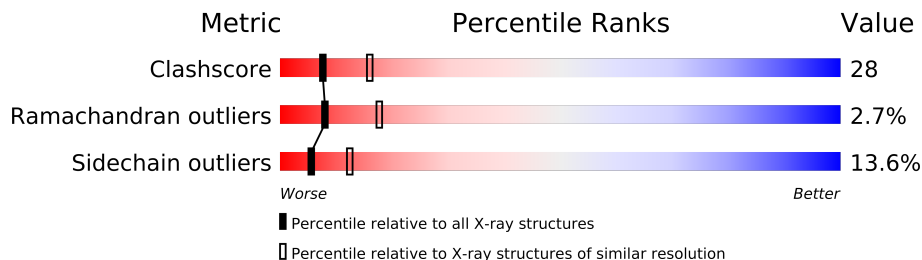
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.67 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))
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	
1	C	315	
2	B	99	
2	D	99	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6026 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2192	1396	378	405	13			
1	C	273	Total	C	N	O	S	0	0	0
			2192	1396	378	405	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	CONFLICT	UNP P11609
C	201	HIS	ASP	CONFLICT	UNP P11609

- Molecule 2 is a protein called CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	D	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

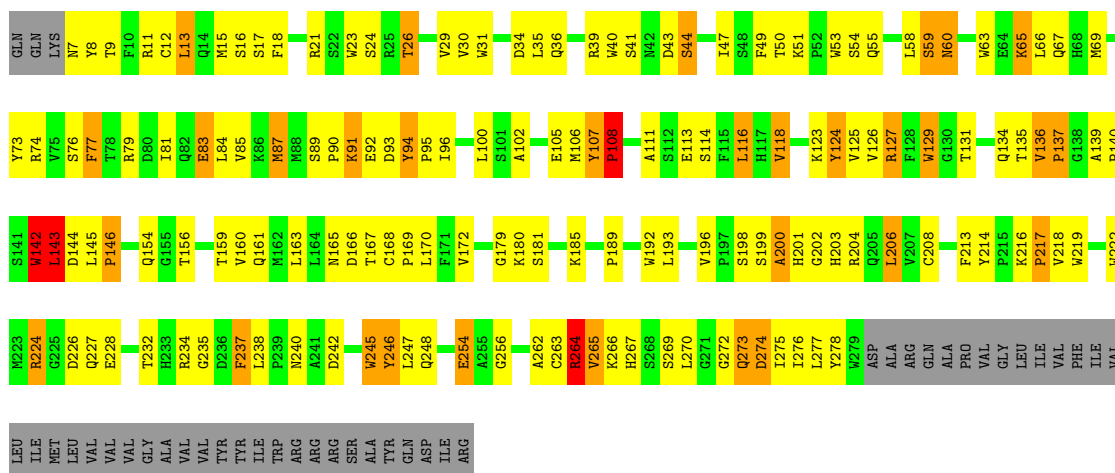
### 3 Residue-property plots

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.

Note EDS was not executed.

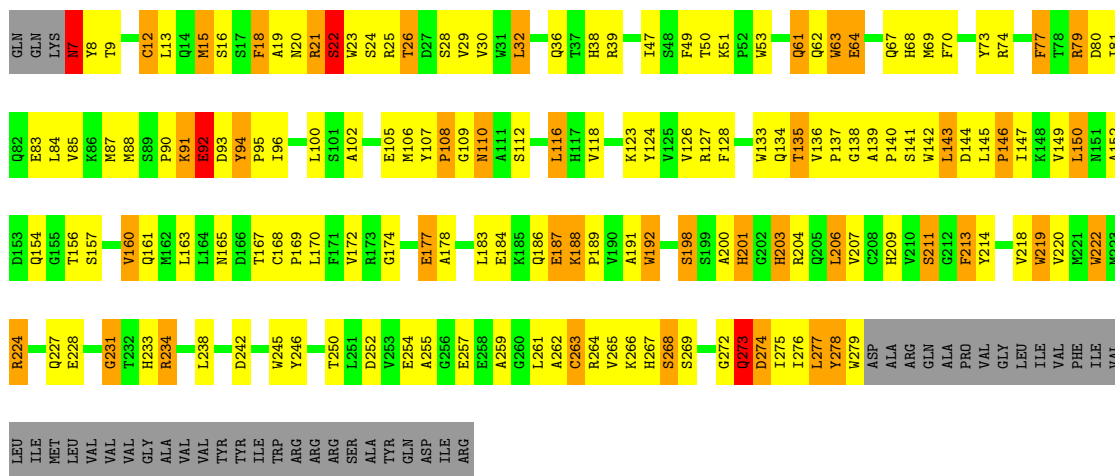
#### • Molecule 1: CD1

Chain A:



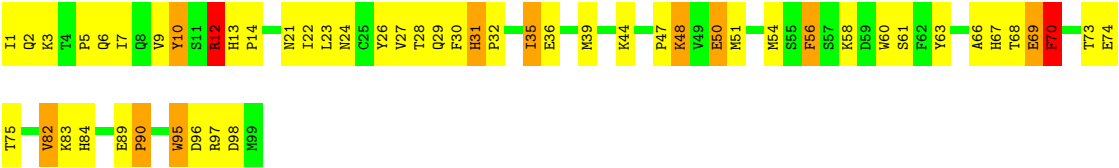
#### • Molecule 1: CD1

Chain C:



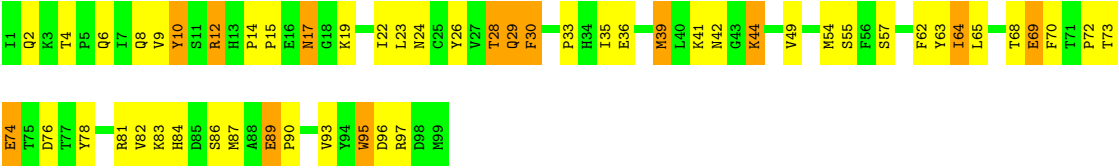
#### • Molecule 2: CD1

Chain B: 



• Molecule 2: CD1

Chain D: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.34Å 76.20Å 103.40Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	10.00 – 2.67	Depositor
% Data completeness (in resolution range)	83.7 (10.00-2.67)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.192 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	1.77	18/2257 (0.8%)	1.63	27/3069 (0.9%)
1	C	1.78	21/2257 (0.9%)	1.51	15/3069 (0.5%)
2	B	1.76	6/847 (0.7%)	1.52	5/1148 (0.4%)
2	D	1.76	5/847 (0.6%)	1.52	8/1148 (0.7%)
All	All	1.77	50/6208 (0.8%)	1.56	55/8434 (0.7%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ARG	CZ-NH1	7.53	1.42	1.33
1	A	264	ARG	CZ-NH2	7.46	1.42	1.33
1	C	278	TYR	CD2-CE2	6.81	1.49	1.39
1	C	22	SER	CA-CB	6.59	1.62	1.52
1	A	124	TYR	CD1-CE1	6.42	1.49	1.39
1	C	7	ASN	N-CA	6.37	1.59	1.46
1	C	25	ARG	CZ-NH2	6.33	1.41	1.33
1	C	222	TRP	CB-CG	-6.31	1.38	1.50
1	A	23	TRP	NE1-CE2	-6.28	1.29	1.37
2	B	26	TYR	CE1-CZ	6.27	1.46	1.38
2	D	8	GLN	N-CA	6.18	1.58	1.46
1	A	256	GLY	N-CA	-6.09	1.36	1.46
1	A	278	TYR	CD1-CE1	-6.06	1.30	1.39
1	A	245	TRP	NE1-CE2	-5.98	1.29	1.37
2	B	10	TYR	CG-CD2	5.97	1.47	1.39
2	D	10	TYR	CG-CD2	-5.96	1.31	1.39
1	C	177	GLU	CD-OE1	5.95	1.32	1.25
2	D	74	GLU	CB-CG	5.85	1.63	1.52
1	A	8	TYR	CG-CD1	-5.78	1.31	1.39
1	C	192	TRP	CG-CD1	-5.76	1.28	1.36
1	C	160	VAL	CA-CB	-5.68	1.42	1.54
1	A	114	SER	CB-OG	-5.62	1.34	1.42
1	C	8	TYR	CD2-CE2	5.60	1.47	1.39
1	C	245	TRP	CB-CG	-5.57	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	GLU	CD-OE1	5.55	1.31	1.25
1	A	245	TRP	CG-CD1	-5.51	1.29	1.36
1	A	269	SER	CB-OG	5.51	1.49	1.42
2	D	89	GLU	CG-CD	-5.49	1.43	1.51
1	C	222	TRP	CG-CD1	5.46	1.44	1.36
1	A	44	SER	CB-OG	-5.46	1.35	1.42
1	C	95	PRO	N-CA	5.42	1.56	1.47
2	D	10	TYR	CE1-CZ	-5.41	1.31	1.38
1	C	231	GLY	N-CA	5.40	1.54	1.46
1	A	224	ARG	CZ-NH1	-5.39	1.26	1.33
1	A	74	ARG	CZ-NH2	-5.38	1.26	1.33
1	C	211	SER	CB-OG	5.35	1.49	1.42
1	A	73	TYR	CG-CD1	5.33	1.46	1.39
2	B	31	HIS	CG-CD2	5.29	1.44	1.35
1	C	184	GLU	CD-OE1	5.29	1.31	1.25
2	B	50	GLU	CD-OE2	5.25	1.31	1.25
1	A	108	PRO	N-CA	5.24	1.56	1.47
1	C	152	ALA	CA-CB	5.19	1.63	1.52
1	C	18	PHE	CG-CD1	-5.19	1.30	1.38
1	C	12	CYS	CB-SG	-5.14	1.73	1.81
1	C	24	SER	CA-CB	5.11	1.60	1.52
2	B	69	GLU	CD-OE2	5.10	1.31	1.25
1	A	129	TRP	NE1-CE2	5.07	1.44	1.37
2	B	89	GLU	CD-OE2	5.03	1.31	1.25
1	C	64	GLU	N-CA	5.01	1.56	1.46
1	A	192	TRP	CZ2-CH2	-5.01	1.27	1.37

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-10.43	115.09	120.30
2	D	81	ARG	NE-CZ-NH2	-8.45	116.08	120.30
2	D	30	PHE	CB-CG-CD1	8.18	126.53	120.80
1	A	74	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	C	204	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	A	264	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	234	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	C	234	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	245	TRP	CE3-CZ3-CH2	6.78	128.66	121.20
1	A	224	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	B	70	PHE	CB-CG-CD1	6.76	125.53	120.80
1	A	129	TRP	CE2-CD2-CG	6.72	112.67	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	234	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	222	TRP	CD1-CG-CD2	-6.55	101.06	106.30
1	A	246	TYR	CG-CD1-CE1	6.55	126.54	121.30
1	A	204	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	11	ARG	NE-CZ-NH2	6.45	123.53	120.30
2	D	95	TRP	CD1-CG-CD2	6.39	111.42	106.30
1	C	110	ASN	N-CA-C	-6.33	93.91	111.00
2	B	12	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	A	107	TYR	CB-CG-CD1	6.22	124.73	121.00
1	A	129	TRP	CD1-CG-CD2	-6.17	101.37	106.30
1	A	246	TYR	CB-CG-CD1	6.09	124.65	121.00
1	A	226	ASP	CB-CG-OD2	-6.06	112.85	118.30
2	D	26	TYR	CB-CG-CD1	6.03	124.62	121.00
1	C	273	GLN	N-CA-C	5.91	126.97	111.00
1	C	77	PHE	CB-CG-CD2	-5.87	116.69	120.80
2	B	95	TRP	CD1-CG-CD2	5.82	110.96	106.30
2	D	30	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	A	8	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	C	94	TYR	C-N-CD	5.74	140.45	128.40
2	B	56	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	A	31	TRP	CG-CD2-CE3	5.67	139.01	133.90
1	A	224	ARG	N-CA-C	-5.63	95.80	111.00
1	A	127	ARG	NE-CZ-NH2	5.62	123.11	120.30
2	B	82	VAL	O-C-N	5.59	131.65	122.70
1	C	213	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	273	GLN	N-CA-C	5.55	125.98	111.00
1	A	129	TRP	CG-CD2-CE3	-5.52	128.94	133.90
2	D	81	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	74	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	254	GLU	N-CA-C	-5.35	96.56	111.00
1	A	237	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	A	73	TYR	CB-CG-CD2	5.34	124.20	121.00
1	A	272	GLY	N-CA-C	-5.34	99.76	113.10
1	C	32	LEU	N-CA-C	-5.32	96.64	111.00
2	D	95	TRP	CD1-NE1-CE2	5.32	113.78	109.00
1	C	63	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	C	272	GLY	N-CA-C	-5.21	100.07	113.10
2	D	69	GLU	N-CA-C	-5.12	97.17	111.00
1	A	11	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	184	GLU	OE1-CD-OE2	-5.11	117.16	123.30
1	A	142	TRP	CD1-NE1-CE2	-5.04	104.47	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2097	120	0
1	C	2192	0	2097	136	0
2	B	821	0	796	41	0
2	D	821	0	796	37	0
All	All	6026	0	5786	325	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (325) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:198:SER:HB2	1:C:201:HIS:HE1	1.26	1.00
1:C:102:ALA:HB2	1:C:116:LEU:HD23	1.43	0.97
1:C:9:THR:HG23	1:C:105:GLU:HG2	1.47	0.96
1:C:88:MET:HG3	1:C:92:GLU:HA	1.47	0.93
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.50	0.92
2:B:83:LYS:HG3	2:B:90:PRO:HG3	1.52	0.92
1:A:262:ALA:HB2	1:A:277:LEU:HD13	1.51	0.89
1:A:265:VAL:HG23	1:A:274:ASP:HB2	1.57	0.86
1:C:36:GLN:O	1:C:51:LYS:HE2	1.77	0.84
1:C:135:THR:HG23	1:C:139:ALA:HB3	1.60	0.83
1:C:189:PRO:HB3	1:C:213:PHE:HB3	1.59	0.82
1:A:118:VAL:HG22	1:A:126:VAL:HB	1.61	0.80
1:C:198:SER:HB2	1:C:201:HIS:CE1	2.14	0.80
1:A:203:HIS:CE1	1:A:254:GLU:HG3	2.18	0.79
1:C:102:ALA:HB2	1:C:116:LEU:CD2	2.13	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:83:LYS:HG2	2:D:90:PRO:HG3	1.65	0.78
2:B:1:ILE:HB	2:B:2:GLN:OE1	1.84	0.78
1:C:156:THR:O	1:C:160:VAL:HG23	1.83	0.76
1:C:18:PHE:HB2	1:C:96:ILE:HG13	1.66	0.76
1:C:106:MET:HG3	1:C:172:VAL:HG11	1.66	0.76
1:C:263:CYS:O	1:C:275:ILE:HA	1.87	0.75
1:C:186:GLN:HE22	1:C:268:SER:HB2	1.51	0.75
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.67	0.75
1:A:140:PRO:HG2	1:A:143:LEU:HD23	1.69	0.74
1:A:201:HIS:CD2	1:A:203:HIS:HB2	2.22	0.74
1:C:88:MET:SD	1:C:91:LYS:O	2.46	0.74
1:C:262:ALA:HB2	1:C:277:LEU:HA	1.70	0.74
1:C:18:PHE:HB2	1:C:96:ILE:CG1	2.18	0.73
1:A:16:SER:HB3	1:A:18:PHE:HE1	1.56	0.71
1:C:47:ILE:HD13	1:C:67:GLN:HG3	1.70	0.71
1:C:145:LEU:HB2	1:C:146:PRO:HD3	1.71	0.71
2:D:89:GLU:HG3	2:D:90:PRO:HD2	1.73	0.70
1:A:216:LYS:HB3	1:A:217:PRO:HD3	1.71	0.70
1:A:102:ALA:HB2	1:A:116:LEU:HD23	1.73	0.70
1:A:159:THR:O	1:A:163:LEU:HG	1.92	0.70
1:C:88:MET:CG	1:C:92:GLU:HA	2.21	0.70
1:C:265:VAL:O	1:C:273:GLN:HB2	1.92	0.69
1:C:32:LEU:HD23	1:C:183:LEU:HD21	1.72	0.69
1:C:238:LEU:HD12	1:C:246:TYR:HD2	1.57	0.69
1:C:102:ALA:CB	1:C:116:LEU:HD23	2.20	0.69
1:A:36:GLN:O	1:A:51:LYS:HE2	1.92	0.69
1:A:262:ALA:CB	1:A:277:LEU:HD13	2.23	0.68
1:C:262:ALA:CB	1:C:277:LEU:HA	2.22	0.68
2:D:49:VAL:HG22	2:D:68:THR:HB	1.75	0.68
1:C:186:GLN:HB3	1:C:269:SER:HB3	1.76	0.67
2:B:29:GLN:HA	2:B:61:SER:HB2	1.76	0.67
1:A:125:VAL:HG23	1:A:126:VAL:HG23	1.76	0.67
1:A:219:TRP:HB3	1:A:266:LYS:HB3	1.76	0.66
2:D:4:THR:HG22	2:D:86:SER:HB2	1.78	0.66
1:C:211:SER:HB2	1:C:246:TYR:HD1	1.61	0.66
1:C:186:GLN:NE2	1:C:268:SER:HB2	2.09	0.66
1:C:84:LEU:HD11	1:C:146:PRO:HB3	1.77	0.66
2:D:28:THR:HG22	2:D:29:GLN:H	1.61	0.66
1:C:118:VAL:CG2	1:C:126:VAL:HB	2.26	0.65
1:C:161:GLN:O	1:C:165:ASN:HB2	1.97	0.65
1:A:118:VAL:CG2	1:A:126:VAL:HB	2.25	0.65
1:C:7:ASN:HA	1:C:106:MET:O	1.95	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:SER:HB3	1:A:18:PHE:CE1	2.31	0.65
1:C:127:ARG:HG2	1:C:134:GLN:HG3	1.80	0.64
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.62	0.64
1:C:133:TRP:CD1	1:C:150:LEU:HG	2.31	0.64
1:C:100:LEU:HD21	1:C:116:LEU:HD21	1.80	0.64
1:A:201:HIS:HD2	1:A:203:HIS:HB2	1.62	0.64
1:A:51:LYS:HB2	1:A:54:SER:OG	1.98	0.63
2:B:50:GLU:HB3	2:B:67:HIS:NE2	2.13	0.63
1:A:65:LYS:HA	1:A:65:LYS:HE3	1.80	0.62
1:A:18:PHE:HB2	1:A:96:ILE:CG1	2.29	0.62
2:B:28:THR:HG22	2:B:29:GLN:H	1.63	0.62
2:D:28:THR:HG23	2:D:63:TYR:HB3	1.81	0.62
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.35	0.62
1:C:168:CYS:HB3	1:C:169:PRO:CD	2.29	0.61
2:D:30:PHE:HZ	2:D:54:MET:CE	2.14	0.60
1:C:219:TRP:HE1	1:C:264:ARG:HG2	1.66	0.60
1:A:161:GLN:O	1:A:165:ASN:HB2	2.01	0.60
1:C:77:PHE:O	1:C:81:ILE:HG12	2.02	0.60
2:B:28:THR:HG23	2:B:63:TYR:HB3	1.84	0.60
1:A:106:MET:HG3	1:A:172:VAL:HG11	1.83	0.60
2:D:10:TYR:CE2	2:D:24:ASN:HB2	2.37	0.60
1:A:41:SER:HB2	1:A:43:ASP:OD1	2.02	0.60
1:A:264:ARG:NH1	1:A:264:ARG:HG2	2.16	0.59
1:C:15:MET:O	1:C:26:THR:HA	2.01	0.59
1:C:39:ARG:HB3	1:C:39:ARG:HH11	1.66	0.59
1:C:116:LEU:HD12	1:C:133:TRP:CH2	2.37	0.59
2:D:70:PHE:HB2	2:D:78:TYR:CE2	2.36	0.59
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.84	0.59
1:C:265:VAL:HB	1:C:274:ASP:OD1	2.03	0.59
1:C:157:SER:O	1:C:161:GLN:HG3	2.03	0.59
1:C:30:VAL:HG22	1:C:38:HIS:HB2	1.85	0.58
1:A:131:THR:HG22	1:A:161:GLN:CD	2.24	0.58
2:D:44:LYS:NZ	2:D:44:LYS:HB2	2.18	0.58
2:B:2:GLN:N	2:B:2:GLN:OE1	2.36	0.58
1:A:47:ILE:CD1	1:A:67:GLN:HG3	2.34	0.58
1:C:84:LEU:CD1	1:C:146:PRO:HB3	2.33	0.58
1:A:100:LEU:HD21	1:A:116:LEU:HD21	1.86	0.58
2:D:35:ILE:HD11	2:D:82:VAL:CG1	2.35	0.57
1:C:264:ARG:HH21	1:C:275:ILE:HD11	1.68	0.57
2:D:97:ARG:O	2:D:97:ARG:HG2	2.04	0.57
1:C:39:ARG:HB3	1:C:39:ARG:NH1	2.19	0.57
1:A:179:GLY:O	1:A:181:SER:N	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:30:PHE:HZ	2:D:54:MET:HE2	1.70	0.57
1:A:237:PHE:HB3	1:A:245:TRP:CE3	2.40	0.56
1:A:240:ASN:OD1	2:B:12:ARG:HG2	2.06	0.56
1:C:69:MET:SD	1:C:163:LEU:HD21	2.45	0.56
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.87	0.56
2:D:17:ASN:OD1	2:D:74:GLU:HG3	2.06	0.56
1:C:106:MET:HG3	1:C:172:VAL:CG1	2.36	0.55
1:A:13:LEU:HB3	2:B:56:PHE:CE2	2.40	0.55
1:A:203:HIS:ND1	1:A:254:GLU:HG3	2.20	0.55
1:A:123:LYS:HD3	1:A:124:TYR:O	2.06	0.55
1:A:265:VAL:CG2	1:A:274:ASP:HB2	2.34	0.55
1:C:29:VAL:HG23	1:C:36:GLN:NE2	2.21	0.55
1:C:79:ARG:HG3	1:C:80:ASP:N	2.20	0.55
2:B:36:GLU:OE1	2:B:36:GLU:HA	2.06	0.55
1:A:222:TRP:HD1	1:A:232:THR:HG23	1.73	0.54
1:A:142:TRP:O	1:A:146:PRO:HD2	2.07	0.54
1:A:15:MET:O	1:A:26:THR:HA	2.07	0.54
1:A:94:TYR:CD1	1:A:94:TYR:O	2.60	0.54
1:A:83:GLU:O	1:A:87:MET:SD	2.66	0.54
1:C:29:VAL:CG2	1:C:36:GLN:NE2	2.70	0.54
2:B:9:VAL:HG11	2:B:95:TRP:HB2	1.89	0.53
2:D:73:THR:OG1	2:D:76:ASP:HB2	2.08	0.53
1:A:94:TYR:O	1:A:96:ILE:N	2.41	0.53
1:A:263:CYS:O	1:A:275:ILE:HA	2.07	0.53
1:C:29:VAL:HG11	2:D:55:SER:OG	2.09	0.53
1:A:60:ASN:N	1:A:60:ASN:OD1	2.41	0.53
1:A:136:VAL:HG22	1:A:137:PRO:HD2	1.91	0.53
1:A:18:PHE:HB2	1:A:96:ILE:HG12	1.88	0.53
1:A:94:TYR:HD1	1:A:94:TYR:O	1.92	0.53
1:C:118:VAL:HG21	1:C:126:VAL:HB	1.90	0.53
1:C:116:LEU:HD12	1:C:133:TRP:CZ3	2.44	0.52
1:C:224:ARG:NH2	1:C:259:ALA:O	2.42	0.52
1:A:156:THR:O	1:A:160:VAL:HG23	2.08	0.52
1:A:13:LEU:HB3	2:B:56:PHE:CZ	2.44	0.52
1:C:88:MET:O	1:C:88:MET:HG3	2.09	0.52
1:A:219:TRP:HZ2	1:A:228:GLU:OE2	1.93	0.52
1:C:140:PRO:O	1:C:143:LEU:HB2	2.10	0.52
1:C:145:LEU:O	1:C:149:VAL:HG23	2.10	0.52
2:B:35:ILE:HD11	2:B:82:VAL:HG13	1.92	0.51
1:A:47:ILE:HD13	1:A:67:GLN:HG3	1.92	0.51
1:C:211:SER:HB2	1:C:246:TYR:CD1	2.42	0.51
1:C:107:TYR:HB2	1:C:110:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:220:VAL:H	1:C:234:ARG:HH21	1.57	0.51
1:C:53:TRP:HB2	1:C:178:ALA:HB1	1.91	0.51
1:C:32:LEU:CD2	1:C:183:LEU:HD21	2.40	0.51
1:A:135:THR:HG23	1:A:139:ALA:HB3	1.93	0.51
1:C:227:GLN:HG2	1:C:228:GLU:O	2.11	0.51
2:B:48:LYS:HE3	2:B:50:GLU:OE1	2.10	0.51
1:A:218:VAL:HG23	1:A:267:HIS:HB2	1.93	0.51
1:C:116:LEU:CD1	1:C:133:TRP:CH2	2.94	0.51
2:B:28:THR:HG22	2:B:29:GLN:N	2.26	0.51
1:C:220:VAL:HG22	1:C:265:VAL:HG13	1.93	0.50
1:A:90:PRO:O	1:A:92:GLU:N	2.38	0.50
2:D:22:ILE:HG23	2:D:68:THR:O	2.11	0.50
2:B:35:ILE:HG13	2:B:83:LYS:O	2.12	0.50
1:A:206:LEU:HB3	1:A:222:TRP:CH2	2.47	0.50
1:C:7:ASN:N	1:C:7:ASN:OD1	2.44	0.50
1:A:198:SER:OG	1:A:203:HIS:O	2.30	0.50
1:C:79:ARG:HG2	1:C:79:ARG:HH11	1.77	0.49
1:A:77:PHE:O	1:A:81:ILE:HG12	2.12	0.49
1:A:200:ALA:O	1:A:201:HIS:HB3	2.12	0.49
1:C:267:HIS:ND1	1:C:269:SER:OG	2.45	0.49
2:D:41:LYS:O	2:D:44:LYS:HE3	2.11	0.49
1:C:238:LEU:HD12	1:C:246:TYR:CD2	2.44	0.49
1:C:94:TYR:O	1:C:96:ILE:N	2.45	0.49
2:B:51:MET:HG2	2:B:66:ALA:HA	1.94	0.49
1:A:237:PHE:CE1	1:A:247:LEU:HD22	2.48	0.49
1:C:257:GLU:C	1:C:259:ALA:H	2.15	0.49
1:C:242:ASP:OD2	2:D:12:ARG:NH1	2.45	0.49
1:C:123:LYS:HD3	1:C:124:TYR:O	2.13	0.49
1:A:18:PHE:HB2	1:A:96:ILE:HG13	1.94	0.48
1:A:107:TYR:HB2	1:A:111:ALA:O	2.13	0.48
2:D:33:PRO:HB3	2:D:62:PHE:CE2	2.48	0.48
1:A:166:ASP:O	1:A:169:PRO:HD2	2.12	0.48
1:A:202:GLY:O	1:A:203:HIS:ND1	2.46	0.48
1:A:224:ARG:O	1:A:227:GLN:HB2	2.13	0.48
2:B:69:GLU:H	2:B:69:GLU:CD	2.16	0.48
1:C:118:VAL:HG22	1:C:126:VAL:HB	1.96	0.48
2:B:73:THR:HG22	2:B:75:THR:H	1.77	0.48
1:A:266:LYS:HE3	1:A:273:GLN:NE2	2.29	0.48
2:D:28:THR:HG23	2:D:63:TYR:CB	2.41	0.48
1:A:47:ILE:H	1:A:47:ILE:HD12	1.78	0.48
1:C:70:PHE:HA	1:C:73:TYR:HB3	1.95	0.48
1:C:206:LEU:HB3	1:C:222:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:LEU:HD21	1:A:214:TYR:CE2	2.48	0.48
1:A:131:THR:HG22	1:A:161:GLN:NE2	2.28	0.48
1:C:254:GLU:HG2	1:C:255:ALA:N	2.29	0.48
1:C:112:SER:OG	1:C:169:PRO:HG3	2.14	0.48
2:D:19:LYS:O	2:D:72:PRO:HD2	2.14	0.48
1:C:50:THR:O	1:C:51:LYS:HG3	2.13	0.47
1:C:219:TRP:HD1	1:C:219:TRP:O	1.98	0.47
1:A:106:MET:HG3	1:A:172:VAL:CG1	2.43	0.47
1:A:135:THR:CG2	1:A:139:ALA:HB3	2.44	0.47
1:C:266:LYS:HE3	1:C:273:GLN:NE2	2.29	0.47
1:A:81:ILE:O	1:A:85:VAL:HG23	2.14	0.47
1:C:188:LYS:HE3	1:C:188:LYS:HB3	1.60	0.47
1:A:216:LYS:HE2	1:A:237:PHE:CG	2.50	0.47
1:C:219:TRP:CD1	1:C:219:TRP:O	2.68	0.47
1:A:216:LYS:HD2	1:A:245:TRP:CE2	2.50	0.47
1:C:174:GLY:O	1:C:177:GLU:HB3	2.15	0.47
1:C:16:SER:HB3	1:C:18:PHE:HE1	1.79	0.46
1:C:220:VAL:N	1:C:234:ARG:HH21	2.12	0.46
1:A:107:TYR:HE2	1:A:113:GLU:HG3	1.80	0.46
1:C:108:PRO:HG2	1:C:109:GLY:H	1.80	0.46
2:D:68:THR:OG1	2:D:69:GLU:N	2.48	0.46
2:D:64:ILE:HG13	2:D:65:LEU:H	1.80	0.46
1:C:219:TRP:C	1:C:219:TRP:CD1	2.88	0.46
2:B:74:GLU:HG2	2:B:75:THR:HG23	1.98	0.46
1:C:20:ASN:C	1:C:22:SER:H	2.18	0.46
2:B:10:TYR:CE2	2:B:24:ASN:HB2	2.51	0.46
1:C:219:TRP:CD1	1:C:266:LYS:HG3	2.50	0.46
1:A:29:VAL:CG2	1:A:36:GLN:NE2	2.79	0.46
1:A:238:LEU:HD12	1:A:246:TYR:HD2	1.81	0.46
2:D:35:ILE:HD11	2:D:82:VAL:HG11	1.97	0.46
1:C:61:GLN:HA	1:C:64:GLU:HG2	1.98	0.46
1:C:201:HIS:NE2	1:C:203:HIS:HB2	2.31	0.46
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.45	0.46
1:A:140:PRO:CG	1:A:143:LEU:HD23	2.42	0.46
1:C:264:ARG:NE	1:C:273:GLN:OE1	2.48	0.46
1:C:267:HIS:HD1	1:C:269:SER:H	1.63	0.46
2:D:84:HIS:HD2	2:D:86:SER:OG	1.98	0.46
1:C:192:TRP:CE3	2:D:14:PRO:HD3	2.51	0.46
1:A:53:TRP:CE2	1:A:179:GLY:HA2	2.51	0.45
2:D:42:ASN:ND2	2:D:76:ASP:OD1	2.49	0.45
1:C:200:ALA:O	1:C:201:HIS:HB3	2.15	0.45
1:C:191:ALA:HA	1:C:209:HIS:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:CYS:O	1:A:248:GLN:HA	2.17	0.45
2:B:96:ASP:O	2:B:98:ASP:N	2.45	0.45
1:C:201:HIS:CE1	1:C:203:HIS:HB2	2.51	0.45
1:C:273:GLN:HB3	1:C:273:GLN:HE21	1.61	0.45
1:C:142:TRP:O	1:C:144:ASP:N	2.49	0.45
1:A:65:LYS:HA	1:A:65:LYS:CE	2.44	0.45
1:C:278:TYR:O	1:C:279:TRP:HB2	2.16	0.45
2:B:58:LYS:HA	2:B:58:LYS:HD2	1.80	0.45
2:B:9:VAL:HG12	2:B:95:TRP:HD1	1.82	0.45
1:C:16:SER:HB3	1:C:18:PHE:CE1	2.52	0.45
2:D:30:PHE:CZ	2:D:54:MET:CE	2.99	0.45
1:A:238:LEU:HB2	1:A:246:TYR:HB3	1.98	0.45
1:A:213:PHE:HE2	1:A:216:LYS:O	2.00	0.45
1:C:138:GLY:O	1:C:140:PRO:HD3	2.17	0.45
1:C:142:TRP:O	1:C:146:PRO:HD2	2.17	0.45
1:A:264:ARG:HD3	1:A:275:ILE:HG12	1.99	0.45
1:C:69:MET:CE	1:C:163:LEU:HD11	2.46	0.45
2:D:39:MET:HB2	2:D:49:VAL:HG21	1.99	0.45
2:B:50:GLU:HB3	2:B:67:HIS:CE1	2.52	0.44
1:A:235:GLY:O	1:A:247:LEU:HD11	2.17	0.44
1:A:140:PRO:HG2	1:A:143:LEU:CD2	2.45	0.44
2:D:23:LEU:HB2	2:D:70:PHE:CD1	2.52	0.44
1:C:136:VAL:HB	1:C:137:PRO:HD2	1.99	0.44
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.86	0.44
1:A:94:TYR:C	1:A:94:TYR:CD1	2.91	0.44
1:A:66:LEU:O	1:A:69:MET:HB2	2.18	0.44
1:A:262:ALA:CB	1:A:277:LEU:HA	2.47	0.44
1:A:265:VAL:O	1:A:273:GLN:HB2	2.18	0.44
1:A:102:ALA:HB2	1:A:116:LEU:CD2	2.44	0.44
2:D:9:VAL:HG12	2:D:23:LEU:HD11	1.99	0.44
1:C:146:PRO:O	1:C:149:VAL:HB	2.18	0.43
2:B:9:VAL:HG12	2:B:95:TRP:CD1	2.53	0.43
2:B:3:LYS:HE2	2:B:31:HIS:CB	2.48	0.43
1:A:193:LEU:HG	1:A:276:ILE:HG21	1.99	0.43
1:C:79:ARG:O	1:C:83:GLU:HG3	2.17	0.43
1:A:267:HIS:HB3	1:A:270:LEU:HD13	1.99	0.43
1:A:39:ARG:HB3	1:A:39:ARG:HH11	1.82	0.43
1:C:266:LYS:HE3	1:C:273:GLN:HE22	1.82	0.43
1:C:207:VAL:HG22	1:C:250:THR:HG22	2.01	0.43
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.29	0.43
1:A:58:LEU:HD12	1:A:63:TRP:HE3	1.83	0.43
1:C:257:GLU:C	1:C:259:ALA:N	2.71	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:22:ILE:HG23	2:B:68:THR:O	2.17	0.43
1:C:19:ALA:HB3	1:C:23:TRP:HB3	2.00	0.43
2:D:9:VAL:HG23	2:D:93:VAL:CG2	2.48	0.43
1:A:107:TYR:HA	1:A:108:PRO:HD3	1.84	0.43
1:A:216:LYS:HB3	1:A:217:PRO:CD	2.46	0.43
1:C:238:LEU:O	1:C:246:TYR:N	2.52	0.43
1:A:59:SER:O	1:A:60:ASN:C	2.56	0.43
2:B:32:PRO:O	2:B:84:HIS:HE1	2.02	0.43
1:A:49:PHE:CE2	1:A:55:GLN:HB2	2.54	0.43
1:C:47:ILE:HD12	1:C:47:ILE:N	2.34	0.42
1:A:60:ASN:O	1:A:63:TRP:N	2.52	0.42
1:A:168:CYS:HB3	1:A:169:PRO:HD3	2.00	0.42
2:B:23:LEU:HD23	2:B:39:MET:HE3	2.00	0.42
2:B:7:ILE:HD11	2:B:82:VAL:HB	2.02	0.42
1:C:67:GLN:HG2	1:C:67:GLN:O	2.18	0.42
1:A:142:TRP:O	1:A:144:ASP:N	2.52	0.42
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.53	0.42
1:C:133:TRP:O	1:C:147:ILE:HD12	2.19	0.42
1:C:220:VAL:H	1:C:234:ARG:NH2	2.17	0.42
2:B:13:HIS:HB3	2:B:14:PRO:HD2	2.02	0.42
1:A:39:ARG:HG2	1:A:40:TRP:N	2.35	0.42
1:A:49:PHE:HE1	1:A:63:TRP:CZ2	2.38	0.42
1:C:224:ARG:NH1	1:C:257:GLU:HG3	2.34	0.42
1:C:140:PRO:HB3	1:C:142:TRP:CZ3	2.54	0.42
1:A:76:SER:HA	1:A:79:ARG:HG2	2.00	0.42
1:C:262:ALA:CB	1:C:277:LEU:HD13	2.50	0.42
2:D:83:LYS:CG	2:D:90:PRO:HG3	2.42	0.42
1:A:9:THR:HG23	1:A:105:GLU:HG2	2.01	0.42
1:C:112:SER:OG	1:C:169:PRO:CG	2.67	0.41
1:A:242:ASP:OD2	2:B:12:ARG:NH1	2.52	0.41
1:A:39:ARG:NH1	1:A:39:ARG:HB3	2.36	0.41
1:C:218:VAL:HG22	1:C:219:TRP:N	2.35	0.41
1:C:79:ARG:NH1	1:C:79:ARG:HG2	2.34	0.41
1:C:53:TRP:HB2	1:C:178:ALA:CB	2.50	0.41
1:A:34:ASP:O	1:A:35:LEU:HD23	2.20	0.41
2:B:23:LEU:HD23	2:B:39:MET:CE	2.51	0.41
1:C:90:PRO:O	1:C:92:GLU:HG2	2.21	0.41
1:A:126:VAL:HG12	1:A:127:ARG:N	2.36	0.41
1:A:94:TYR:O	1:A:96:ILE:HG23	2.19	0.41
2:B:12:ARG:HE	2:B:13:HIS:CE1	2.38	0.41
2:B:3:LYS:HE2	2:B:31:HIS:HB3	2.03	0.41
1:A:262:ALA:HB2	1:A:277:LEU:HA	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:18:PHE:HB2	1:C:96:ILE:HG12	2.00	0.41
2:B:68:THR:OG1	2:B:69:GLU:N	2.53	0.41
1:A:238:LEU:HD12	1:A:246:TYR:CD2	2.55	0.41
1:A:143:LEU:HD13	1:A:143:LEU:HA	1.85	0.41
1:A:50:THR:O	1:A:51:LYS:HD3	2.21	0.41
1:A:15:MET:HE3	2:B:54:MET:O	2.21	0.41
1:C:49:PHE:HE1	1:C:63:TRP:CZ2	2.38	0.41
1:C:134:GLN:HA	1:C:147:ILE:HD12	2.02	0.40
1:C:262:ALA:HB2	1:C:277:LEU:HD13	2.03	0.40
1:A:265:VAL:O	1:A:273:GLN:HG3	2.21	0.40
1:C:128:PHE:CD1	1:C:160:VAL:HG11	2.56	0.40
1:C:187:GLU:HB2	1:C:214:TYR:HB3	2.02	0.40
1:C:231:GLY:O	1:C:233:HIS:ND1	2.53	0.40
1:C:192:TRP:CZ3	2:D:14:PRO:HD3	2.57	0.40
1:A:17:SER:O	1:A:24:SER:HA	2.22	0.40
2:D:95:TRP:CE2	2:D:96:ASP:O	2.74	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	271/315 (86%)	229 (84%)	33 (12%)	9 (3%)	6	12
1	C	271/315 (86%)	232 (86%)	33 (12%)	6 (2%)	10	24
2	B	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	7	14
2	D	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	11	25
All	All	736/828 (89%)	635 (86%)	81 (11%)	20 (3%)	8	18

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	199	SER

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Mol	Chain	Res	Type
2	B	97	ARG
2	D	29	GLN
1	A	91	LYS
1	A	108	PRO
1	A	200	ALA
1	C	21	ARG
1	C	92	GLU
1	C	143	LEU
1	A	143	LEU
1	C	141	SER
1	A	21	ARG
1	A	95	PRO
2	B	60	TRP
1	C	198	SER
1	C	108	PRO
1	A	217	PRO
2	B	47	PRO
2	D	15	PRO

### 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	238/274 (87%)	203 (85%)	35 (15%)	4	11
1	C	238/274 (87%)	201 (84%)	37 (16%)	4	9
2	B	94/94 (100%)	87 (93%)	7 (7%)	20	41
2	D	94/94 (100%)	83 (88%)	11 (12%)	8	17
All	All	664/736 (90%)	574 (86%)	90 (14%)	5	12

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	CYS
1	A	13	LEU
1	A	26	THR

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Mol	Chain	Res	Type
1	A	30	VAL
1	A	44	SER
1	A	59	SER
1	A	60	ASN
1	A	65	LYS
1	A	77	PHE
1	A	83	GLU
1	A	84	LEU
1	A	87	MET
1	A	89	SER
1	A	91	LYS
1	A	93	ASP
1	A	94	TYR
1	A	116	LEU
1	A	118	VAL
1	A	134	GLN
1	A	136	VAL
1	A	137	PRO
1	A	142	TRP
1	A	143	LEU
1	A	145	LEU
1	A	146	PRO
1	A	154	GLN
1	A	167	THR
1	A	170	LEU
1	A	185	LYS
1	A	196	VAL
1	A	206	LEU
1	A	264	ARG
1	A	265	VAL
1	A	274	ASP
2	B	6	GLN
2	B	12	ARG
2	B	35	ILE
2	B	44	LYS
2	B	48	LYS
2	B	70	PHE
2	B	90	PRO
1	C	7	ASN
1	C	12	CYS
1	C	13	LEU
1	C	15	MET

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Mol	Chain	Res	Type
1	C	21	ARG
1	C	22	SER
1	C	26	THR
1	C	28	SER
1	C	61	GLN
1	C	62	GLN
1	C	68	HIS
1	C	79	ARG
1	C	85	VAL
1	C	87	MET
1	C	91	LYS
1	C	92	GLU
1	C	116	LEU
1	C	135	THR
1	C	146	PRO
1	C	150	LEU
1	C	154	GLN
1	C	167	THR
1	C	170	LEU
1	C	188	LYS
1	C	201	HIS
1	C	203	HIS
1	C	206	LEU
1	C	219	TRP
1	C	224	ARG
1	C	252	ASP
1	C	261	LEU
1	C	263	CYS
1	C	268	SER
1	C	273	GLN
1	C	274	ASP
1	C	276	ILE
1	C	277	LEU
2	D	2	GLN
2	D	6	GLN
2	D	12	ARG
2	D	17	ASN
2	D	28	THR
2	D	36	GLU
2	D	39	MET
2	D	44	LYS
2	D	57	SER

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Mol	Chain	Res	Type
2	D	64	ILE
2	D	87	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	110	ASN
1	A	186	GLN
2	B	84	HIS
1	C	7	ASN
1	C	36	GLN
1	C	186	GLN
1	C	201	HIS
2	D	6	GLN
2	D	38	GLN
2	D	84	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.