



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:27 AM GMT

PDB ID : 3SIR
Title : Crystal Structure of drICE
Authors : Li, X.; Wang, J.; Shi, Y.
Deposited on : 2011-06-20
Resolution : 2.68 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

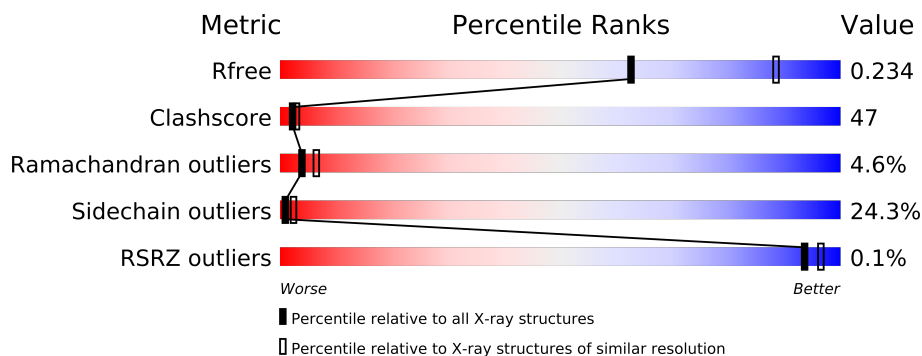
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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


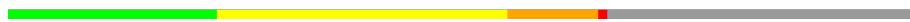


The reported resolution of this entry is 2.68 Å.

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}	66092	2010 (2.70-2.66)
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
1	C	259	
1	D	259	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5766 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 Caspase.

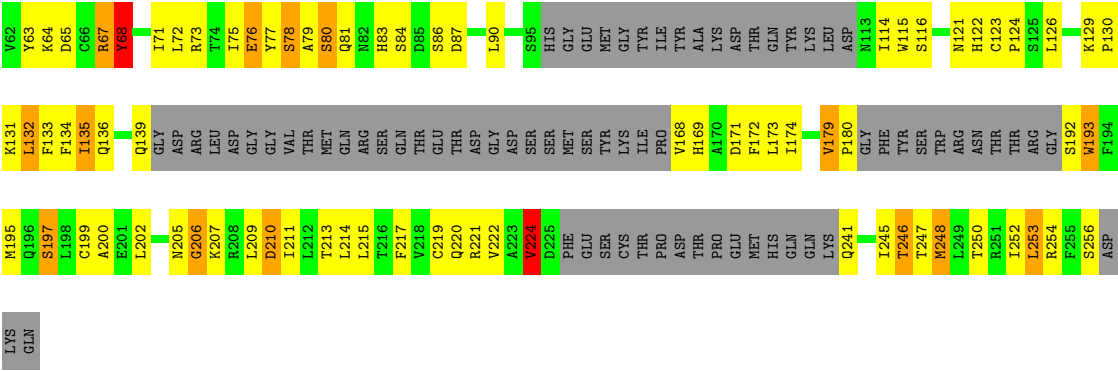
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1727	1102	300	312	13			
1	B	172	Total	C	N	O	S	0	0	0
			1377	882	236	246	13			
1	C	162	Total	C	N	O	S	0	0	0
			1298	830	224	232	12			
1	D	169	Total	C	N	O	S	0	0	0
			1361	873	234	244	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	SEE REMARK 999	UNP 001382
A	2	LEU	-	SEE REMARK 999	UNP 001382
A	3	GLY	-	SEE REMARK 999	UNP 001382
A	4	SER	-	SEE REMARK 999	UNP 001382
A	78	SER	ALA	ENGINEERED MUTATION	UNP 001382
B	1	ALA	-	SEE REMARK 999	UNP 001382
B	2	LEU	-	SEE REMARK 999	UNP 001382
B	3	GLY	-	SEE REMARK 999	UNP 001382
B	4	SER	-	SEE REMARK 999	UNP 001382
B	78	SER	ALA	ENGINEERED MUTATION	UNP 001382
C	1	ALA	-	SEE REMARK 999	UNP 001382
C	2	LEU	-	SEE REMARK 999	UNP 001382
C	3	GLY	-	SEE REMARK 999	UNP 001382
C	4	SER	-	SEE REMARK 999	UNP 001382
C	78	SER	ALA	ENGINEERED MUTATION	UNP 001382
D	1	ALA	-	SEE REMARK 999	UNP 001382
D	2	LEU	-	SEE REMARK 999	UNP 001382
D	3	GLY	-	SEE REMARK 999	UNP 001382
D	4	SER	-	SEE REMARK 999	UNP 001382
D	78	SER	ALA	ENGINEERED MUTATION	UNP 001382

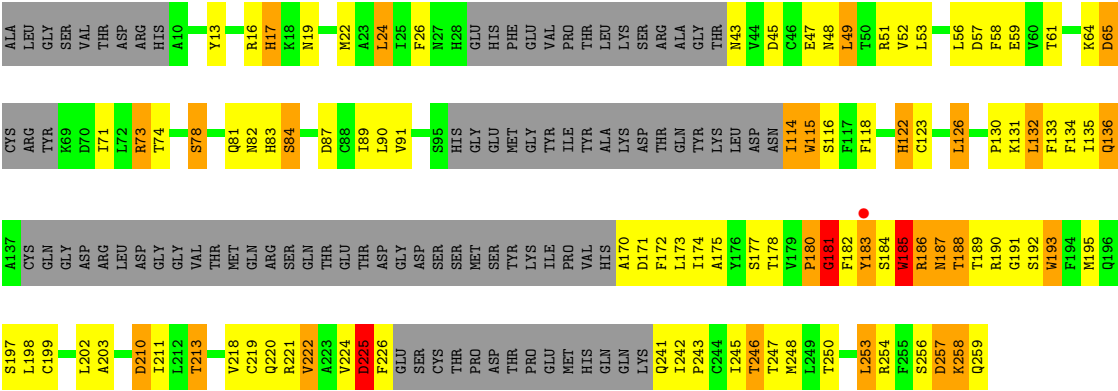
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		



● Molecule 1: Caspase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	56.02Å 56.02Å 287.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.97 – 2.68 45.97 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.97-2.68) 98.8 (45.97-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.235 0.164 , 0.234	Depositor DCC
R_{free} test set	1400 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.2	EDS
Estimated twinning fraction	0.294 for H, K, L 0.213 for -H, H+K, -L 0.214 for K, H, -L 0.279 for -H, -K, L 0.457 for -h,-k,l 0.417 for h,-h-k,-l 0.416 for -k,-h,-l	Xtriage
Reported twinning fraction	0.294 for H, K, L 0.213 for -H, H+K, -L 0.214 for K, H, -L 0.279 for -H, -K, L	Depositor
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 27934 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5766	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.26	0/1765	0.45	0/2384
1	B	0.25	0/1402	0.43	0/1891
1	C	0.25	0/1320	0.42	0/1781
1	D	0.24	0/1386	0.42	0/1869
All	All	0.25	0/5873	0.43	0/7925

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	7
1	C	0	2
1	D	0	4
All	All	0	21

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Peptide
1	A	183	TYR	Peptide
1	A	187	ASN	Peptide
1	A	190	ARG	Peptide
1	A	2	LEU	Peptide
1	A	241	GLN	Peptide
1	A	65	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	97	GLY	Peptide
1	B	166	ILE	Peptide
1	B	167	PRO	Peptide
1	B	168	VAL	Peptide
1	B	189	THR	Peptide
1	B	190	ARG	Peptide
1	B	223	ALA	Peptide
1	B	67	ARG	Peptide
1	C	44	VAL	Peptide
1	C	67	ARG	Peptide
1	D	136	GLN	Peptide
1	D	181	GLY	Peptide
1	D	182	PHE	Peptide
1	D	225	ASP	Peptide

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	1727	0	1694	221	0
1	B	1377	0	1375	126	0
1	C	1298	0	1296	106	0
1	D	1361	0	1353	114	0
2	A	3	0	0	0	0
All	All	5766	0	5718	545	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 47.

All (545) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:LEU:CA	1:A:114:ILE:HD11	1.52	1.36
1:A:109:TYR:CA	1:A:112:ASP:OD2	1.74	1.35
1:A:7:ASP:O	1:A:9:HIS:N	1.60	1.34
1:D:210:ASP:OD2	1:D:213:THR:HG23	1.19	1.32

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:LEU:O	1:A:114:ILE:CD1	1.80	1.28
1:A:109:TYR:HA	1:A:112:ASP:OD2	1.16	1.28
1:A:111:LEU:O	1:A:114:ILE:HD12	1.31	1.25
1:C:77:TYR:O	1:C:80:SER:HB2	1.38	1.20
1:B:15:MET:CE	1:B:253:LEU:HD11	1.74	1.17
1:A:111:LEU:C	1:A:114:ILE:HD11	1.66	1.13
1:A:98:GLU:HB3	1:A:182:PHE:O	1.45	1.13
1:A:111:LEU:HA	1:A:114:ILE:HD11	1.18	1.12
1:C:78:SER:HA	1:C:81:GLN:HE21	0.99	1.12
1:A:2:LEU:O	1:A:2:LEU:HD22	1.50	1.09
1:D:73:ARG:HG3	1:D:73:ARG:HH11	1.03	1.09
1:D:210:ASP:OD2	1:D:213:THR:CG2	2.04	1.04
1:A:241:GLN:HG2	1:A:241:GLN:O	1.53	1.03
1:D:64:LYS:O	1:D:65:ASP:HB3	1.58	1.00
1:B:52:VAL:HG13	1:B:203:ALA:HB2	1.43	1.00
1:B:15:MET:HE3	1:B:253:LEU:HD11	1.44	0.99
1:D:22:MET:CE	1:D:83:HIS:HE1	1.75	0.99
1:C:78:SER:HA	1:C:81:GLN:NE2	1.76	0.98
1:A:6:THR:C	1:A:7:ASP:OD1	2.01	0.98
1:A:111:LEU:C	1:A:114:ILE:CD1	2.26	0.97
1:C:210:ASP:OD2	1:C:213:THR:HG23	1.65	0.96
1:B:167:PRO:HB2	1:B:168:VAL:HG23	1.46	0.96
1:A:27:ASN:ND2	1:A:46:CYS:SG	2.37	0.96
1:A:56:LEU:O	1:A:57:ASP:HB2	1.62	0.95
1:B:15:MET:HE2	1:B:253:LEU:HD11	1.42	0.95
1:B:167:PRO:HB2	1:B:168:VAL:CG2	1.95	0.95
1:A:224:VAL:CG1	1:A:224:VAL:O	2.16	0.94
1:B:218:VAL:O	1:B:222:VAL:HG12	1.67	0.94
1:D:224:VAL:CG1	1:D:224:VAL:O	2.15	0.94
1:D:78:SER:HA	1:D:81:GLN:HE21	1.31	0.94
1:A:168:VAL:HA	1:A:248:MET:CE	1.97	0.94
1:A:72:LEU:HD11	1:A:111:LEU:CD2	1.96	0.94
1:D:22:MET:HE3	1:D:83:HIS:HE1	1.30	0.93
1:A:184:SER:O	1:A:185:TRP:HB2	1.66	0.93
1:A:28:HIS:O	1:A:96:HIS:HD2	1.52	0.93
1:C:27:ASN:HD22	1:C:27:ASN:N	1.67	0.92
1:A:254:ARG:HB2	1:A:254:ARG:NH1	1.83	0.92
1:D:188:THR:O	1:D:190:ARG:N	2.01	0.92
1:B:226:PHE:CE2	1:B:241:GLN:NE2	2.37	0.92
1:C:68:TYR:HD2	1:C:68:TYR:N	1.66	0.92
1:D:221:ARG:O	1:D:225:ASP:HB2	1.70	0.92
1:D:47:GLU:O	1:D:51:ARG:HG2	1.71	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:VAL:HG12	1:A:168:VAL:O	1.71	0.90
1:D:73:ARG:HG3	1:D:73:ARG:NH1	1.72	0.89
1:A:111:LEU:HA	1:A:114:ILE:CD1	2.02	0.89
1:A:114:ILE:H	1:A:114:ILE:HD12	1.37	0.89
1:A:109:TYR:N	1:A:112:ASP:OD2	2.04	0.89
1:A:90:LEU:HD11	1:A:134:PHE:CE1	2.06	0.89
1:D:22:MET:CE	1:D:83:HIS:CE1	2.55	0.88
1:B:15:MET:CE	1:B:253:LEU:CD1	2.51	0.88
1:D:73:ARG:CG	1:D:73:ARG:HH11	1.88	0.87
1:B:15:MET:SD	1:B:87:ASP:HB3	2.14	0.86
1:D:22:MET:HE3	1:D:83:HIS:CE1	2.09	0.86
1:B:72:LEU:HD22	1:B:114:ILE:HG23	1.55	0.86
1:C:68:TYR:N	1:C:68:TYR:CD2	2.41	0.86
1:D:89:ILE:O	1:D:132:LEU:CD2	2.24	0.85
1:C:67:ARG:HA	1:C:68:TYR:CD2	2.12	0.85
1:A:168:VAL:HA	1:A:248:MET:HE2	1.58	0.84
1:A:23:ALA:C	1:A:24:LEU:HD23	1.97	0.84
1:B:24:LEU:HB2	1:B:26:PHE:HE2	1.42	0.84
1:B:64:LYS:O	1:B:65:ASP:HB3	1.78	0.84
1:A:111:LEU:CA	1:A:114:ILE:CD1	2.48	0.83
1:A:111:LEU:HD23	1:A:111:LEU:H	1.41	0.83
1:B:164:TYR:CE1	1:B:166:ILE:HG23	2.13	0.83
1:B:15:MET:HE3	1:B:253:LEU:CD1	2.08	0.83
1:C:17:HIS:HB2	1:C:87:ASP:OD1	1.79	0.83
1:B:164:TYR:HE1	1:B:166:ILE:CG2	1.92	0.83
1:A:254:ARG:HH11	1:A:254:ARG:CB	1.91	0.83
1:A:241:GLN:CG	1:A:241:GLN:O	2.25	0.83
1:C:72:LEU:HD22	1:C:114:ILE:HG12	1.59	0.82
1:A:90:LEU:HD11	1:A:134:PHE:HE1	1.41	0.82
1:A:183:TYR:CD2	1:A:184:SER:HA	2.13	0.82
1:D:224:VAL:HG13	1:D:224:VAL:O	1.77	0.81
1:D:225:ASP:O	1:D:226:PHE:HB2	1.77	0.81
1:C:78:SER:CA	1:C:81:GLN:HE21	1.88	0.81
1:A:72:LEU:HD11	1:A:111:LEU:HD23	1.62	0.81
1:B:167:PRO:CB	1:B:168:VAL:HG23	2.10	0.81
1:A:109:TYR:O	1:A:113:ASN:ND2	2.14	0.81
1:A:111:LEU:HD23	1:A:111:LEU:N	1.96	0.80
1:A:143:LEU:HD12	1:A:164:TYR:O	1.83	0.79
1:C:173:LEU:C	1:C:173:LEU:HD23	2.01	0.79
1:B:15:MET:HE2	1:B:253:LEU:CD1	2.13	0.79
1:C:67:ARG:HA	1:C:68:TYR:HD2	1.47	0.79
1:C:43:ASN:O	1:C:47:GLU:HG3	1.82	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:THR:O	1:A:7:ASP:CG	2.21	0.79
1:A:193:TRP:O	1:A:197:SER:OG	2.00	0.78
1:A:136:GLN:NE2	1:A:195:MET:HG2	1.99	0.78
1:D:17:HIS:HB2	1:D:87:ASP:OD1	1.84	0.78
1:A:224:VAL:HG13	1:A:224:VAL:O	1.84	0.78
1:A:24:LEU:HD23	1:A:24:LEU:N	1.98	0.78
1:A:98:GLU:CB	1:A:182:PHE:O	2.30	0.77
1:A:28:HIS:O	1:A:96:HIS:CD2	2.36	0.77
1:C:246:THR:HB	1:D:246:THR:HB	1.66	0.77
1:D:132:LEU:H	1:D:132:LEU:HD22	1.49	0.77
1:A:182:PHE:N	1:A:182:PHE:HD1	1.83	0.77
1:C:77:TYR:O	1:C:80:SER:CB	2.26	0.77
1:C:193:TRP:O	1:C:197:SER:OG	2.03	0.77
1:A:167:PRO:O	1:A:168:VAL:HB	1.84	0.77
1:A:5:VAL:HG21	1:B:209:LEU:HD11	1.66	0.76
1:D:115:TRP:N	1:D:115:TRP:CD1	2.52	0.76
1:B:48:ASN:O	1:B:52:VAL:HG23	1.85	0.76
1:B:125:SER:O	1:B:129:LYS:NZ	2.18	0.76
1:D:132:LEU:N	1:D:132:LEU:HD22	2.00	0.76
1:A:192:SER:O	1:A:196:GLN:HG3	1.86	0.76
1:B:115:TRP:O	1:B:117:PHE:N	2.19	0.76
1:A:2:LEU:O	1:A:2:LEU:CD2	2.32	0.76
1:B:24:LEU:HB2	1:B:26:PHE:CE2	2.21	0.76
1:A:135:ILE:N	1:A:135:ILE:HD13	2.00	0.75
1:B:164:TYR:HE1	1:B:166:ILE:HG23	1.50	0.75
1:A:142:ARG:HB2	1:A:163:SER:HB2	1.67	0.75
1:D:90:LEU:HD23	1:D:91:VAL:N	2.01	0.75
1:D:22:MET:HE1	1:D:83:HIS:CE1	2.21	0.75
1:A:49:LEU:HG	1:A:195:MET:HE1	1.68	0.75
1:A:110:LYS:HA	1:A:113:ASN:ND2	2.01	0.75
1:A:108:GLN:C	1:A:112:ASP:OD2	2.25	0.74
1:A:199:CYS:O	1:A:203:ALA:CB	2.36	0.74
1:C:71:ILE:O	1:C:75:ILE:HG13	1.86	0.74
1:D:24:LEU:HD23	1:D:24:LEU:N	2.03	0.73
1:A:90:LEU:CD1	1:A:134:PHE:HE1	2.01	0.73
1:C:224:VAL:O	1:C:224:VAL:HG13	1.89	0.72
1:D:89:ILE:O	1:D:132:LEU:HD23	1.87	0.72
1:A:224:VAL:HG12	1:A:224:VAL:O	1.90	0.72
1:D:185:TRP:C	1:D:187:ASN:H	1.92	0.72
1:C:67:ARG:CA	1:C:68:TYR:HD2	2.01	0.72
1:A:101:TYR:O	1:A:102:ILE:HD12	1.89	0.72
1:A:7:ASP:HB2	1:B:220:GLN:NE2	2.04	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:114:ILE:HB	1:D:115:TRP:CD1	2.27	0.70
1:D:115:TRP:HD1	1:D:115:TRP:N	1.90	0.69
1:A:182:PHE:N	1:A:182:PHE:CD1	2.55	0.69
1:C:210:ASP:OD2	1:C:213:THR:CG2	2.40	0.69
1:A:110:LYS:O	1:A:111:LEU:C	2.30	0.69
1:A:6:THR:C	1:A:7:ASP:CG	2.51	0.69
1:A:135:ILE:CD1	1:A:135:ILE:N	2.54	0.69
1:C:67:ARG:C	1:C:68:TYR:HD2	1.95	0.69
1:B:220:GLN:O	1:B:224:VAL:HB	1.92	0.69
1:D:185:TRP:O	1:D:187:ASN:N	2.23	0.69
1:A:13:TYR:OH	1:A:171:ASP:OD1	2.08	0.69
1:B:250:THR:O	1:B:251:ARG:HG3	1.93	0.69
1:B:167:PRO:HB2	1:B:168:VAL:CA	2.22	0.68
1:D:43:ASN:O	1:D:47:GLU:HG3	1.93	0.68
1:A:253:LEU:HD12	1:A:254:ARG:N	2.08	0.68
1:A:168:VAL:O	1:A:168:VAL:CG1	2.41	0.68
1:A:183:TYR:CE2	1:A:184:SER:HA	2.28	0.68
1:D:118:PHE:HB3	1:D:131:LYS:HD3	1.75	0.68
1:A:218:VAL:O	1:A:222:VAL:HG12	1.93	0.68
1:B:24:LEU:N	1:B:24:LEU:HD23	2.08	0.68
1:D:64:LYS:O	1:D:65:ASP:CB	2.36	0.67
1:C:22:MET:CE	1:C:81:GLN:OE1	2.42	0.67
1:D:114:ILE:HB	1:D:115:TRP:HD1	1.59	0.67
1:C:27:ASN:ND2	1:C:27:ASN:N	2.40	0.67
1:A:22:MET:HB3	1:A:24:LEU:HD21	1.76	0.67
1:A:173:LEU:C	1:A:173:LEU:HD23	2.15	0.67
1:A:129:LYS:O	1:A:131:LYS:NZ	2.28	0.67
1:B:226:PHE:HB3	1:B:227:GLU:OE2	1.95	0.67
1:D:224:VAL:HG12	1:D:224:VAL:O	1.95	0.66
1:B:193:TRP:O	1:B:197:SER:OG	2.13	0.66
1:A:98:GLU:HB3	1:A:182:PHE:C	2.14	0.66
1:A:191:GLY:O	1:A:196:GLN:NE2	2.29	0.66
1:A:168:VAL:HA	1:A:248:MET:HE3	1.75	0.66
1:A:101:TYR:C	1:A:102:ILE:HD12	2.16	0.66
1:A:184:SER:O	1:A:185:TRP:CB	2.43	0.66
1:D:89:ILE:O	1:D:132:LEU:HD22	1.95	0.66
1:C:77:TYR:C	1:C:80:SER:HB2	2.16	0.66
1:B:218:VAL:O	1:B:222:VAL:CG1	2.43	0.66
1:A:199:CYS:O	1:A:203:ALA:HB3	1.96	0.66
1:A:71:ILE:O	1:A:75:ILE:HG13	1.95	0.65
1:B:115:TRP:C	1:B:117:PHE:H	2.00	0.65
1:A:49:LEU:HG	1:A:195:MET:CE	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:193:TRP:H	1:C:193:TRP:HE3	1.43	0.65
1:A:7:ASP:OD1	1:A:7:ASP:N	2.30	0.65
1:B:135:ILE:CD1	1:B:135:ILE:N	2.59	0.65
1:C:67:ARG:CA	1:C:68:TYR:CD2	2.78	0.65
1:D:218:VAL:O	1:D:222:VAL:HG12	1.95	0.65
1:A:254:ARG:NH1	1:A:254:ARG:CB	2.52	0.65
1:C:168:VAL:HA	1:C:248:MET:CE	2.26	0.64
1:A:250:THR:O	1:B:220:GLN:HB2	1.97	0.64
1:B:133:PHE:HB2	1:B:174:ILE:HG13	1.79	0.64
1:A:20:ARG:NH1	1:A:87:ASP:OD2	2.31	0.64
1:C:173:LEU:C	1:C:174:ILE:HD12	2.18	0.64
1:A:7:ASP:C	1:A:9:HIS:N	2.43	0.64
1:B:222:VAL:HG11	1:B:243:PRO:HD2	1.78	0.64
1:A:2:LEU:HD21	1:A:11:ALA:HB1	1.80	0.63
1:B:250:THR:O	1:B:251:ARG:CG	2.47	0.63
1:D:221:ARG:O	1:D:225:ASP:CB	2.46	0.63
1:B:228:SER:O	1:B:229:CYS:SG	2.57	0.63
1:C:13:TYR:OH	1:C:171:ASP:OD1	2.08	0.63
1:B:167:PRO:CG	1:B:168:VAL:HG23	2.29	0.62
1:A:78:SER:HA	1:A:81:GLN:HG3	1.80	0.62
1:B:134:PHE:C	1:B:135:ILE:HD12	2.20	0.62
1:A:20:ARG:O	1:A:87:ASP:HB2	2.00	0.62
1:A:30:HIS:CD2	1:A:30:HIS:H	2.18	0.62
1:C:22:MET:HE2	1:C:81:GLN:OE1	1.99	0.61
1:B:202:LEU:HD23	1:B:214:LEU:HD21	1.82	0.61
1:D:187:ASN:O	1:D:188:THR:O	2.17	0.61
1:B:24:LEU:CB	1:B:26:PHE:CE2	2.83	0.61
1:B:52:VAL:CG1	1:B:203:ALA:HB2	2.25	0.61
1:B:194:PHE:CD1	1:B:243:PRO:HG3	2.35	0.61
1:A:184:SER:HB3	1:A:185:TRP:CE3	2.36	0.61
1:A:2:LEU:HD11	1:A:252:ILE:HD13	1.82	0.60
1:A:104:ALA:O	1:A:107:THR:OG1	2.19	0.60
1:A:250:THR:C	1:A:251:ARG:HG2	2.21	0.60
1:C:136:GLN:HE21	1:C:195:MET:HG2	1.65	0.60
1:B:164:TYR:HE1	1:B:166:ILE:HG21	1.65	0.60
1:C:205:ASN:HB3	1:C:209:LEU:HD12	1.82	0.60
1:A:205:ASN:HB3	1:A:209:LEU:HD12	1.83	0.60
1:B:13:TYR:CD1	1:B:130:PRO:HD3	2.37	0.59
1:A:72:LEU:CD1	1:A:110:LYS:HB3	2.32	0.59
1:A:108:GLN:O	1:A:112:ASP:CG	2.41	0.59
1:A:8:ARG:HB2	1:B:224:VAL:CG1	2.33	0.59
1:A:201:GLU:O	1:A:202:LEU:C	2.41	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:49:LEU:HG	1:D:195:MET:HE1	1.84	0.59
1:A:111:LEU:N	1:A:111:LEU:CD2	2.65	0.59
1:C:168:VAL:HA	1:C:248:MET:HE2	1.83	0.59
1:A:145:GLY:CA	1:A:166:ILE:HD12	2.32	0.59
1:B:72:LEU:CD2	1:B:114:ILE:HG23	2.31	0.59
1:B:173:LEU:HD23	1:B:174:ILE:N	2.17	0.59
1:B:123:CYS:SG	1:B:126:LEU:HD12	2.42	0.59
1:A:96:HIS:O	1:A:97:GLY:O	2.21	0.59
1:B:115:TRP:N	1:B:115:TRP:CD1	2.71	0.58
1:D:173:LEU:C	1:D:173:LEU:HD23	2.23	0.58
1:C:205:ASN:O	1:C:207:LYS:N	2.35	0.58
1:C:202:LEU:O	1:C:206:GLY:HA3	2.03	0.58
1:A:110:LYS:HA	1:A:113:ASN:HD22	1.67	0.58
1:B:47:GLU:O	1:B:50:THR:HB	2.02	0.58
1:D:198:LEU:HG	1:D:202:LEU:HD12	1.86	0.58
1:B:135:ILE:HD12	1:B:135:ILE:N	2.19	0.58
1:B:136:GLN:NE2	1:B:195:MET:HG2	2.18	0.58
1:D:185:TRP:C	1:D:187:ASN:N	2.57	0.58
1:A:242:ILE:HG12	1:A:243:PRO:N	2.18	0.57
1:D:65:ASP:C	1:D:65:ASP:OD2	2.42	0.57
1:B:164:TYR:CE1	1:B:166:ILE:CG2	2.77	0.57
1:A:93:ILE:O	1:A:94:LEU:HD23	2.05	0.57
1:D:183:TYR:N	1:D:183:TYR:CD2	2.73	0.57
1:A:107:THR:O	1:A:110:LYS:N	2.38	0.57
1:C:67:ARG:HA	1:C:68:TYR:CE2	2.39	0.56
1:A:2:LEU:C	1:A:2:LEU:HD22	2.18	0.56
1:B:64:LYS:O	1:B:65:ASP:CB	2.51	0.56
1:A:218:VAL:O	1:A:222:VAL:CG1	2.52	0.56
1:C:173:LEU:C	1:C:173:LEU:CD2	2.74	0.56
1:C:248:MET:HB2	1:D:242:ILE:HD13	1.87	0.56
1:A:242:ILE:HG12	1:A:243:PRO:HD2	1.86	0.56
1:B:88:CYS:HB2	1:B:130:PRO:O	2.05	0.56
1:D:123:CYS:SG	1:D:126:LEU:HD12	2.46	0.56
1:A:254:ARG:HB3	1:A:254:ARG:HH11	1.67	0.56
1:A:184:SER:C	1:A:185:TRP:HE3	2.09	0.56
1:A:72:LEU:CD1	1:A:111:LEU:HD23	2.34	0.55
1:B:48:ASN:O	1:B:49:LEU:C	2.45	0.55
1:C:135:ILE:CD1	1:C:135:ILE:N	2.69	0.55
1:A:168:VAL:CA	1:A:248:MET:CE	2.78	0.55
1:A:242:ILE:HG12	1:A:243:PRO:CD	2.36	0.55
1:C:123:CYS:SG	1:C:126:LEU:HD12	2.45	0.55
1:B:136:GLN:NE2	1:B:192:SER:OG	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:78:SER:HA	1:D:81:GLN:NE2	2.13	0.55
1:A:173:LEU:HD23	1:A:173:LEU:O	2.06	0.55
1:D:134:PHE:C	1:D:135:ILE:HD12	2.27	0.55
1:A:30:HIS:CD2	1:A:30:HIS:N	2.73	0.55
1:D:254:ARG:HB2	1:D:254:ARG:CZ	2.34	0.55
1:D:122:HIS:N	1:D:122:HIS:CD2	2.74	0.55
1:D:193:TRP:H	1:D:193:TRP:HE3	1.52	0.55
1:C:174:ILE:HD12	1:C:174:ILE:N	2.21	0.55
1:B:65:ASP:OD2	1:B:65:ASP:O	2.25	0.55
1:B:115:TRP:CH2	1:B:166:ILE:HG22	2.41	0.55
1:A:113:ASN:O	1:A:115:TRP:N	2.39	0.55
1:A:72:LEU:O	1:A:75:ILE:HB	2.07	0.55
1:A:134:PHE:CD2	1:A:175:ALA:HB3	2.42	0.55
1:A:134:PHE:C	1:A:135:ILE:HD13	2.27	0.55
1:A:199:CYS:O	1:A:203:ALA:HB2	2.06	0.55
1:B:167:PRO:HB2	1:B:168:VAL:HA	1.89	0.55
1:B:222:VAL:HG11	1:B:243:PRO:CD	2.37	0.54
1:A:209:LEU:HD22	1:A:213:THR:OG1	2.07	0.54
1:C:135:ILE:N	1:C:135:ILE:HD12	2.21	0.54
1:C:129:LYS:O	1:C:131:LYS:NZ	2.40	0.54
1:B:115:TRP:C	1:B:117:PHE:N	2.60	0.54
1:A:142:ARG:HD3	1:A:163:SER:CB	2.38	0.54
1:C:220:GLN:HB2	1:D:250:THR:O	2.06	0.54
1:C:47:GLU:O	1:C:50:THR:HB	2.08	0.54
1:D:253:LEU:C	1:D:253:LEU:HD12	2.28	0.54
1:B:167:PRO:HG2	1:B:168:VAL:HG23	1.90	0.54
1:D:90:LEU:C	1:D:90:LEU:HD23	2.28	0.54
1:A:115:TRP:N	1:A:115:TRP:CD1	2.75	0.54
1:D:135:ILE:N	1:D:135:ILE:HD12	2.23	0.54
1:A:72:LEU:CD1	1:A:111:LEU:CD2	2.81	0.53
1:D:220:GLN:O	1:D:224:VAL:HB	2.08	0.53
1:A:245:ILE:O	1:B:246:THR:HA	2.08	0.53
1:A:69:LYS:HD3	1:A:110:LYS:NZ	2.24	0.53
1:C:130:PRO:CG	1:C:253:LEU:HD22	2.39	0.53
1:C:247:THR:N	1:D:245:ILE:O	2.37	0.53
1:A:83:HIS:HB3	1:A:86:SER:HB2	1.91	0.53
1:B:226:PHE:CZ	1:B:241:GLN:NE2	2.71	0.53
1:A:170:ALA:O	1:A:171:ASP:HB2	2.09	0.53
1:A:252:ILE:HD11	1:B:217:PHE:HZ	1.73	0.53
1:A:108:GLN:O	1:A:109:TYR:C	2.48	0.53
1:D:45:ASP:OD1	1:D:191:GLY:CA	2.57	0.53
1:C:132:LEU:H	1:C:132:LEU:HD22	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:72:LEU:CD2	1:C:114:ILE:HG12	2.35	0.52
1:B:20:ARG:HA	1:B:87:ASP:OD2	2.09	0.52
1:D:52:VAL:CG1	1:D:202:LEU:HB3	2.40	0.52
1:C:22:MET:HE1	1:C:81:GLN:OE1	2.08	0.52
1:C:136:GLN:NE2	1:C:195:MET:HG3	2.23	0.52
1:D:219:CYS:SG	1:D:245:ILE:HD12	2.49	0.52
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.91	0.52
1:C:121:ASN:O	1:C:124:PRO:HD3	2.09	0.52
1:D:53:LEU:O	1:D:58:PHE:HB2	2.10	0.52
1:C:25:ILE:HD12	1:C:60:VAL:CG1	2.39	0.52
1:D:136:GLN:NE2	1:D:192:SER:OG	2.43	0.52
1:A:56:LEU:O	1:A:57:ASP:CB	2.46	0.52
1:A:145:GLY:N	1:A:166:ILE:HD12	2.25	0.52
1:C:13:TYR:CD2	1:C:130:PRO:HG3	2.45	0.52
1:A:250:THR:HB	1:B:220:GLN:HG3	1.91	0.52
1:D:193:TRP:CD1	1:D:226:PHE:CB	2.93	0.52
1:A:24:LEU:CD2	1:A:24:LEU:N	2.70	0.52
1:B:88:CYS:HB3	1:B:130:PRO:HG2	1.91	0.52
1:A:136:GLN:HE22	1:A:195:MET:HG2	1.73	0.52
1:B:224:VAL:HG12	1:B:225:ASP:OD1	2.09	0.51
1:D:180:PRO:O	1:D:181:GLY:O	2.28	0.51
1:B:210:ASP:OD2	1:B:213:THR:HG23	2.09	0.51
1:A:114:ILE:H	1:A:114:ILE:CD1	2.05	0.51
1:A:69:LYS:HD3	1:A:110:LYS:HZ3	1.75	0.51
1:C:67:ARG:C	1:C:68:TYR:CD2	2.78	0.51
1:B:90:LEU:HD11	1:B:134:PHE:CE1	2.46	0.51
1:A:108:GLN:O	1:A:112:ASP:OD2	2.28	0.51
1:C:136:GLN:NE2	1:C:195:MET:CG	2.73	0.51
1:D:254:ARG:NH1	1:D:254:ARG:CB	2.74	0.51
1:D:193:TRP:CD1	1:D:226:PHE:HB3	2.46	0.51
1:B:177:SER:HB3	1:B:194:PHE:CD2	2.46	0.51
1:A:109:TYR:C	1:A:112:ASP:OD2	2.45	0.50
1:A:2:LEU:HD11	1:A:252:ILE:CD1	2.40	0.50
1:C:217:PHE:O	1:C:221:ARG:HG3	2.12	0.50
1:A:6:THR:O	1:A:7:ASP:OD1	2.21	0.50
1:A:253:LEU:C	1:A:253:LEU:HD12	2.32	0.50
1:A:184:SER:HB3	1:A:185:TRP:HE3	1.75	0.50
1:A:2:LEU:CD1	1:A:252:ILE:HD13	2.42	0.50
1:A:82:ASN:C	1:A:82:ASN:OD1	2.49	0.50
1:A:137:ALA:O	1:A:179:VAL:N	2.24	0.50
1:D:193:TRP:CD1	1:D:226:PHE:CG	3.00	0.50
1:B:68:TYR:N	1:B:68:TYR:CD1	2.80	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:21:GLY:HA2	1:B:86:SER:HB3	1.93	0.49
1:C:52:VAL:HG21	1:C:199:CYS:HB3	1.95	0.49
1:A:247:THR:N	1:B:245:ILE:O	2.45	0.49
1:B:25:ILE:CD1	1:B:49:LEU:HD13	2.41	0.49
1:D:49:LEU:HD22	1:D:53:LEU:HG	1.94	0.49
1:A:72:LEU:HD12	1:A:110:LYS:HB3	1.95	0.49
1:C:224:VAL:CG1	1:C:224:VAL:O	2.60	0.49
1:C:213:THR:OG1	1:C:214:LEU:N	2.46	0.49
1:A:145:GLY:HA3	1:A:166:ILE:HD12	1.94	0.49
1:D:187:ASN:C	1:D:188:THR:O	2.49	0.49
1:C:246:THR:HA	1:D:246:THR:HA	1.95	0.49
1:B:129:LYS:O	1:B:131:LYS:NZ	2.45	0.49
1:A:222:VAL:CG2	1:A:222:VAL:O	2.60	0.49
1:C:250:THR:O	1:D:220:GLN:HB2	2.13	0.49
1:C:168:VAL:HA	1:C:248:MET:HE1	1.93	0.49
1:A:53:LEU:O	1:A:58:PHE:HB2	2.13	0.49
1:A:193:TRP:HE3	1:A:193:TRP:H	1.58	0.49
1:A:125:SER:O	1:A:129:LYS:NZ	2.40	0.49
1:B:132:LEU:HB3	1:B:134:PHE:CE1	2.48	0.49
1:A:110:LYS:CA	1:A:113:ASN:ND2	2.73	0.49
1:A:72:LEU:HD13	1:A:110:LYS:HB3	1.93	0.49
1:A:2:LEU:C	1:A:2:LEU:CD2	2.80	0.49
1:A:144:ASP:HB3	1:B:165:LYS:HA	1.95	0.49
1:A:48:ASN:O	1:A:49:LEU:C	2.51	0.48
1:C:134:PHE:C	1:C:135:ILE:HD12	2.33	0.48
1:B:207:LYS:HG2	1:B:255:PHE:O	2.13	0.48
1:D:193:TRP:CD1	1:D:226:PHE:CD2	3.01	0.48
1:C:22:MET:HE1	1:C:81:GLN:CD	2.34	0.48
1:C:136:GLN:HE21	1:C:195:MET:CG	2.26	0.48
1:B:52:VAL:HG21	1:B:199:CYS:HB3	1.95	0.48
1:A:144:ASP:O	1:A:165:LYS:HA	2.12	0.48
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.71	0.48
1:B:219:CYS:SG	1:B:245:ILE:HD12	2.53	0.48
1:D:257:ASP:CG	1:D:258:LYS:H	2.17	0.48
1:A:134:PHE:C	1:A:135:ILE:CD1	2.82	0.48
1:D:49:LEU:HA	1:D:49:LEU:HD23	1.66	0.48
1:C:19:ASN:O	1:C:86:SER:HA	2.14	0.48
1:A:254:ARG:HB2	1:A:254:ARG:CZ	2.43	0.48
1:A:47:GLU:O	1:A:50:THR:HB	2.14	0.48
1:A:183:TYR:CE1	1:D:203:ALA:CB	2.96	0.48
1:D:56:LEU:O	1:D:57:ASP:HB2	2.13	0.48
1:C:219:CYS:SG	1:C:245:ILE:CD1	3.02	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:ASN:CB	1:A:209:LEU:HD12	2.44	0.47
1:B:202:LEU:O	1:B:206:GLY:N	2.45	0.47
1:B:95:SER:C	1:B:96:HIS:HD1	2.18	0.47
1:D:193:TRP:HD1	1:D:226:PHE:CD2	2.32	0.47
1:C:48:ASN:O	1:C:52:VAL:HG23	2.15	0.47
1:A:138:CYS:HB2	1:A:141:ASP:OD2	2.14	0.47
1:B:201:GLU:O	1:B:202:LEU:C	2.52	0.47
1:A:202:LEU:O	1:A:206:GLY:HA3	2.14	0.47
1:A:126:LEU:HD23	1:A:129:LYS:HD2	1.96	0.47
1:A:185:TRP:HE3	1:A:185:TRP:N	2.13	0.47
1:D:26:PHE:CD1	1:D:71:ILE:HG12	2.49	0.47
1:B:22:MET:CE	1:B:83:HIS:HE1	2.28	0.47
1:A:166:ILE:CG2	1:A:167:PRO:HD2	2.45	0.47
1:A:184:SER:HB2	1:D:48:ASN:OD1	2.14	0.47
1:C:20:ARG:HA	1:C:87:ASP:OD2	2.14	0.47
1:D:17:HIS:ND1	1:D:87:ASP:HA	2.29	0.47
1:B:174:ILE:O	1:B:174:ILE:HG22	2.13	0.47
1:D:195:MET:HA	1:D:195:MET:HE3	1.96	0.47
1:D:74:THR:O	1:D:78:SER:OG	2.32	0.47
1:D:118:PHE:O	1:D:131:LYS:HE2	2.15	0.47
1:C:168:VAL:HG12	1:C:168:VAL:O	2.14	0.47
1:C:25:ILE:HD12	1:C:60:VAL:HG13	1.96	0.47
1:D:13:TYR:OH	1:D:171:ASP:OD1	2.30	0.47
1:A:201:GLU:O	1:A:203:ALA:N	2.48	0.47
1:A:184:SER:C	1:A:185:TRP:CE3	2.88	0.47
1:C:49:LEU:HB2	1:C:195:MET:HE1	1.97	0.46
1:C:219:CYS:SG	1:C:245:ILE:HD12	2.55	0.46
1:A:52:VAL:O	1:A:56:LEU:HG	2.15	0.46
1:A:28:HIS:NE2	1:A:68:TYR:HD1	2.13	0.46
1:A:8:ARG:HG2	1:B:221:ARG:HH12	1.79	0.46
1:A:65:ASP:OD2	1:A:70:ASP:OD2	2.34	0.46
1:D:170:ALA:O	1:D:171:ASP:HB2	2.15	0.46
1:A:110:LYS:CA	1:A:113:ASN:HD22	2.28	0.46
1:A:110:LYS:O	1:A:114:ILE:HG13	2.16	0.46
1:B:132:LEU:HB3	1:B:134:PHE:HE1	1.81	0.46
1:D:187:ASN:O	1:D:188:THR:C	2.55	0.45
1:C:199:CYS:O	1:C:200:ALA:C	2.54	0.45
1:D:133:PHE:HB3	1:D:135:ILE:HD11	1.98	0.45
1:A:50:THR:O	1:A:54:LYS:HG3	2.16	0.45
1:C:26:PHE:CE1	1:C:63:TYR:CD1	3.04	0.45
1:C:22:MET:CE	1:C:83:HIS:HE1	2.30	0.45
1:B:195:MET:HA	1:B:195:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:ILE:HG23	1:A:167:PRO:HD2	1.98	0.45
1:A:8:ARG:O	1:A:9:HIS:CD2	2.68	0.45
1:D:48:ASN:HB3	1:D:199:CYS:SG	2.56	0.45
1:A:222:VAL:HG23	1:A:222:VAL:O	2.16	0.45
1:A:114:ILE:N	1:A:114:ILE:HD12	2.19	0.45
1:A:210:ASP:HB3	1:A:254:ARG:NH2	2.32	0.45
1:B:83:HIS:H	1:B:125:SER:HB2	1.82	0.45
1:C:211:ILE:HB	1:C:253:LEU:HB3	1.99	0.45
1:A:188:THR:O	1:A:189:THR:C	2.55	0.45
1:C:193:TRP:CE3	1:C:193:TRP:N	2.75	0.45
1:C:15:MET:HG3	1:C:254:ARG:O	2.17	0.45
1:B:202:LEU:HD23	1:B:214:LEU:CD2	2.46	0.44
1:B:72:LEU:HD22	1:B:114:ILE:CG2	2.37	0.44
1:A:142:ARG:HD3	1:A:163:SER:HB3	1.99	0.44
1:D:82:ASN:OD1	1:D:84:SER:HB2	2.16	0.44
1:B:253:LEU:HD12	1:B:254:ARG:N	2.32	0.44
1:A:8:ARG:HG3	1:B:225:ASP:OD1	2.17	0.44
1:C:202:LEU:O	1:C:206:GLY:CA	2.65	0.44
1:B:177:SER:OG	1:B:178:THR:N	2.50	0.44
1:B:209:LEU:HD22	1:B:213:THR:OG1	2.17	0.44
1:C:52:VAL:HG11	1:C:202:LEU:HB2	1.99	0.44
1:D:116:SER:O	1:D:122:HIS:CG	2.71	0.44
1:B:23:ALA:C	1:B:24:LEU:HD23	2.38	0.44
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.78	0.44
1:B:25:ILE:HD13	1:B:49:LEU:HD13	1.99	0.43
1:D:78:SER:CA	1:D:81:GLN:HE21	2.17	0.43
1:A:179:VAL:HG22	1:A:180:PRO:HD2	1.99	0.43
1:A:184:SER:CB	1:D:48:ASN:OD1	2.66	0.43
1:A:131:LYS:HD2	1:A:172:PHE:CE1	2.53	0.43
1:D:254:ARG:HB3	1:D:254:ARG:HH11	1.82	0.43
1:B:10:ALA:O	1:B:251:ARG:HD3	2.19	0.43
1:C:211:ILE:CG2	1:C:253:LEU:HB3	2.48	0.43
1:B:22:MET:HE3	1:B:83:HIS:HE1	1.83	0.43
1:A:187:ASN:O	1:A:188:THR:C	2.56	0.43
1:C:76:GLU:O	1:C:79:ALA:HB3	2.17	0.43
1:A:182:PHE:H	1:A:182:PHE:HD1	1.65	0.43
1:B:26:PHE:CD2	1:B:26:PHE:N	2.87	0.43
1:C:130:PRO:HB3	1:C:253:LEU:CD2	2.48	0.43
1:D:254:ARG:NH1	1:D:254:ARG:HB2	2.33	0.43
1:A:165:LYS:HG2	1:A:165:LYS:H	1.55	0.43
1:A:26:PHE:CG	1:A:71:ILE:HG23	2.54	0.43
1:D:210:ASP:O	1:D:211:ILE:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:PRO:HB2	1:B:168:VAL:CB	2.49	0.43
1:A:205:ASN:O	1:A:206:GLY:C	2.57	0.43
1:A:126:LEU:HA	1:A:129:LYS:HD2	2.00	0.43
1:C:77:TYR:C	1:C:80:SER:H	2.22	0.43
1:A:22:MET:HB3	1:A:24:LEU:CD2	2.48	0.43
1:D:134:PHE:CD2	1:D:175:ALA:HB3	2.54	0.43
1:D:174:ILE:HD12	1:D:174:ILE:N	2.34	0.43
1:B:68:TYR:O	1:B:72:LEU:HG	2.18	0.43
1:C:173:LEU:HD23	1:C:174:ILE:N	2.34	0.43
1:A:138:CYS:C	1:A:140:GLY:H	2.22	0.43
1:A:8:ARG:HB2	1:B:224:VAL:HG11	2.00	0.43
1:B:214:LEU:O	1:B:218:VAL:HG23	2.19	0.43
1:D:52:VAL:HG11	1:D:202:LEU:HB3	2.01	0.43
1:C:83:HIS:HB3	1:C:86:SER:HB2	2.01	0.42
1:A:17:HIS:HB2	1:A:87:ASP:OD1	2.19	0.42
1:C:210:ASP:HB2	1:C:252:ILE:HG23	2.01	0.42
1:B:13:TYR:CE1	1:B:130:PRO:HD3	2.54	0.42
1:A:186:ARG:HG3	1:A:186:ARG:O	2.20	0.42
1:A:30:HIS:O	1:A:31:PHE:CG	2.72	0.42
1:D:185:TRP:HB3	1:D:186:ARG:H	1.49	0.42
1:C:132:LEU:HD22	1:C:132:LEU:N	2.35	0.42
1:A:215:LEU:HB3	1:A:245:ILE:CD1	2.49	0.42
1:C:116:SER:O	1:C:122:HIS:CG	2.73	0.42
1:B:253:LEU:HD12	1:B:253:LEU:C	2.40	0.42
1:B:45:ASP:HB3	1:B:195:MET:HG3	2.01	0.42
1:D:132:LEU:CD2	1:D:132:LEU:H	2.25	0.42
1:B:49:LEU:HG	1:B:195:MET:HE1	2.02	0.42
1:A:144:ASP:C	1:A:166:ILE:HD12	2.40	0.42
1:B:250:THR:C	1:B:251:ARG:HG3	2.39	0.42
1:A:173:LEU:C	1:A:173:LEU:CD2	2.85	0.42
1:D:13:TYR:CD1	1:D:130:PRO:HD3	2.54	0.42
1:A:109:TYR:O	1:A:112:ASP:N	2.53	0.42
1:A:98:GLU:CG	1:A:182:PHE:O	2.67	0.42
1:B:72:LEU:CD2	1:B:114:ILE:CG2	2.96	0.42
1:C:115:TRP:HB3	1:C:172:PHE:HE2	1.85	0.42
1:C:133:PHE:HB2	1:C:174:ILE:HG13	2.02	0.42
1:D:195:MET:HE3	1:D:195:MET:CA	2.49	0.42
1:D:183:TYR:HD2	1:D:183:TYR:N	2.16	0.42
1:B:226:PHE:CB	1:B:227:GLU:OE2	2.67	0.42
1:B:173:LEU:HD23	1:B:173:LEU:C	2.40	0.42
1:A:139:GLN:HG3	1:A:178:THR:HB	2.02	0.42
1:A:98:GLU:HG2	1:A:182:PHE:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:132:LEU:N	1:D:132:LEU:CD2	2.73	0.41
1:B:66:CYS:HB2	1:B:67:ARG:H	1.49	0.41
1:A:252:ILE:HG21	1:A:254:ARG:HH22	1.85	0.41
1:A:184:SER:HB3	1:A:185:TRP:CZ3	2.55	0.41
1:C:68:TYR:O	1:C:71:ILE:HB	2.20	0.41
1:A:195:MET:CE	1:A:198:LEU:HD23	2.50	0.41
1:D:115:TRP:HB3	1:D:172:PHE:HE2	1.84	0.41
1:D:254:ARG:CB	1:D:254:ARG:CZ	2.98	0.41
1:C:173:LEU:HD23	1:C:173:LEU:O	2.20	0.41
1:A:118:PHE:HB3	1:A:131:LYS:HD3	2.01	0.41
1:C:205:ASN:O	1:C:206:GLY:C	2.58	0.41
1:B:195:MET:HE3	1:B:195:MET:CA	2.50	0.41
1:D:122:HIS:CD2	1:D:122:HIS:H	2.38	0.41
1:B:216:THR:O	1:B:219:CYS:HB2	2.20	0.41
1:B:219:CYS:HB3	1:B:242:ILE:HD11	2.03	0.41
1:C:46:CYS:SG	1:C:46:CYS:O	2.78	0.41
1:C:22:MET:SD	1:C:83:HIS:HE1	2.44	0.41
1:A:201:GLU:C	1:A:203:ALA:N	2.75	0.41
1:A:242:ILE:CG1	1:A:243:PRO:HD2	2.51	0.41
1:A:93:ILE:C	1:A:94:LEU:HD23	2.40	0.41
1:C:211:ILE:O	1:C:211:ILE:HG13	2.20	0.41
1:B:248:MET:O	1:B:249:LEU:C	2.59	0.41
1:C:23:ALA:HA	1:C:90:LEU:O	2.21	0.41
1:A:2:LEU:HG	1:A:252:ILE:HD11	2.03	0.40
1:C:213:THR:O	1:C:214:LEU:C	2.59	0.40
1:A:136:GLN:HE21	1:A:195:MET:HG2	1.80	0.40
1:D:242:ILE:CG1	1:D:243:PRO:HD2	2.51	0.40
1:C:211:ILE:O	1:C:215:LEU:HD12	2.20	0.40
1:D:219:CYS:SG	1:D:245:ILE:CD1	3.09	0.40
1:B:211:ILE:O	1:B:215:LEU:HG	2.20	0.40
1:A:6:THR:HB	1:A:7:ASP:H	1.58	0.40
1:C:248:MET:HB2	1:D:242:ILE:CD1	2.51	0.40
1:D:52:VAL:HG11	1:D:202:LEU:CB	2.52	0.40
1:D:123:CYS:O	1:D:126:LEU:O	2.39	0.40
1:B:46:CYS:O	1:B:50:THR:OG1	2.30	0.40
1:A:192:SER:OG	1:A:195:MET:HB2	2.22	0.40
1:C:51:ARG:O	1:C:54:LYS:N	2.54	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	206/259 (80%)	162 (79%)	32 (16%)	12 (6%)	3	3
1	B	160/259 (62%)	135 (84%)	20 (12%)	5 (3%)	7	14
1	C	150/259 (58%)	130 (87%)	15 (10%)	5 (3%)	6	12
1	D	157/259 (61%)	137 (87%)	11 (7%)	9 (6%)	3	4
All	All	673/1036 (65%)	564 (84%)	78 (12%)	31 (5%)	4	6

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	HIS
1	A	57	ASP
1	A	97	GLY
1	B	68	TYR
1	B	167	PRO
1	C	68	TYR
1	D	17	HIS
1	D	186	ARG
1	D	188	THR
1	D	189	THR
1	D	257	ASP
1	A	202	LEU
1	B	116	SER
1	C	206	GLY
1	D	181	GLY
1	D	185	TRP
1	A	119	THR
1	A	185	TRP
1	A	206	GLY
1	A	224	VAL
1	B	65	ASP
1	C	45	ASP
1	D	187	ASN

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	9	HIS
1	A	49	LEU
1	B	67	ARG
1	C	224	VAL
1	C	84	SER
1	D	180	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	188/229 (82%)	138 (73%)	50 (27%)	1	2
1	B	154/229 (67%)	115 (75%)	39 (25%)	1	2
1	C	145/229 (63%)	113 (78%)	32 (22%)	1	3
1	D	150/229 (66%)	116 (77%)	34 (23%)	1	3
All	All	637/916 (70%)	482 (76%)	155 (24%)	1	2

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	7	ASP
1	A	16	ARG
1	A	19	ASN
1	A	24	LEU
1	A	28	HIS
1	A	30	HIS
1	A	44	VAL
1	A	49	LEU
1	A	57	ASP
1	A	59	GLU
1	A	61	THR
1	A	64	LYS
1	A	66	CYS
1	A	73	ARG

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Mol	Chain	Res	Type
1	A	78	SER
1	A	80	SER
1	A	98	GLU
1	A	99	MET
1	A	105	LYS
1	A	107	THR
1	A	111	LEU
1	A	114	ILE
1	A	115	TRP
1	A	132	LEU
1	A	135	ILE
1	A	136	GLN
1	A	139	GLN
1	A	144	ASP
1	A	165	LYS
1	A	178	THR
1	A	179	VAL
1	A	182	PHE
1	A	185	TRP
1	A	186	ARG
1	A	189	THR
1	A	190	ARG
1	A	197	SER
1	A	210	ASP
1	A	221	ARG
1	A	222	VAL
1	A	225	ASP
1	A	241	GLN
1	A	242	ILE
1	A	244	CYS
1	A	246	THR
1	A	247	THR
1	A	251	ARG
1	A	253	LEU
1	A	256	SER
1	B	12	GLU
1	B	18	LYS
1	B	24	LEU
1	B	44	VAL
1	B	49	LEU
1	B	51	ARG
1	B	52	VAL

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Mol	Chain	Res	Type
1	B	57	ASP
1	B	59	GLU
1	B	61	THR
1	B	64	LYS
1	B	66	CYS
1	B	67	ARG
1	B	68	TYR
1	B	78	SER
1	B	80	SER
1	B	96	HIS
1	B	114	ILE
1	B	115	TRP
1	B	131	LYS
1	B	135	ILE
1	B	138	CYS
1	B	165	LYS
1	B	169	HIS
1	B	178	THR
1	B	179	VAL
1	B	189	THR
1	B	197	SER
1	B	210	ASP
1	B	211	ILE
1	B	222	VAL
1	B	226	PHE
1	B	228	SER
1	B	241	GLN
1	B	246	THR
1	B	247	THR
1	B	248	MET
1	B	253	LEU
1	B	256	SER
1	C	12	GLU
1	C	16	ARG
1	C	19	ASN
1	C	27	ASN
1	C	28	HIS
1	C	49	LEU
1	C	57	ASP
1	C	59	GLU
1	C	61	THR
1	C	64	LYS

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Mol	Chain	Res	Type
1	C	65	ASP
1	C	68	TYR
1	C	73	ARG
1	C	76	GLU
1	C	78	SER
1	C	80	SER
1	C	132	LEU
1	C	135	ILE
1	C	139	GLN
1	C	169	HIS
1	C	179	VAL
1	C	192	SER
1	C	193	TRP
1	C	197	SER
1	C	210	ASP
1	C	222	VAL
1	C	224	VAL
1	C	241	GLN
1	C	246	THR
1	C	248	MET
1	C	253	LEU
1	C	256	SER
1	D	16	ARG
1	D	19	ASN
1	D	24	LEU
1	D	49	LEU
1	D	59	GLU
1	D	61	THR
1	D	65	ASP
1	D	73	ARG
1	D	78	SER
1	D	84	SER
1	D	114	ILE
1	D	115	TRP
1	D	122	HIS
1	D	126	LEU
1	D	132	LEU
1	D	177	SER
1	D	178	THR
1	D	183	TYR
1	D	184	SER
1	D	185	TRP

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Mol	Chain	Res	Type
1	D	193	TRP
1	D	197	SER
1	D	210	ASP
1	D	213	THR
1	D	222	VAL
1	D	225	ASP
1	D	241	GLN
1	D	246	THR
1	D	247	THR
1	D	248	MET
1	D	253	LEU
1	D	256	SER
1	D	258	LYS
1	D	259	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	27	ASN
1	A	30	HIS
1	A	96	HIS
1	A	113	ASN
1	A	136	GLN
1	B	83	HIS
1	B	136	GLN
1	B	220	GLN
1	C	27	ASN
1	C	48	ASN
1	C	83	HIS
1	C	136	GLN
1	C	139	GLN
1	D	81	GLN
1	D	83	HIS
1	D	122	HIS
1	D	136	GLN
1	D	259	GLN

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 ⓘ

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	214/259 (82%)	-0.27	0 100 100	2, 41, 55, 63	0
1	B	172/259 (66%)	-0.25	0 100 100	28, 43, 60, 73	0
1	C	162/259 (62%)	-0.26	0 100 100	27, 42, 57, 65	0
1	D	169/259 (65%)	-0.27	1 (0%) 86 90	24, 44, 62, 73	0
All	All	717/1036 (69%)	-0.26	1 (0%) 93 96	2, 42, 60, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	TYR	3.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.