Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 02:25 am BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

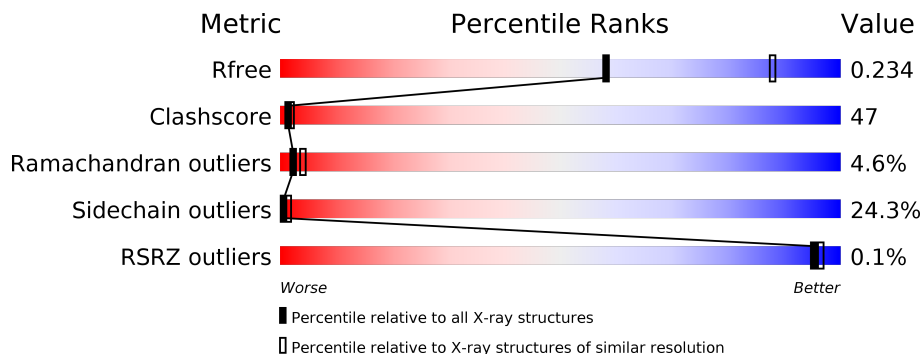|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		47
Ramachandran outliers		4.6%
Sidechain outliers		24.3%
RSRZ outliers		0.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	25% 40% 15% • 17%
1	B	259	23% 32% 10% • 34%
1	C	259	22% 33% 7% • 37%
1	D	259	26% 28% 10% • 35%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5766 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 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 O01382
A	2	LEU	-	SEE REMARK 999	UNP O01382
A	3	GLY	-	SEE REMARK 999	UNP O01382
A	4	SER	-	SEE REMARK 999	UNP O01382
A	78	SER	ALA	ENGINEERED MUTATION	UNP O01382
B	1	ALA	-	SEE REMARK 999	UNP O01382
B	2	LEU	-	SEE REMARK 999	UNP O01382
B	3	GLY	-	SEE REMARK 999	UNP O01382
B	4	SER	-	SEE REMARK 999	UNP O01382
B	78	SER	ALA	ENGINEERED MUTATION	UNP O01382
C	1	ALA	-	SEE REMARK 999	UNP O01382
C	2	LEU	-	SEE REMARK 999	UNP O01382
C	3	GLY	-	SEE REMARK 999	UNP O01382
C	4	SER	-	SEE REMARK 999	UNP O01382
C	78	SER	ALA	ENGINEERED MUTATION	UNP O01382
D	1	ALA	-	SEE REMARK 999	UNP O01382
D	2	LEU	-	SEE REMARK 999	UNP O01382
D	3	GLY	-	SEE REMARK 999	UNP O01382
D	4	SER	-	SEE REMARK 999	UNP O01382
D	78	SER	ALA	ENGINEERED MUTATION	UNP O01382

• Molecule 2 is water.

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

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
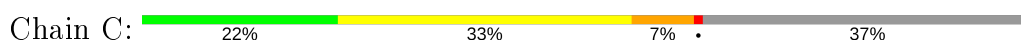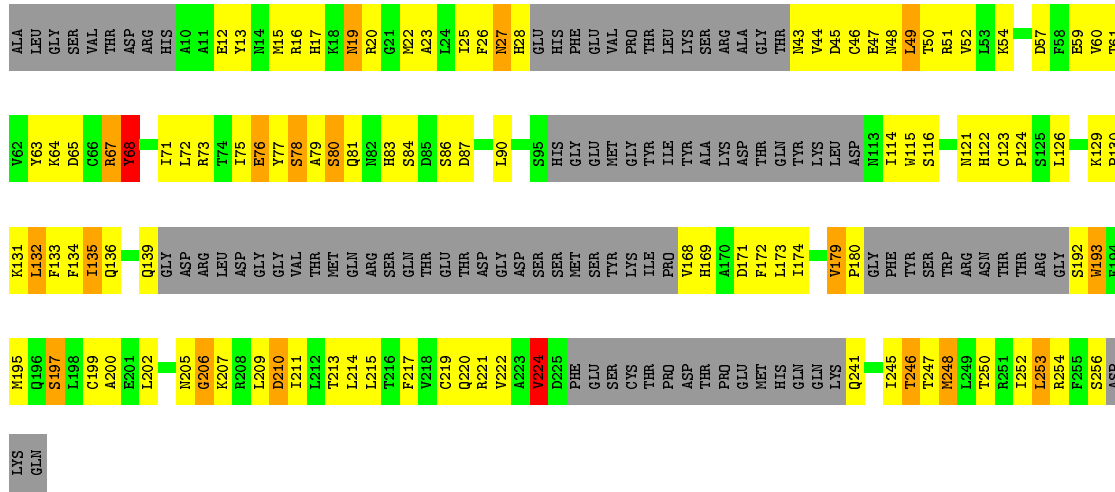
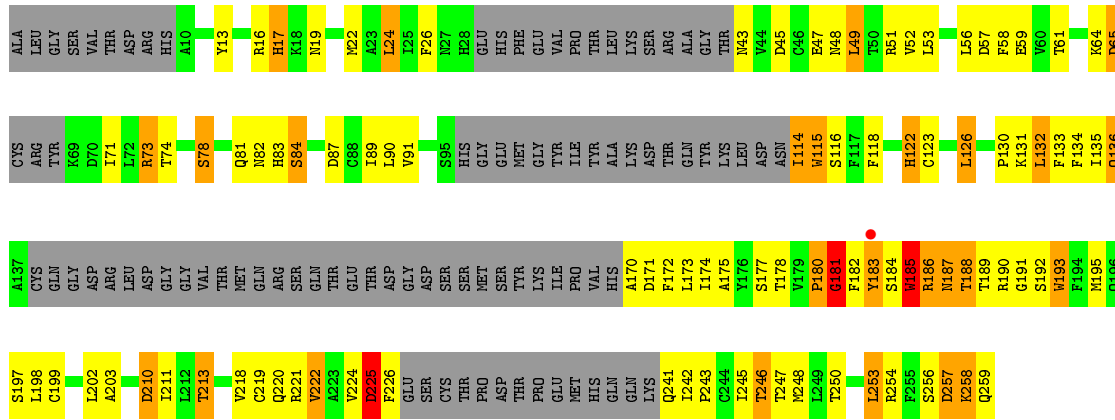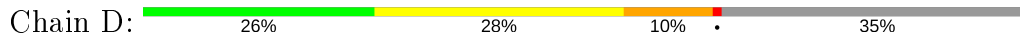- Molecule 1: Caspase

Chain A:

- Molecule 1: Caspase

Chain B:

- Molecule 1: Caspase

Chain C:

• Molecule 1: Caspase

Chain D:

| 26% | 28% | 10% | • | 35% |
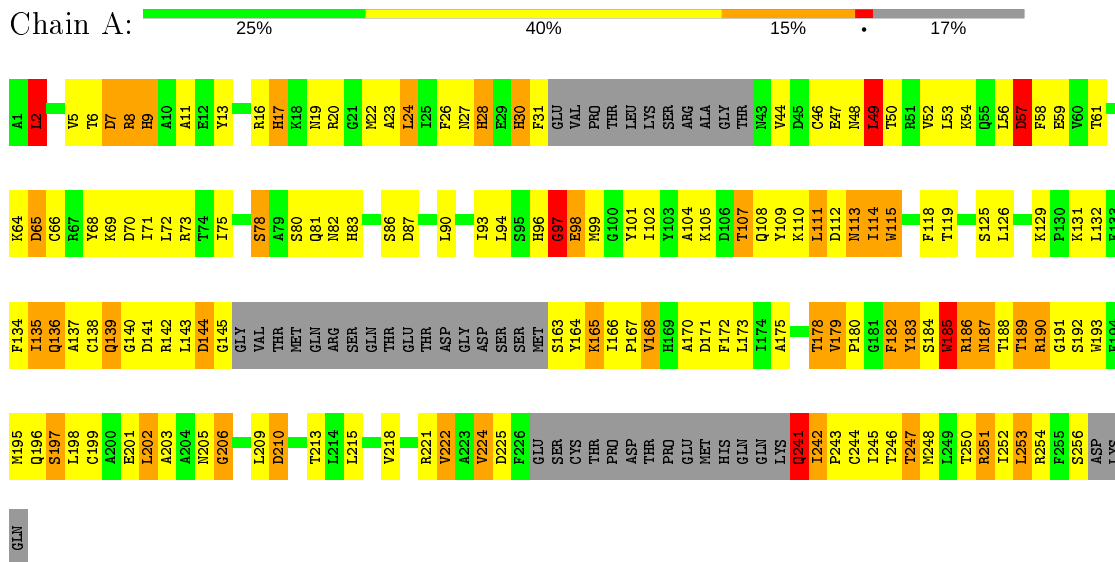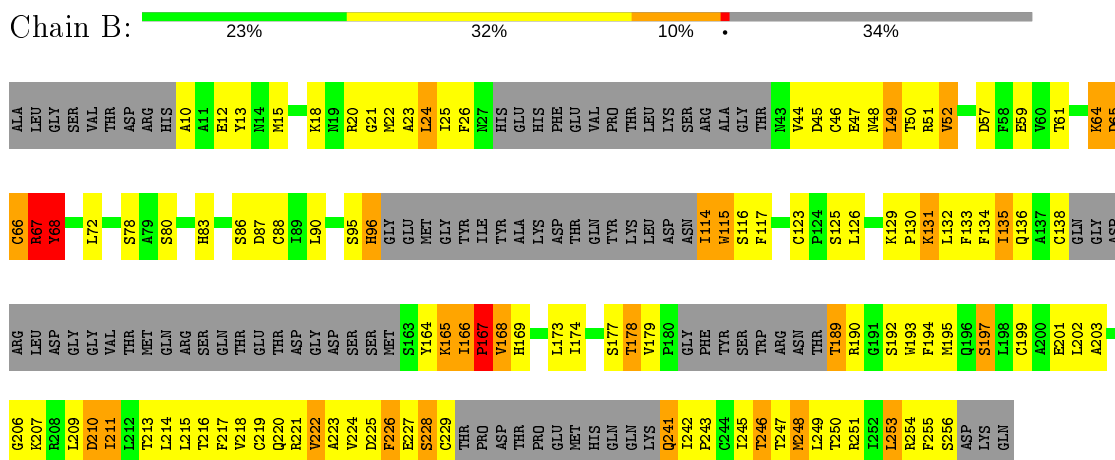
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 20.8	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	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
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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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 Too-close contacts (i)

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	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

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 47.

All (545) 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: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	Interatomic distance (Å)	Clash overlap (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:O	1:D:224:VAL:CG1	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:B:226:PHE:CE2	1:B:241:GLN:NE2	2.37	0.92
1:D:188:THR:O	1:D:190:ARG:N	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLU:O	1:D:51:ARG:HG2	1.71	0.91
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:241:GLN:CG	1:A:241:GLN:O	2.25	0.83
1:A:254:ARG:HH11	1:A:254:ARG:CB	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ASN:O	1:C:47:GLU:HG3	1.82	0.79
1:C:67:ARG:HA	1:C:68:TYR:HD2	1.47	0.79
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:28:HIS:O	1:A:96:HIS:CD2	2.36	0.77
1:A:98:GLU:CB	1:A:182:PHE:O	2.30	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:A:192:SER:O	1:A:196:GLN:HG3	1.86	0.76
1:D:132:LEU:N	1:D:132:LEU:HD22	2.00	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:A:49:LEU:HG	1:A:195:MET:HE1	1.68	0.75
1:D:22:MET:HE1	1:D:83:HIS:CE1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TYR:O	1:A:102:ILE:HD12	1.89	0.72
1:C:67:ARG:CA	1:C:68:TYR:HD2	2.01	0.72
1:A:7:ASP:HB2	1:B:220:GLN:NE2	2.04	0.71
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: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:A:218:VAL:O	1:A:222:VAL:HG12	1.93	0.68
1:A:253:LEU:HD12	1:A:254:ARG:N	2.08	0.68
1:D:118:PHE:HB3	1:D:131:LYS:HD3	1.75	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:A:22:MET:HB3	1:A:24:LEU:HD21	1.76	0.67
1:C:27:ASN:ND2	1:C:27:ASN:N	2.40	0.67
1:A:129:LYS:O	1:A:131:LYS:NZ	2.28	0.67
1:A:173:LEU:C	1:A:173:LEU:HD23	2.15	0.67
1:B:226:PHE:HB3	1:B:227:GLU:OE2	1.95	0.67
1:B:193:TRP:O	1:B:197:SER:OG	2.13	0.66
1:D:224:VAL:HG12	1:D:224:VAL:O	1.95	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:101:TYR:C	1:A:102:ILE:HD12	2.16	0.66
1:A:168:VAL:HA	1:A:248:MET:HE3	1.75	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:A:199:CYS:O	1:A:203:ALA:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:O	1:B:222:VAL:CG1	2.43	0.66
1:A:49:LEU:HG	1:A:195:MET:CE	2.26	0.65
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: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:A:20:ARG:O	1:A:87:ASP:HB2	2.00	0.62
1:B:134:PHE:C	1:B:135:ILE:HD12	2.20	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:A:184:SER:HB3	1:A:185:TRP:CE3	2.36	0.61
1:B:194:PHE:CD1	1:B:243:PRO:HG3	2.35	0.61
1:B:52:VAL:CG1	1:B:203:ALA:HB2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:123:CYS:SG	1:B:126:LEU:HD12	2.42	0.59
1:B:173:LEU:HD23	1:B:174:ILE:N	2.17	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:B:164:TYR:CE1	1:B:166:ILE:CG2	2.77	0.57
1:D:65:ASP:C	1:D:65:ASP:OD2	2.42	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:218:VAL:O	1:A:222:VAL:CG1	2.52	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: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:184:SER:C	1:A:185:TRP:HE3	2.09	0.56
1:A:254:ARG:HB3	1:A:254:ARG:HH11	1.67	0.56
1:A:72:LEU:CD1	1:A:111:LEU:HD23	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:O	1:B:49:LEU:C	2.45	0.55
1:C:135:ILE:N	1:C:135:ILE:CD1	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:A:173:LEU:O	1:A:173:LEU:HD23	2.06	0.55
1:B:136:GLN:NE2	1:B:192:SER:OG	2.39	0.55
1:D:134:PHE:C	1:D:135:ILE:HD12	2.27	0.55
1:D:78:SER:HA	1:D:81:GLN:NE2	2.13	0.55
1:A:30:HIS:CD2	1:A:30:HIS:N	2.73	0.55
1:D:122:HIS:N	1:D:122:HIS:CD2	2.74	0.55
1:D:254:ARG:HB2	1:D:254:ARG:CZ	2.34	0.55
1:C:174:ILE:HD12	1:C:174:ILE:N	2.21	0.55
1:D:193:TRP:H	1:D:193:TRP:HE3	1.52	0.55
1:B:115:TRP:CH2	1:B:166:ILE:HG22	2.41	0.55
1:B:65:ASP:OD2	1:B:65:ASP:O	2.25	0.55
1:A:113:ASN:O	1:A:115:TRP:N	2.39	0.55
1:A:134:PHE:CD2	1:A:175:ALA:HB3	2.42	0.55
1:A:72:LEU:O	1:A:75:ILE:HB	2.07	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:129:LYS:O	1:C:131:LYS:NZ	2.40	0.54
1:C:135:ILE:N	1:C:135:ILE:HD12	2.21	0.54
1:A:142:ARG:HD3	1:A:163:SER:CB	2.38	0.54
1:B:115:TRP:C	1:B:117:PHE:N	2.60	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:A:245:ILE:O	1:B:246:THR:HA	2.08	0.53
1:D:220:GLN:O	1:D:224:VAL:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:HIS:HB3	1:A:86:SER:HB2	1.91	0.53
1:A:170:ALA:O	1:A:171:ASP:HB2	2.09	0.53
1:B:226:PHE:CZ	1:B:241:GLN:NE2	2.71	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
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:136:GLN:NE2	1:C:195:MET:HG3	2.23	0.52
1:C:22:MET:HE1	1:C:81:GLN:OE1	2.08	0.52
1:D:219:CYS:SG	1:D:245:ILE:HD12	2.49	0.52
1:C:121:ASN:O	1:C:124:PRO:HD3	2.09	0.52
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.91	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:D:53:LEU:O	1:D:58:PHE:HB2	2.10	0.52
1:A:145:GLY:N	1:A:166:ILE:HD12	2.25	0.52
1:A:56:LEU:O	1:A:57:ASP:CB	2.46	0.52
1:C:13:TYR:CD2	1:C:130:PRO:HG3	2.45	0.52
1:A:24:LEU:CD2	1:A:24:LEU:N	2.70	0.52
1:A:250:THR:HB	1:B:220:GLN:HG3	1.91	0.52
1:B:88:CYS:HB3	1:B:130:PRO:HG2	1.91	0.52
1:D:193:TRP:CD1	1:D:226:PHE:CB	2.93	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:B:90:LEU:HD11	1:B:134:PHE:CE1	2.46	0.51
1:C:67:ARG:C	1:C:68:TYR:CD2	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:HB3	1:A:185:TRP:HE3	1.75	0.50
1:A:253:LEU:C	1:A:253:LEU:HD12	2.32	0.50
1:A:6:THR:O	1:A:7:ASP:OD1	2.21	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:B:68:TYR:N	1:B:68:TYR:CD1	2.80	0.50
1:D:193:TRP:CD1	1:D:226:PHE:CG	3.00	0.50
1:B:21:GLY:HA2	1:B:86:SER:HB3	1.93	0.49
1:A:247:THR:N	1:B:245:ILE:O	2.45	0.49
1:C:52:VAL:HG21	1:C:199:CYS:HB3	1.95	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:A:145:GLY:HA3	1:A:166:ILE:HD12	1.94	0.49
1:A:222:VAL:O	1:A:222:VAL:CG2	2.60	0.49
1:B:129:LYS:O	1:B:131:LYS:NZ	2.45	0.49
1:C:213:THR:OG1	1:C:214:LEU:N	2.46	0.49
1:C:246:THR:HA	1:D:246:THR:HA	1.95	0.49
1:D:187:ASN:C	1:D:188:THR:O	2.49	0.49
1:A:53:LEU:O	1:A:58:PHE:HB2	2.13	0.49
1:C:168:VAL:HA	1:C:248:MET:HE1	1.93	0.49
1:C:250:THR:O	1:D:220:GLN:HB2	2.13	0.49
1:A:125:SER:O	1:A:129:LYS:NZ	2.40	0.49
1:A:193:TRP:HE3	1:A:193:TRP:H	1.58	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:2:LEU:C	1:A:2:LEU:CD2	2.80	0.49
1:A:72:LEU:HD13	1:A:110:LYS:HB3	1.93	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:B:207:LYS:HG2	1:B:255:PHE:O	2.13	0.48
1:C:134:PHE:C	1:C:135:ILE:HD12	2.33	0.48
1:D:193:TRP:CD1	1:D:226:PHE:CD2	3.01	0.48
1:C:136:GLN:HE21	1:C:195:MET:CG	2.26	0.48
1:C:22:MET:HE1	1:C:81:GLN:CD	2.34	0.48
1:A:144:ASP:O	1:A:165:LYS:HA	2.12	0.48
1:B:52:VAL:HG21	1:B:199:CYS:HB3	1.95	0.48
1:B:219:CYS:SG	1:B:245:ILE:HD12	2.53	0.48
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:19:ASN:O	1:C:86:SER:HA	2.14	0.48
1:C:219:CYS:SG	1:C:245:ILE:CD1	3.02	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: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:A:138:CYS:HB2	1:A:141:ASP:OD2	2.14	0.47
1:C:48:ASN:O	1:C:52:VAL:HG23	2.15	0.47
1:D:193:TRP:HD1	1:D:226:PHE:CD2	2.32	0.47
1:A:126:LEU:HD23	1:A:129:LYS:HD2	1.96	0.47
1:A:202:LEU:O	1:A:206:GLY:HA3	2.14	0.47
1:B:201:GLU:O	1:B:202:LEU:C	2.52	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:D:195:MET:HE3	1:D:195:MET:HA	1.96	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:B:174:ILE:HG22	1:B:174:ILE:O	2.13	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: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:118:PHE:O	1:D:131:LYS:HE2	2.15	0.47
1:D:13:TYR:OH	1:D:171:ASP:OD1	2.30	0.47
1:D:74:THR:O	1:D:78:SER:OG	2.32	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:219:CYS:SG	1:C:245:ILE:HD12	2.55	0.46
1:C:49:LEU:HB2	1:C:195:MET:HE1	1.97	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:65:ASP:OD2	1:A:70:ASP:OD2	2.34	0.46
1:A:8:ARG:HG2	1:B:221:ARG:HH12	1.79	0.46
1:D:170:ALA:O	1:D:171:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:50:THR:O	1:A:54:LYS:HG3	2.16	0.45
1:C:199:CYS:O	1:C:200:ALA:C	2.54	0.45
1:C:26:PHE:CE1	1:C:63:TYR:CD1	3.04	0.45
1:D:133:PHE:HB3	1:D:135:ILE:HD11	1.98	0.45
1:D:187:ASN:O	1:D:188:THR:C	2.55	0.45
1:A:166:ILE:HG23	1:A:167:PRO:HD2	1.98	0.45
1:B:195:MET:HA	1:B:195:MET:HE3	1.98	0.45
1:C:22:MET:CE	1:C:83:HIS:HE1	2.30	0.45
1:A:8:ARG:O	1:A:9:HIS:CD2	2.68	0.45
1:A:222:VAL:HG23	1:A:222:VAL:O	2.16	0.45
1:D:48:ASN:HB3	1:D:199:CYS:SG	2.56	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:A:188:THR:O	1:A:189:THR:C	2.55	0.45
1:C:211:ILE:HB	1:C:253:LEU:HB3	1.99	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:A:142:ARG:HD3	1:A:163:SER:HB3	1.99	0.44
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: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:A:179:VAL:HG22	1:A:180:PRO:HD2	1.99	0.43
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:131:LYS:HD2	1:A:172:PHE:CE1	2.53	0.43
1:A:184:SER:CB	1:D:48:ASN:OD1	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ILE:CG2	1:C:253:LEU:HB3	2.48	0.43
1:A:187:ASN:O	1:A:188:THR:C	2.56	0.43
1:B:22:MET:HE3	1:B:83:HIS:HE1	1.83	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:126:LEU:HA	1:A:129:LYS:HD2	2.00	0.43
1:A:205:ASN:O	1:A:206:GLY:C	2.57	0.43
1:A:26:PHE:CG	1:A:71:ILE:HG23	2.54	0.43
1:B:167:PRO:HB2	1:B:168:VAL:CB	2.49	0.43
1:D:210:ASP:O	1:D:211:ILE:C	2.57	0.43
1:A:22:MET:HB3	1:A:24:LEU:CD2	2.48	0.43
1:C:77:TYR:C	1:C:80:SER:H	2.22	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:A:138:CYS:C	1:A:140:GLY:H	2.22	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: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:A:17:HIS:HB2	1:A:87:ASP:OD1	2.19	0.42
1:C:83:HIS:HB3	1:C:86:SER:HB2	2.01	0.42
1:A:186:ARG:HG3	1:A:186:ARG:O	2.20	0.42
1:B:13:TYR:CE1	1:B:130:PRO:HD3	2.54	0.42
1:C:210:ASP:HB2	1:C:252:ILE:HG23	2.01	0.42
1:A:30:HIS:O	1:A:31:PHE:CG	2.72	0.42
1:C:132:LEU:N	1:C:132:LEU:HD22	2.35	0.42
1:D:185:TRP:HB3	1:D:186:ARG:H	1.49	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:45:ASP:HB3	1:B:195:MET:HG3	2.01	0.42
1:B:253:LEU:HD12	1:B:253:LEU:C	2.40	0.42
1:D:132:LEU:CD2	1:D:132:LEU:H	2.25	0.42
1:A:144:ASP:C	1:A:166:ILE:HD12	2.40	0.42
1:A:173:LEU:C	1:A:173:LEU:CD2	2.85	0.42
1:B:49:LEU:HG	1:B:195:MET:HE1	2.02	0.42
1:B:250:THR:C	1:B:251:ARG:HG3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:183:TYR:HD2	1:D:183:TYR:N	2.16	0.42
1:D:195:MET:HE3	1:D:195:MET:CA	2.49	0.42
1:A:139:GLN:HG3	1:A:178:THR:HB	2.02	0.42
1:B:173:LEU:HD23	1:B:173:LEU:C	2.40	0.42
1:B:226:PHE:CB	1:B:227:GLU:OE2	2.67	0.42
1:A:98:GLU:HG2	1:A:182:PHE:O	2.19	0.41
1:D:132:LEU:CD2	1:D:132:LEU:N	2.73	0.41
1:B:66:CYS:HB2	1:B:67:ARG:H	1.49	0.41
1:A:184:SER:HB3	1:A:185:TRP:CZ3	2.55	0.41
1:A:195:MET:CE	1:A:198:LEU:HD23	2.50	0.41
1:A:252:ILE:HG21	1:A:254:ARG:HH22	1.85	0.41
1:C:68:TYR:O	1:C:71:ILE:HB	2.20	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:A:118:PHE:HB3	1:A:131:LYS:HD3	2.01	0.41
1:C:173:LEU:HD23	1:C:173:LEU:O	2.20	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:A:93:ILE:C	1:A:94:LEU:HD23	2.40	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:B:248:MET:O	1:B:249:LEU:C	2.59	0.41
1:C:211:ILE:O	1:C:211:ILE:HG13	2.20	0.41
1:C:23:ALA:HA	1:C:90:LEU:O	2.21	0.41
1:A:136:GLN:HE21	1:A:195:MET:HG2	1.80	0.40
1:A:2:LEU:HG	1:A:252:ILE:HD11	2.03	0.40
1:B:211:ILE:O	1:B:215:LEU:HG	2.20	0.40
1:C:213:THR:O	1:C:214:LEU:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:CG1	1:D:243:PRO:HD2	2.51	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:123:CYS:O	1:D:126:LEU:O	2.39	0.40
1:D:52:VAL:HG11	1:D:202:LEU:CB	2.52	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 (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	206/259 (80%)	162 (79%)	32 (16%)	12 (6%)	1	2
1	B	160/259 (62%)	135 (84%)	20 (12%)	5 (3%)	4	8
1	C	150/259 (58%)	130 (87%)	15 (10%)	5 (3%)	4	7
1	D	157/259 (61%)	137 (87%)	11 (7%)	9 (6%)	1	2
All	All	673/1036 (65%)	564 (84%)	78 (12%)	31 (5%)	2	4

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

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Mol	Chain	Res	Type
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
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 (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	188/229 (82%)	138 (73%)	50 (27%)	0	1
1	B	154/229 (67%)	115 (75%)	39 (25%)	0	1
1	C	145/229 (63%)	113 (78%)	32 (22%)	1	2
1	D	150/229 (66%)	116 (77%)	34 (23%)	1	2
All	All	637/916 (70%)	482 (76%)	155 (24%)	0	1

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Continued from previous page...

Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	214/259 (82%)	-0.31	0	100	100	2, 41, 55, 63	0
1	B	172/259 (66%)	-0.29	0	100	100	28, 43, 60, 73	0
1	C	162/259 (62%)	-0.30	0	100	100	27, 42, 57, 65	0
1	D	169/259 (65%)	-0.32	1 (0%)	89	90	24, 44, 62, 73	0
All	All	717/1036 (69%)	-0.31	1 (0%)	95	96	2, 42, 60, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	TYR	2.8

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.