Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:14 am BST

PDB ID	:	3U9B
Title	:	Structure of apo-CATI
Authors	:	Biswas, T.; Garneau-Tsodikova, S.; Tsodikov, O.V.
Deposited on	:	2011-10-18
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

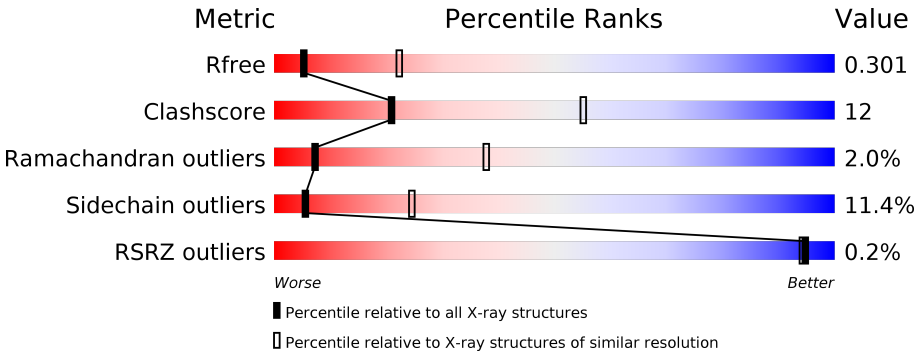
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	219	64% 27% 6%
1	B	219	58% 34% 5%
1	C	219	66% 29%
1	D	219	65% 28%
1	E	219	% 70% 23%
1	F	219	71% 23%

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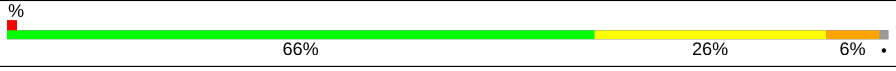
Mol	Chain	Length	Quality of chain
1	G	219	
1	H	219	
1	I	219	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15981 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 Chloramphenicol acetyltransferase.

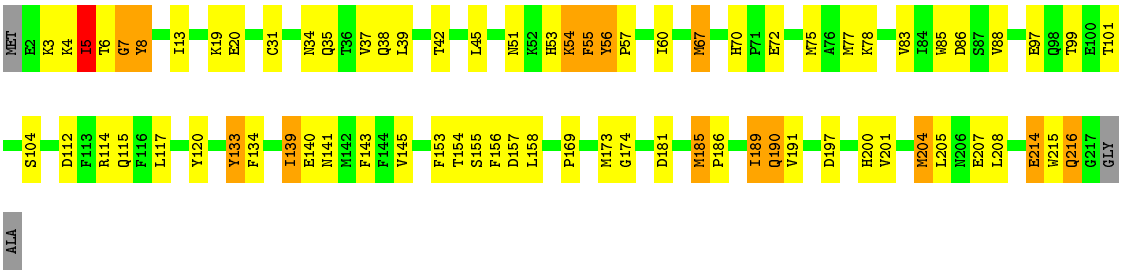
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1786	1160	294	319	13			
1	B	216	Total	C	N	O	S	0	0	0
			1786	1160	294	319	13			
1	C	216	Total	C	N	O	S	0	0	0
			1786	1160	294	319	13			
1	D	213	Total	C	N	O	S	0	0	0
			1767	1148	290	316	13			
1	E	213	Total	C	N	O	S	0	0	0
			1767	1148	290	316	13			
1	F	212	Total	C	N	O	S	0	0	0
			1759	1142	289	315	13			
1	G	214	Total	C	N	O	S	0	0	0
			1772	1151	291	317	13			
1	H	216	Total	C	N	O	S	0	0	0
			1786	1160	294	319	13			
1	I	214	Total	C	N	O	S	0	0	0
			1772	1151	291	317	13			

3 Residue-property plots (i)

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

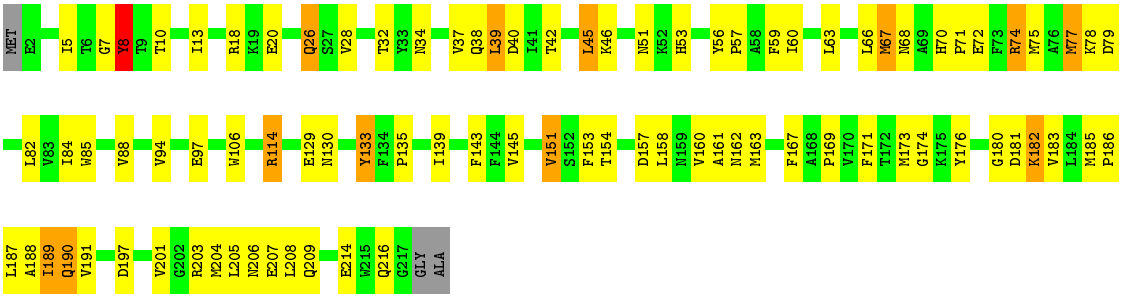
- Molecule 1: Chloramphenicol acetyltransferase

Chain A:



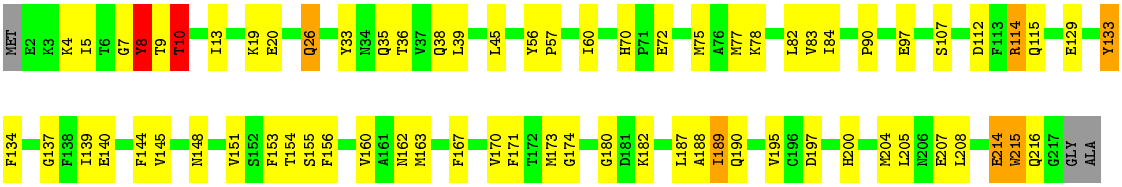
- Molecule 1: Chloramphenicol acetyltransferase

Chain B:



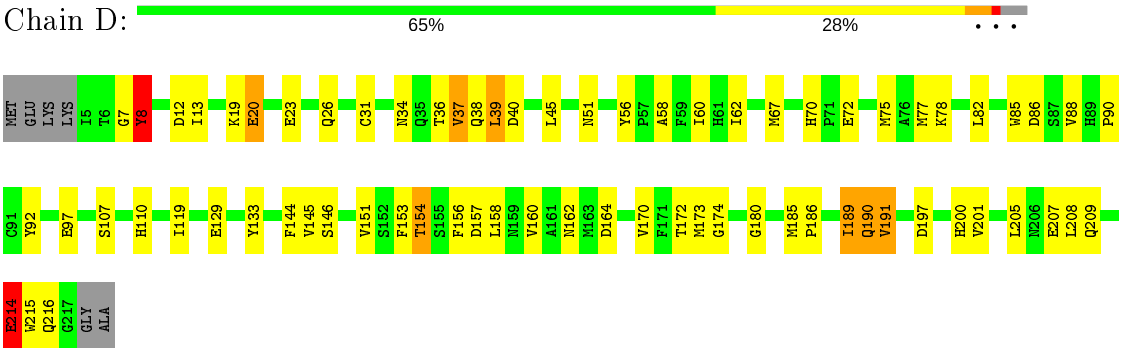
- Molecule 1: Chloramphenicol acetyltransferase

Chain C:



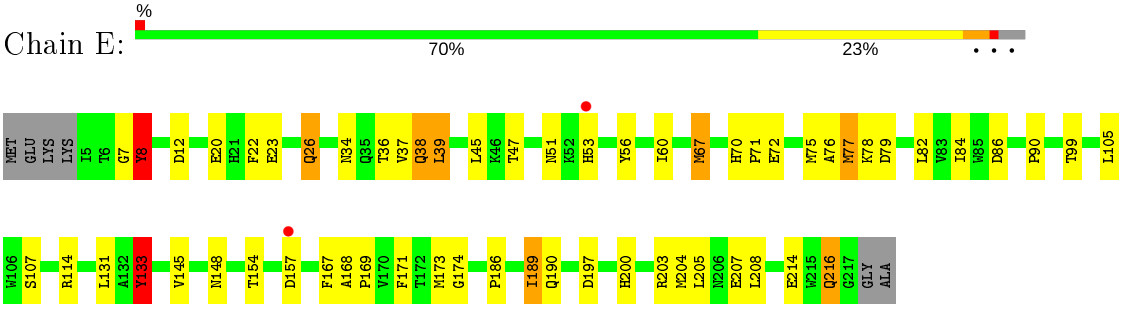
- Molecule 1: Chloramphenicol acetyltransferase

Chain D:



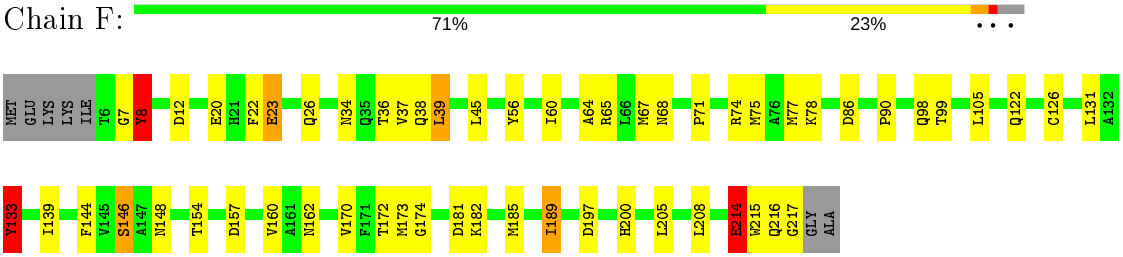
• Molecule 1: Chloramphenicol acetyltransferase

Chain E:



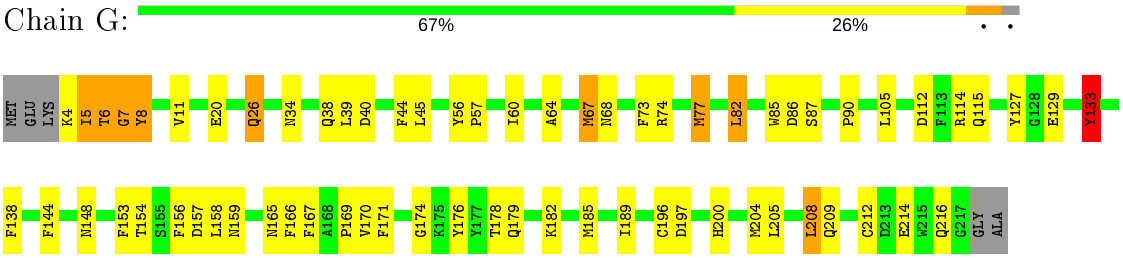
• Molecule 1: Chloramphenicol acetyltransferase

Chain F:



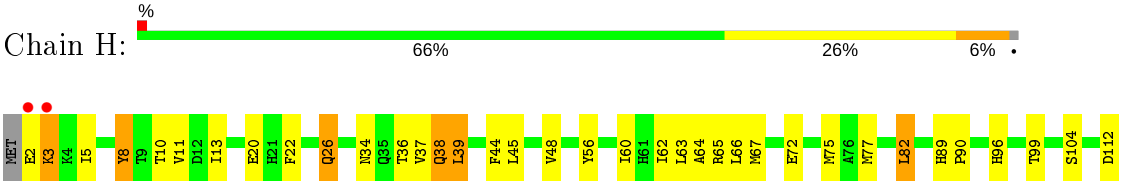
• Molecule 1: Chloramphenicol acetyltransferase

Chain G:



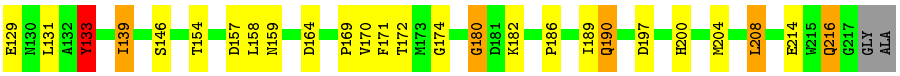
• Molecule 1: Chloramphenicol acetyltransferase

Chain H:



- Molecule 1: Chloramphenicol acetyltransferase

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.16Å 102.74Å 114.09Å 90.00° 119.94° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 49.43 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-3.20) 97.7 (49.43-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.301 0.236 , 0.301	Depositor DCC
R_{free} test set	1912 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.854	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 24.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.125 for -h-l,k,h 0.125 for l,k,-h-l 0.045 for -h-l,-k,l 0.045 for l,-k,h 0.049 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15981	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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	0.46	0/1845	0.58	0/2504
1	B	0.49	0/1845	0.59	0/2504
1	C	0.56	4/1845 (0.2%)	0.59	0/2504
1	D	0.38	0/1826	0.54	0/2479
1	E	0.41	0/1826	0.54	0/2479
1	F	0.39	0/1818	0.54	0/2468
1	G	0.38	0/1831	0.55	1/2486 (0.0%)
1	H	0.73	3/1845 (0.2%)	0.53	0/2504
1	I	0.40	0/1831	0.57	2/2486 (0.1%)
All	All	0.48	7/16512 (0.0%)	0.56	3/22414 (0.0%)

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	C	0	1
1	I	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	3	LYS	CA-CB	22.24	2.02	1.53
1	C	8	TYR	CG-CD1	10.07	1.52	1.39
1	H	2	GLU	N-CA	9.40	1.65	1.46
1	H	2	GLU	CA-CB	8.78	1.73	1.53
1	C	8	TYR	CE2-CZ	7.81	1.48	1.38
1	C	10	THR	C-O	6.38	1.35	1.23
1	C	8	TYR	CE1-CZ	5.92	1.46	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	208	LEU	CA-CB-CG	5.51	127.96	115.30
1	I	8	TYR	CA-CB-CG	5.42	123.70	113.40
1	G	208	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	7	GLY	Mainchain
1	I	8	TYR	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	1786	0	1672	53	0
1	B	1786	0	1672	63	0
1	C	1786	0	1672	43	0
1	D	1767	0	1655	42	0
1	E	1767	0	1655	44	0
1	F	1759	0	1644	37	0
1	G	1772	0	1657	48	0
1	H	1786	0	1672	50	0
1	I	1772	0	1657	36	0
All	All	15981	0	14956	378	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 12.

All (378) 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:H:3:LYS:CA	1:H:3:LYS:CB	2.02	1.35
1:F:7:GLY:O	1:F:8:TYR:HB2	1.57	0.99
1:A:6:THR:HG22	1:A:7:GLY:H	1.33	0.93
1:H:197:ASP:H	1:H:200:HIS:HD2	1.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:HB3	1:A:57:PRO:HD3	1.52	0.91
1:A:7:GLY:HA3	1:A:86:ASP:H	1.37	0.89
1:E:197:ASP:H	1:E:200:HIS:HD2	1.19	0.87
1:H:197:ASP:H	1:H:200:HIS:CD2	1.92	0.87
1:G:5:ILE:HD12	1:G:6:THR:H	1.38	0.85
1:I:26:GLN:HE21	1:I:26:GLN:HA	1.44	0.83
1:E:26:GLN:HA	1:E:26:GLN:HE21	1.44	0.83
1:F:197:ASP:H	1:F:200:HIS:HD2	1.30	0.79
1:D:7:GLY:HA2	1:D:86:ASP:H	1.50	0.77
1:D:154:THR:O	1:F:154:THR:HG23	1.86	0.75
1:A:197:ASP:H	1:A:200:HIS:HD2	1.31	0.74
1:I:197:ASP:H	1:I:200:HIS:HD2	1.35	0.74
1:G:5:ILE:HD12	1:G:6:THR:N	2.03	0.73
1:D:174:GLY:HA3	1:D:186:PRO:HG2	1.70	0.73
1:H:197:ASP:N	1:H:200:HIS:HD2	1.83	0.73
1:H:191:VAL:HG21	1:H:201:VAL:HG21	1.72	0.72
1:E:56:TYR:O	1:E:60:ILE:HG12	1.89	0.71
1:H:56:TYR:O	1:H:60:ILE:HG12	1.90	0.71
1:A:154:THR:HG23	1:B:154:THR:O	1.91	0.70
1:H:170:VAL:HB	1:H:190:GLN:HB3	1.74	0.69
1:B:130:ASN:HD22	1:B:135:PRO:HB3	1.57	0.69
1:G:40:ASP:HB3	1:G:209:GLN:HE22	1.58	0.69
1:F:56:TYR:O	1:F:60:ILE:HG12	1.93	0.69
1:H:174:GLY:HA3	1:H:186:PRO:HG2	1.75	0.68
1:D:56:TYR:O	1:D:60:ILE:HG12	1.93	0.68
1:A:157:ASP:OD2	1:B:157:ASP:HB2	1.93	0.68
1:A:57:PRO:HG3	1:A:120:TYR:CE2	2.29	0.68
1:H:99:THR:HG21	1:H:131:LEU:HD22	1.75	0.67
1:E:39:LEU:HD11	1:E:208:LEU:HD11	1.76	0.67
1:H:113:PHE:HB3	1:H:114:ARG:HH21	1.59	0.67
1:G:154:THR:HG21	1:H:38:GLN:HE22	1.61	0.66
1:C:9:THR:O	1:C:10:THR:O	2.13	0.66
1:H:26:GLN:HE21	1:H:26:GLN:HA	1.61	0.65
1:B:34:ASN:ND2	1:B:190:GLN:HB2	2.11	0.65
1:C:197:ASP:H	1:C:200:HIS:HD2	1.42	0.65
1:D:157:ASP:OD2	1:F:157:ASP:HB3	1.97	0.65
1:C:56:TYR:O	1:C:60:ILE:HG12	1.97	0.65
1:I:75:MET:HG2	1:I:84:ILE:HG12	1.78	0.65
1:H:62:ILE:HD12	1:H:211:TYR:HB3	1.79	0.65
1:B:189:ILE:HD12	1:B:189:ILE:H	1.62	0.64
1:G:154:THR:HG21	1:H:38:GLN:NE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:LEU:HD11	1:F:208:LEU:CD1	2.28	0.63
1:G:154:THR:HG23	1:H:154:THR:O	1.98	0.63
1:A:154:THR:O	1:C:154:THR:HG23	1.98	0.63
1:B:75:MET:SD	1:B:82:LEU:HD21	2.39	0.63
1:B:133:TYR:CE1	1:C:20:GLU:HB2	2.34	0.63
1:G:7:GLY:HA3	1:G:86:ASP:H	1.62	0.62
1:D:70:HIS:HE1	1:D:207:GLU:OE1	1.83	0.62
1:E:77:MET:HE3	1:E:167:PHE:HE2	1.63	0.62
1:A:7:GLY:O	1:A:85:TRP:HA	2.00	0.61
1:C:189:ILE:HD11	1:C:205:LEU:HD11	1.82	0.61
1:C:8:TYR:HB3	1:C:83:VAL:HB	1.81	0.61
1:H:166:PHE:HE2	1:H:190:GLN:HE21	1.49	0.61
1:G:11:VAL:HB	1:G:82:LEU:HD23	1.83	0.61
1:E:26:GLN:HA	1:E:26:GLN:NE2	2.13	0.61
1:A:6:THR:HG22	1:A:7:GLY:N	2.10	0.61
1:B:70:HIS:HE1	1:B:207:GLU:OE1	1.82	0.60
1:C:215:TRP:CE3	1:C:215:TRP:HA	2.34	0.60
1:A:56:TYR:HB3	1:A:57:PRO:CD	2.29	0.60
1:B:26:GLN:HA	1:B:26:GLN:HE21	1.67	0.60
1:A:6:THR:HG21	1:A:141:ASN:ND2	2.15	0.60
1:A:13:ILE:O	1:A:19:LYS:HB2	2.01	0.59
1:E:39:LEU:HD11	1:E:208:LEU:CD1	2.32	0.59
1:B:56:TYR:HB3	1:B:57:PRO:HD3	1.85	0.59
1:I:67:MET:HE3	1:I:169:PRO:HG2	1.84	0.59
1:B:68:ASN:HA	1:B:74:ARG:HD3	1.84	0.59
1:H:34:ASN:HD21	1:H:190:GLN:HB2	1.68	0.58
1:H:11:VAL:HB	1:H:82:LEU:HD23	1.86	0.58
1:E:133:TYR:CE1	1:F:20:GLU:HB2	2.39	0.58
1:A:174:GLY:HA3	1:A:186:PRO:HG2	1.86	0.57
1:A:70:HIS:HE1	1:A:207:GLU:OE1	1.86	0.57
1:I:99:THR:HG21	1:I:131:LEU:HD22	1.85	0.57
1:A:145:VAL:CG1	1:A:173:MET:HE3	2.35	0.57
1:H:39:LEU:HD11	1:H:208:LEU:CD1	2.35	0.57
1:H:38:GLN:HG3	1:H:177:TYR:OH	2.04	0.57
1:G:4:LYS:O	1:G:5:ILE:HG23	2.04	0.56
1:C:8:TYR:CD2	1:C:8:TYR:N	2.72	0.56
1:I:133:TYR:CD1	1:I:133:TYR:N	2.73	0.56
1:C:215:TRP:HE3	1:C:215:TRP:HA	1.70	0.56
1:B:56:TYR:HB3	1:B:57:PRO:CD	2.36	0.56
1:C:153:PHE:CE1	1:C:156:PHE:HB2	2.41	0.56
1:F:39:LEU:HD11	1:F:208:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:LEU:HD12	1:H:208:LEU:HD23	1.88	0.56
1:I:13:ILE:O	1:I:19:LYS:HB2	2.06	0.56
1:B:56:TYR:O	1:B:60:ILE:HG12	2.07	0.55
1:H:72:GLU:HA	1:H:75:MET:CE	2.36	0.55
1:F:197:ASP:H	1:F:200:HIS:CD2	2.17	0.55
1:E:7:GLY:HA2	1:E:86:ASP:HB2	1.89	0.55
1:G:26:GLN:HA	1:G:26:GLN:NE2	2.21	0.55
1:I:146:SER:HB2	1:I:172:THR:HG23	1.88	0.55
1:A:189:ILE:H	1:A:189:ILE:HD12	1.72	0.55
1:E:37:VAL:HG21	1:E:205:LEU:HD13	1.87	0.55
1:E:20:GLU:HA	1:E:23:GLU:HB2	1.88	0.54
1:G:56:TYR:O	1:G:60:ILE:HG12	2.07	0.54
1:D:7:GLY:HA2	1:D:86:ASP:N	2.20	0.54
1:C:134:PHE:HB3	1:C:137:GLY:HA2	1.88	0.54
1:G:77:MET:HE2	1:G:82:LEU:HA	1.88	0.54
1:H:72:GLU:HG3	1:H:200:HIS:HB3	1.88	0.54
1:A:6:THR:CG2	1:A:7:GLY:H	2.12	0.54
1:G:133:TYR:N	1:G:133:TYR:CD1	2.76	0.54
1:H:44:PHE:HB2	1:H:212:CYS:HB3	1.90	0.54
1:G:34:ASN:ND2	1:G:158:LEU:H	2.05	0.54
1:A:55:PHE:CD2	1:A:55:PHE:C	2.81	0.54
1:B:187:LEU:HG	1:B:188:ALA:N	2.23	0.54
1:H:134:PHE:HB3	1:H:137:GLY:HA2	1.90	0.54
1:H:215:TRP:HB3	1:H:216:GLN:OE1	2.07	0.53
1:B:189:ILE:N	1:B:189:ILE:HD12	2.23	0.53
1:A:173:MET:HB2	1:A:185:MET:CE	2.39	0.53
1:I:67:MET:HE3	1:I:169:PRO:CG	2.38	0.53
1:E:197:ASP:H	1:E:200:HIS:CD2	2.11	0.53
1:A:38:GLN:HE21	1:C:154:THR:HG21	1.74	0.53
1:B:180:GLY:C	1:B:182:LYS:H	2.13	0.52
1:H:72:GLU:HA	1:H:75:MET:HE3	1.90	0.52
1:B:151:VAL:HG22	1:B:153:PHE:HB3	1.90	0.52
1:B:176:TYR:HB3	1:B:185:MET:HG3	1.91	0.52
1:B:77:MET:HE3	1:B:167:PHE:HE2	1.74	0.52
1:B:189:ILE:HD11	1:B:205:LEU:HD11	1.90	0.52
1:B:7:GLY:O	1:B:8:TYR:HB2	2.08	0.52
1:A:189:ILE:HD11	1:A:205:LEU:HD11	1.91	0.52
1:A:55:PHE:C	1:A:55:PHE:HD2	2.13	0.52
1:G:112:ASP:HB3	1:G:115:GLN:HB2	1.92	0.52
1:C:70:HIS:HE1	1:C:207:GLU:OE1	1.92	0.52
1:D:191:VAL:HG21	1:D:201:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ASN:HA	1:F:74:ARG:HD3	1.91	0.52
1:G:26:GLN:HA	1:G:26:GLN:HE21	1.75	0.52
1:B:67:MET:HE3	1:B:169:PRO:HG2	1.91	0.51
1:A:88:VAL:HG12	1:A:143:PHE:HD1	1.75	0.51
1:D:110:HIS:HE1	1:D:119:ILE:HG13	1.75	0.51
1:F:7:GLY:HA2	1:F:86:ASP:CG	2.30	0.51
1:G:5:ILE:CD1	1:G:6:THR:N	2.72	0.51
1:H:159:ASN:HD21	1:I:159:ASN:ND2	2.08	0.51
1:B:75:MET:HG2	1:B:84:ILE:HG12	1.93	0.51
1:C:8:TYR:CE2	1:C:78:LYS:HE3	2.45	0.51
1:G:77:MET:HE3	1:G:167:PHE:HE2	1.75	0.51
1:H:60:ILE:CD1	1:H:145:VAL:HG11	2.41	0.51
1:C:72:GLU:HA	1:C:75:MET:HE2	1.93	0.51
1:D:13:ILE:O	1:D:19:LYS:HB2	2.11	0.51
1:E:22:PHE:CE1	1:E:82:LEU:HD12	2.46	0.51
1:G:64:ALA:HB2	1:G:90:PRO:HG3	1.92	0.51
1:A:34:ASN:ND2	1:A:158:LEU:H	2.08	0.51
1:B:174:GLY:HA3	1:B:186:PRO:HG2	1.92	0.51
1:H:34:ASN:HB2	1:H:157:ASP:OD2	2.11	0.51
1:C:75:MET:CE	1:C:195:VAL:HB	2.41	0.51
1:F:173:MET:SD	1:F:185:MET:HE1	2.51	0.51
1:G:67:MET:CE	1:G:171:PHE:HE1	2.23	0.51
1:B:59:PHE:CE2	1:B:63:LEU:HD21	2.46	0.51
1:B:39:LEU:CD2	1:B:209:GLN:OE1	2.59	0.50
1:D:197:ASP:H	1:D:200:HIS:HD2	1.57	0.50
1:E:78:LYS:HG3	1:E:79:ASP:H	1.76	0.50
1:D:153:PHE:CE1	1:D:156:PHE:HB2	2.47	0.50
1:F:146:SER:HB3	1:F:172:THR:HG23	1.92	0.50
1:B:34:ASN:HD21	1:B:190:GLN:HB2	1.77	0.50
1:G:157:ASP:OD2	1:I:157:ASP:HB3	2.10	0.50
1:H:154:THR:HG23	1:I:154:THR:O	2.11	0.50
1:I:71:PRO:HB2	1:I:84:ILE:HD13	1.94	0.50
1:D:170:VAL:HB	1:D:190:GLN:HB3	1.94	0.50
1:C:145:VAL:CG1	1:C:173:MET:HE3	2.41	0.50
1:C:75:MET:HE1	1:C:195:VAL:HB	1.92	0.50
1:F:20:GLU:HA	1:F:23:GLU:HB2	1.94	0.50
1:F:22:PHE:O	1:F:26:GLN:HB2	2.12	0.50
1:G:44:PHE:HB2	1:G:212:CYS:HB3	1.93	0.50
1:A:215:TRP:HB3	1:A:216:GLN:OE1	2.12	0.49
1:B:45:LEU:HD11	1:B:176:TYR:CE1	2.46	0.49
1:A:133:TYR:CE1	1:B:20:GLU:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:HE2	1:B:189:ILE:HG13	1.75	0.49
1:I:68:ASN:HA	1:I:74:ARG:HH11	1.76	0.49
1:E:34:ASN:HB2	1:E:157:ASP:OD2	2.12	0.49
1:E:7:GLY:HA2	1:E:86:ASP:H	1.77	0.49
1:G:144:PHE:HB2	1:G:170:VAL:HG22	1.94	0.49
1:G:197:ASP:H	1:G:200:HIS:CD2	2.30	0.49
1:G:196:CYS:HA	1:G:200:HIS:HD2	1.76	0.49
1:D:56:TYR:CE1	1:D:60:ILE:HD11	2.48	0.49
1:F:64:ALA:HB2	1:F:90:PRO:HG3	1.94	0.49
1:I:105:LEU:HD13	1:I:127:TYR:HB2	1.94	0.49
1:D:19:LYS:O	1:D:23:GLU:HB2	2.13	0.48
1:E:67:MET:HE2	1:E:171:PHE:HE1	1.78	0.48
1:I:197:ASP:H	1:I:200:HIS:CD2	2.24	0.48
1:B:143:PHE:HB2	1:B:169:PRO:HD2	1.95	0.48
1:A:191:VAL:HG21	1:A:201:VAL:CG2	2.44	0.48
1:A:56:TYR:CE1	1:A:60:ILE:HD11	2.48	0.48
1:B:154:THR:HG23	1:C:36:THR:HB	1.96	0.48
1:E:71:PRO:HB3	1:E:84:ILE:HD13	1.95	0.48
1:A:173:MET:HB2	1:A:185:MET:HE1	1.94	0.48
1:A:31:CYS:CB	1:C:160:VAL:HA	2.44	0.48
1:A:31:CYS:HB3	1:C:160:VAL:HA	1.94	0.48
1:D:189:ILE:HD11	1:D:205:LEU:HD11	1.96	0.48
1:B:34:ASN:ND2	1:B:158:LEU:H	2.11	0.48
1:E:26:GLN:CA	1:E:26:GLN:HE21	2.12	0.48
1:F:144:PHE:HB2	1:F:170:VAL:HG22	1.95	0.48
1:G:67:MET:HE2	1:G:171:PHE:HE1	1.79	0.48
1:B:191:VAL:HG21	1:B:201:VAL:HG21	1.96	0.47
1:A:197:ASP:N	1:A:200:HIS:HD2	2.06	0.47
1:E:154:THR:HG23	1:F:154:THR:O	2.15	0.47
1:F:197:ASP:N	1:F:200:HIS:HD2	2.06	0.47
1:F:148:ASN:O	1:F:174:GLY:HA2	2.13	0.47
1:F:37:VAL:HG21	1:F:205:LEU:HD13	1.96	0.47
1:A:99:THR:HG23	1:A:101:THR:OG1	2.14	0.47
1:B:88:VAL:HG12	1:B:143:PHE:HD1	1.80	0.47
1:H:65:ARG:HH11	1:H:217:GLY:HA2	1.79	0.47
1:B:37:VAL:HG21	1:B:205:LEU:HD13	1.95	0.47
1:D:154:THR:O	1:F:154:THR:CG2	2.60	0.47
1:G:26:GLN:OE1	1:G:167:PHE:HZ	1.97	0.47
1:C:13:ILE:O	1:C:19:LYS:HB2	2.14	0.47
1:B:161:ALA:HB2	1:C:163:MET:SD	2.55	0.47
1:E:145:VAL:CG1	1:E:173:MET:HE3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:THR:HG22	1:F:36:THR:O	2.14	0.47
1:G:189:ILE:HD11	1:G:205:LEU:HD21	1.96	0.46
1:G:8:TYR:H	1:G:85:TRP:HA	1.80	0.46
1:B:145:VAL:HG11	1:B:173:MET:HE3	1.96	0.46
1:C:26:GLN:HE21	1:C:26:GLN:HA	1.81	0.46
1:F:133:TYR:N	1:F:133:TYR:CD1	2.83	0.46
1:A:67:MET:HE3	1:A:169:PRO:CG	2.46	0.46
1:A:190:GLN:HG3	1:A:190:GLN:O	2.15	0.46
1:A:55:PHE:O	1:A:55:PHE:HD2	1.97	0.46
1:G:34:ASN:HA	1:G:189:ILE:O	2.15	0.46
1:H:96:HIS:HB2	1:H:99:THR:HG22	1.98	0.46
1:B:13:ILE:HG13	1:B:13:ILE:H	1.57	0.46
1:B:173:MET:HB2	1:B:185:MET:CE	2.46	0.46
1:B:78:LYS:HD3	1:B:85:TRP:HH2	1.81	0.46
1:D:56:TYR:OH	1:D:92:TYR:HB2	2.15	0.46
1:G:68:ASN:HA	1:G:74:ARG:HH11	1.80	0.46
1:D:110:HIS:CE1	1:D:119:ILE:HG13	2.51	0.46
1:D:36:THR:O	1:F:154:THR:HG22	2.16	0.46
1:D:20:GLU:HB3	1:F:133:TYR:CE1	2.50	0.46
1:A:72:GLU:HA	1:A:75:MET:CE	2.46	0.46
1:B:145:VAL:CG1	1:B:173:MET:HE3	2.46	0.46
1:D:144:PHE:HB2	1:D:170:VAL:HG22	1.98	0.46
1:G:176:TYR:HB3	1:G:185:MET:HG3	1.97	0.45
1:B:18:ARG:NH2	1:B:197:ASP:OD1	2.46	0.45
1:I:180:GLY:C	1:I:182:LYS:H	2.20	0.45
1:I:8:TYR:CZ	1:I:78:LYS:HG2	2.52	0.45
1:B:180:GLY:C	1:B:182:LYS:N	2.70	0.45
1:E:76:ALA:HA	1:E:167:PHE:HB2	1.98	0.45
1:G:133:TYR:CZ	1:H:20:GLU:HG3	2.52	0.45
1:D:8:TYR:H	1:D:85:TRP:HA	1.81	0.45
1:G:148:ASN:O	1:G:174:GLY:HA2	2.16	0.45
1:D:37:VAL:HG21	1:D:205:LEU:HD13	1.98	0.45
1:F:214:GLU:HB3	1:F:215:TRP:H	1.66	0.45
1:A:8:TYR:CE2	1:A:78:LYS:HE3	2.50	0.45
1:E:99:THR:HG21	1:E:131:LEU:HD22	1.98	0.45
1:D:162:ASN:HD21	1:D:164:ASP:HB2	1.81	0.45
1:E:77:MET:HE3	1:E:167:PHE:CE2	2.49	0.45
1:E:75:MET:HG2	1:E:84:ILE:HG12	1.97	0.45
1:I:56:TYR:O	1:I:60:ILE:HG12	2.17	0.45
1:A:112:ASP:HB3	1:A:115:GLN:HB2	1.99	0.45
1:A:51:ASN:ND2	1:A:216:GLN:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLY:O	1:B:8:TYR:CB	2.64	0.45
1:A:35:GLN:HA	1:C:155:SER:O	2.18	0.45
1:E:114:ARG:HH21	1:E:216:GLN:HE22	1.65	0.45
1:D:39:LEU:HD11	1:D:208:LEU:CD1	2.47	0.44
1:F:34:ASN:HB2	1:F:157:ASP:OD2	2.17	0.44
1:B:190:GLN:HG3	1:B:190:GLN:O	2.16	0.44
1:I:11:VAL:HB	1:I:82:LEU:HD23	2.00	0.44
1:A:153:PHE:CE1	1:A:156:PHE:HB2	2.53	0.44
1:C:56:TYR:HB3	1:C:57:PRO:CD	2.47	0.44
1:I:26:GLN:NE2	1:I:26:GLN:HA	2.24	0.44
1:A:139:ILE:HD13	1:A:140:GLU:H	1.83	0.44
1:D:90:PRO:HD2	1:D:107:SER:O	2.17	0.44
1:B:70:HIS:HB3	1:B:72:GLU:CD	2.38	0.44
1:C:144:PHE:HB2	1:C:170:VAL:HG22	1.98	0.44
1:C:9:THR:HB	1:C:84:ILE:HB	1.99	0.44
1:E:189:ILE:HD11	1:E:205:LEU:HD21	2.00	0.44
1:E:47:THR:O	1:E:51:ASN:ND2	2.51	0.44
1:G:165:ASN:O	1:G:167:PHE:N	2.51	0.44
1:I:171:PHE:HZ	1:I:204:MET:HE1	1.83	0.44
1:B:106:TRP:CE2	1:B:139:ILE:HG13	2.52	0.43
1:C:171:PHE:HD2	1:C:187:LEU:HD11	1.82	0.43
1:D:8:TYR:CE2	1:D:78:LYS:HE3	2.52	0.43
1:G:105:LEU:HD13	1:G:127:TYR:HB2	1.99	0.43
1:B:78:LYS:HD3	1:B:85:TRP:CH2	2.53	0.43
1:G:67:MET:HE3	1:G:169:PRO:HG3	1.99	0.43
1:H:64:ALA:HB2	1:H:90:PRO:HG3	2.00	0.43
1:D:197:ASP:H	1:D:200:HIS:CD2	2.35	0.43
1:C:90:PRO:HD2	1:C:107:SER:O	2.18	0.43
1:C:56:TYR:HB3	1:C:57:PRO:HD3	2.00	0.43
1:G:158:LEU:HD22	1:G:170:VAL:HG11	2.01	0.43
1:B:114:ARG:HG2	1:B:114:ARG:H	1.68	0.43
1:B:66:LEU:HB3	1:B:204:MET:HE2	2.01	0.43
1:D:173:MET:HB2	1:D:185:MET:HE2	2.01	0.43
1:D:72:GLU:HA	1:D:75:MET:CE	2.49	0.43
1:H:133:TYR:N	1:H:133:TYR:CD1	2.86	0.43
1:H:153:PHE:CE1	1:H:186:PRO:HB2	2.54	0.43
1:H:66:LEU:CD1	1:H:208:LEU:HD23	2.48	0.43
1:A:19:LYS:HG3	1:A:20:GLU:N	2.33	0.43
1:F:39:LEU:HD11	1:F:208:LEU:HD12	2.00	0.43
1:G:56:TYR:HB3	1:G:57:PRO:CD	2.49	0.43
1:I:216:GLN:CD	1:I:216:GLN:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:CE2	1:B:189:ILE:HG13	2.53	0.43
1:D:173:MET:HB2	1:D:185:MET:CE	2.49	0.43
1:H:114:ARG:HE	1:H:114:ARG:H	1.66	0.43
1:A:104:SER:HB2	1:A:134:PHE:CE1	2.54	0.42
1:G:154:THR:HG22	1:H:36:THR:O	2.19	0.42
1:C:148:ASN:O	1:C:174:GLY:HA2	2.19	0.42
1:C:153:PHE:CD1	1:C:156:PHE:HB2	2.55	0.42
1:I:67:MET:HE2	1:I:171:PHE:HE1	1.84	0.42
1:C:75:MET:O	1:C:167:PHE:HB2	2.19	0.42
1:C:214:GLU:HB3	1:C:215:TRP:H	1.73	0.42
1:D:40:ASP:HB3	1:D:209:GLN:HE22	1.84	0.42
1:A:4:LYS:O	1:A:5:ILE:HB	2.18	0.42
1:D:34:ASN:ND2	1:D:158:LEU:H	2.17	0.42
1:E:78:LYS:HG3	1:E:79:ASP:N	2.34	0.42
1:F:99:THR:HG21	1:F:131:LEU:HD22	2.00	0.42
1:H:112:ASP:OD1	1:H:114:ARG:HG2	2.20	0.42
1:I:34:ASN:HB2	1:I:157:ASP:OD2	2.20	0.42
1:A:70:HIS:HB3	1:A:72:GLU:OE1	2.20	0.42
1:B:151:VAL:HG11	1:C:35:GLN:OE1	2.20	0.42
1:B:40:ASP:HB3	1:B:209:GLN:NE2	2.35	0.42
1:B:78:LYS:HG3	1:B:79:ASP:N	2.35	0.42
1:H:189:ILE:CD1	1:H:205:LEU:HD11	2.50	0.42
1:B:45:LEU:HD12	1:B:183:VAL:HG11	2.00	0.42
1:B:51:ASN:HB2	1:B:53:HIS:ND1	2.35	0.42
1:F:189:ILE:HD11	1:F:205:LEU:HD21	2.02	0.42
1:I:174:GLY:HA3	1:I:186:PRO:HG2	2.02	0.42
1:A:201:VAL:O	1:A:204:MET:HG3	2.19	0.42
1:A:72:GLU:HA	1:A:75:MET:HE1	2.02	0.42
1:B:171:PHE:HE2	1:B:189:ILE:CG1	2.33	0.42
1:E:168:ALA:HA	1:E:169:PRO:HD3	1.89	0.42
1:E:174:GLY:HA3	1:E:186:PRO:HG2	2.01	0.42
1:G:67:MET:HE3	1:G:169:PRO:CG	2.50	0.42
1:G:56:TYR:HB3	1:G:57:PRO:HD3	2.02	0.42
1:G:20:GLU:HB2	1:I:133:TYR:CD1	2.54	0.42
1:D:214:GLU:HB3	1:D:215:TRP:H	1.59	0.41
1:E:114:ARG:HH21	1:E:216:GLN:NE2	2.18	0.41
1:G:153:PHE:CD1	1:G:156:PHE:HB2	2.55	0.41
1:H:13:ILE:HG13	1:H:13:ILE:H	1.69	0.41
1:B:173:MET:HB2	1:B:185:MET:HE2	2.01	0.41
1:C:36:THR:HG23	1:C:188:ALA:HB2	2.02	0.41
1:E:8:TYR:HE2	1:E:78:LYS:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLU:HB3	1:F:133:TYR:CD1	2.56	0.41
1:A:155:SER:HB2	1:C:155:SER:HB2	2.03	0.41
1:E:51:ASN:C	1:E:53:HIS:H	2.22	0.41
1:E:67:MET:HE3	1:E:169:PRO:HG2	2.02	0.41
1:F:122:GLN:O	1:F:126:CYS:HB3	2.20	0.41
1:F:71:PRO:O	1:F:75:MET:HG3	2.21	0.41
1:C:114:ARG:H	1:C:114:ARG:HG2	1.65	0.41
1:E:148:ASN:O	1:E:174:GLY:HA2	2.21	0.41
1:G:159:ASN:HA	1:I:159:ASN:ND2	2.35	0.41
1:H:63:LEU:HD23	1:H:208:LEU:HD21	2.03	0.41
1:I:170:VAL:HB	1:I:190:GLN:HG3	2.01	0.41
1:B:130:ASN:ND2	1:B:135:PRO:HB3	2.30	0.41
1:G:73:PHE:CZ	1:G:204:MET:HG2	2.55	0.41
1:H:191:VAL:HG21	1:H:201:VAL:CG2	2.47	0.41
1:A:54:LYS:HG3	1:A:55:PHE:N	2.36	0.41
1:D:58:ALA:O	1:D:62:ILE:HG12	2.20	0.41
1:D:154:THR:HG23	1:E:36:THR:HB	2.02	0.41
1:B:203:ARG:HA	1:B:206:ASN:HB2	2.03	0.41
1:C:112:ASP:HB3	1:C:115:GLN:HB2	2.02	0.41
1:E:7:GLY:O	1:E:8:TYR:CB	2.68	0.41
1:H:22:PHE:O	1:H:26:GLN:HB2	2.21	0.41
1:I:139:ILE:HD13	1:I:139:ILE:HA	1.93	0.41
1:I:44:PHE:CE2	1:I:48:VAL:HG21	2.56	0.41
1:B:32:THR:HG23	1:B:163:MET:CE	2.51	0.41
1:D:154:THR:HG21	1:E:38:GLN:NE2	2.36	0.41
1:H:189:ILE:HD11	1:H:205:LEU:HD21	2.03	0.41
1:C:13:ILE:H	1:C:13:ILE:HG13	1.64	0.40
1:D:60:ILE:HD13	1:D:145:VAL:HG11	2.03	0.40
1:E:90:PRO:HD2	1:E:107:SER:O	2.21	0.40
1:G:154:THR:O	1:I:154:THR:HG23	2.20	0.40
1:I:22:PHE:O	1:I:26:GLN:HB2	2.21	0.40
1:E:72:GLU:HA	1:E:75:MET:HE3	2.02	0.40
1:F:65:ARG:HH12	1:F:217:GLY:HA2	1.86	0.40
1:G:159:ASN:HA	1:I:159:ASN:HD21	1.87	0.40
1:H:139:ILE:HD13	1:H:139:ILE:HA	1.96	0.40
1:I:158:LEU:HD22	1:I:170:VAL:HG11	2.02	0.40
1:B:32:THR:HG23	1:B:163:MET:HE2	2.03	0.40
1:H:89:HIS:HA	1:H:90:PRO:HD3	1.98	0.40
1:A:173:MET:HB2	1:A:185:MET:HE2	2.04	0.40
1:C:189:ILE:HD12	1:C:189:ILE:H	1.87	0.40
1:D:31:CYS:CB	1:F:160:VAL:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:HIS:HE1	1:E:207:GLU:OE1	2.04	0.40
1:I:204:MET:HE2	1:I:204:MET:HB2	1.97	0.40
1:E:204:MET:O	1:E:208:LEU:HB2	2.21	0.40
1:D:20:GLU:CB	1:F:133:TYR:CE1	3.05	0.40
1:H:62:ILE:HG22	1:H:208:LEU:HD22	2.03	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	214/219 (98%)	197 (92%)	12 (6%)	5 (2%)	6	34
1	B	214/219 (98%)	190 (89%)	18 (8%)	6 (3%)	5	29
1	C	214/219 (98%)	192 (90%)	18 (8%)	4 (2%)	8	39
1	D	211/219 (96%)	196 (93%)	12 (6%)	3 (1%)	11	46
1	E	211/219 (96%)	197 (93%)	11 (5%)	3 (1%)	11	46
1	F	210/219 (96%)	193 (92%)	12 (6%)	5 (2%)	6	34
1	G	212/219 (97%)	189 (89%)	18 (8%)	5 (2%)	6	34
1	H	214/219 (98%)	194 (91%)	15 (7%)	5 (2%)	6	34
1	I	212/219 (97%)	198 (93%)	11 (5%)	3 (1%)	11	46
All	All	1912/1971 (97%)	1746 (91%)	127 (7%)	39 (2%)	7	38

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	B	8	TYR
1	B	28	VAL

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Mol	Chain	Res	Type
1	C	10	THR
1	F	8	TYR
1	G	5	ILE
1	G	133	TYR
1	H	133	TYR
1	I	28	VAL
1	I	133	TYR
1	A	3	LYS
1	A	7	GLY
1	A	56	TYR
1	B	10	THR
1	C	133	TYR
1	C	180	GLY
1	E	8	TYR
1	F	133	TYR
1	F	181	ASP
1	G	7	GLY
1	A	214	GLU
1	E	133	TYR
1	E	214	GLU
1	G	166	PHE
1	H	10	THR
1	H	166	PHE
1	I	180	GLY
1	B	5	ILE
1	B	74	ARG
1	D	8	TYR
1	F	214	GLU
1	C	5	ILE
1	F	78	LYS
1	G	6	THR
1	H	5	ILE
1	H	8	TYR
1	D	214	GLU
1	B	71	PRO
1	D	180	GLY

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	191/194 (98%)	166 (87%)	25 (13%)	4 19
1	B	191/194 (98%)	167 (87%)	24 (13%)	4 21
1	C	191/194 (98%)	165 (86%)	26 (14%)	3 17
1	D	190/194 (98%)	164 (86%)	26 (14%)	3 17
1	E	190/194 (98%)	176 (93%)	14 (7%)	13 46
1	F	189/194 (97%)	171 (90%)	18 (10%)	8 32
1	G	190/194 (98%)	171 (90%)	19 (10%)	7 30
1	H	191/194 (98%)	168 (88%)	23 (12%)	5 22
1	I	190/194 (98%)	169 (89%)	21 (11%)	6 25
All	All	1713/1746 (98%)	1517 (89%)	196 (11%)	5 24

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	TYR
1	A	37	VAL
1	A	39	LEU
1	A	42	THR
1	A	45	LEU
1	A	53	HIS
1	A	54	LYS
1	A	55	PHE
1	A	67	MET
1	A	77	MET
1	A	83	VAL
1	A	97	GLU
1	A	114	ARG
1	A	117	LEU
1	A	133	TYR
1	A	139	ILE
1	A	181	ASP
1	A	185	MET
1	A	189	ILE
1	A	190	GLN
1	A	204	MET
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	214	GLU
1	A	216	GLN
1	B	8	TYR
1	B	26	GLN
1	B	38	GLN
1	B	39	LEU
1	B	42	THR
1	B	45	LEU
1	B	46	LYS
1	B	67	MET
1	B	77	MET
1	B	94	VAL
1	B	97	GLU
1	B	114	ARG
1	B	129	GLU
1	B	133	TYR
1	B	151	VAL
1	B	160	VAL
1	B	162	ASN
1	B	181	ASP
1	B	182	LYS
1	B	189	ILE
1	B	190	GLN
1	B	208	LEU
1	B	214	GLU
1	B	216	GLN
1	C	4	LYS
1	C	8	TYR
1	C	10	THR
1	C	26	GLN
1	C	33	TYR
1	C	38	GLN
1	C	39	LEU
1	C	45	LEU
1	C	77	MET
1	C	82	LEU
1	C	97	GLU
1	C	114	ARG
1	C	129	GLU
1	C	133	TYR
1	C	139	ILE
1	C	140	GLU

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Mol	Chain	Res	Type
1	C	151	VAL
1	C	162	ASN
1	C	182	LYS
1	C	189	ILE
1	C	190	GLN
1	C	204	MET
1	C	208	LEU
1	C	214	GLU
1	C	215	TRP
1	C	216	GLN
1	D	8	TYR
1	D	12	ASP
1	D	20	GLU
1	D	26	GLN
1	D	37	VAL
1	D	38	GLN
1	D	39	LEU
1	D	45	LEU
1	D	51	ASN
1	D	67	MET
1	D	77	MET
1	D	82	LEU
1	D	88	VAL
1	D	97	GLU
1	D	129	GLU
1	D	133	TYR
1	D	146	SER
1	D	151	VAL
1	D	154	THR
1	D	160	VAL
1	D	172	THR
1	D	189	ILE
1	D	190	GLN
1	D	191	VAL
1	D	214	GLU
1	D	216	GLN
1	E	8	TYR
1	E	12	ASP
1	E	26	GLN
1	E	38	GLN
1	E	39	LEU
1	E	45	LEU

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Mol	Chain	Res	Type
1	E	67	MET
1	E	77	MET
1	E	105	LEU
1	E	133	TYR
1	E	189	ILE
1	E	190	GLN
1	E	203	ARG
1	E	216	GLN
1	F	8	TYR
1	F	12	ASP
1	F	23	GLU
1	F	38	GLN
1	F	39	LEU
1	F	45	LEU
1	F	67	MET
1	F	77	MET
1	F	98	GLN
1	F	105	LEU
1	F	133	TYR
1	F	139	ILE
1	F	146	SER
1	F	162	ASN
1	F	182	LYS
1	F	189	ILE
1	F	214	GLU
1	F	216	GLN
1	G	8	TYR
1	G	26	GLN
1	G	38	GLN
1	G	39	LEU
1	G	45	LEU
1	G	67	MET
1	G	77	MET
1	G	82	LEU
1	G	87	SER
1	G	114	ARG
1	G	129	GLU
1	G	133	TYR
1	G	138	PHE
1	G	178	THR
1	G	179	GLN
1	G	182	LYS

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Mol	Chain	Res	Type
1	G	208	LEU
1	G	214	GLU
1	G	216	GLN
1	H	8	TYR
1	H	26	GLN
1	H	37	VAL
1	H	38	GLN
1	H	39	LEU
1	H	45	LEU
1	H	48	VAL
1	H	67	MET
1	H	77	MET
1	H	82	LEU
1	H	104	SER
1	H	114	ARG
1	H	129	GLU
1	H	133	TYR
1	H	139	ILE
1	H	140	GLU
1	H	159	ASN
1	H	160	VAL
1	H	162	ASN
1	H	189	ILE
1	H	191	VAL
1	H	214	GLU
1	H	216	GLN
1	I	5	ILE
1	I	8	TYR
1	I	26	GLN
1	I	37	VAL
1	I	39	LEU
1	I	45	LEU
1	I	67	MET
1	I	77	MET
1	I	82	LEU
1	I	103	SER
1	I	105	LEU
1	I	111	ASP
1	I	129	GLU
1	I	133	TYR
1	I	139	ILE
1	I	164	ASP

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Mol	Chain	Res	Type
1	I	189	ILE
1	I	190	GLN
1	I	208	LEU
1	I	214	GLU
1	I	216	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	38	GLN
1	A	53	HIS
1	A	61	HIS
1	A	70	HIS
1	A	159	ASN
1	A	200	HIS
1	B	26	GLN
1	B	34	ASN
1	B	38	GLN
1	B	51	ASN
1	B	70	HIS
1	B	130	ASN
1	B	159	ASN
1	B	162	ASN
1	B	165	ASN
1	C	34	ASN
1	C	70	HIS
1	C	159	ASN
1	C	200	HIS
1	C	206	ASN
1	D	26	GLN
1	D	34	ASN
1	D	70	HIS
1	D	110	HIS
1	D	159	ASN
1	D	200	HIS
1	D	209	GLN
1	E	26	GLN
1	E	38	GLN
1	E	70	HIS
1	E	110	HIS
1	E	165	ASN

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Mol	Chain	Res	Type
1	E	200	HIS
1	E	216	GLN
1	F	26	GLN
1	F	159	ASN
1	F	162	ASN
1	F	200	HIS
1	G	26	GLN
1	G	34	ASN
1	G	53	HIS
1	G	70	HIS
1	G	200	HIS
1	G	209	GLN
1	H	53	HIS
1	H	61	HIS
1	H	70	HIS
1	H	118	HIS
1	H	162	ASN
1	H	165	ASN
1	H	200	HIS
1	I	26	GLN
1	I	70	HIS
1	I	159	ASN
1	I	162	ASN
1	I	200	HIS
1	I	216	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	216/219 (98%)	-0.30	0 100 100	49, 70, 98, 114	0
1	B	216/219 (98%)	-0.21	0 100 100	35, 65, 98, 113	0
1	C	216/219 (98%)	-0.29	0 100 100	51, 72, 98, 110	0
1	D	213/219 (97%)	-0.25	0 100 100	61, 78, 105, 118	0
1	E	213/219 (97%)	-0.28	2 (0%) 84 75	54, 73, 101, 115	0
1	F	212/219 (96%)	-0.24	0 100 100	60, 83, 114, 124	0
1	G	214/219 (97%)	-0.21	0 100 100	59, 83, 110, 123	0
1	H	216/219 (98%)	-0.24	2 (0%) 84 75	61, 81, 100, 111	0
1	I	214/219 (97%)	-0.26	0 100 100	60, 78, 96, 103	0
All	All	1930/1971 (97%)	-0.25	4 (0%) 95 94	35, 76, 104, 124	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	53	HIS	2.5
1	H	3	LYS	2.5
1	E	157	ASP	2.4
1	H	2	GLU	2.2

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.