



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:35 am BST

PDB ID : 1C6V
Title : SIV INTEGRASE (CATALYTIC DOMAIN + DNA BINDING DOMAIN COMPRISING RESIDUES 50-293) MUTANT WITH PHE 185 REPLACED BY HIS (F185H)
Authors : Chen, Z.; Yan, Y.; Munshi, S.; Li, Y.; Zrurgy-Murphy, J.; Xu, B.; Witmer, M.; Felock, P.; Wolfe, A.; Sardana, V.; Emini, E.A.; Hazuda, D.; Kuo, L.C.
Deposited on : 1999-12-21
Resolution : 3.00 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

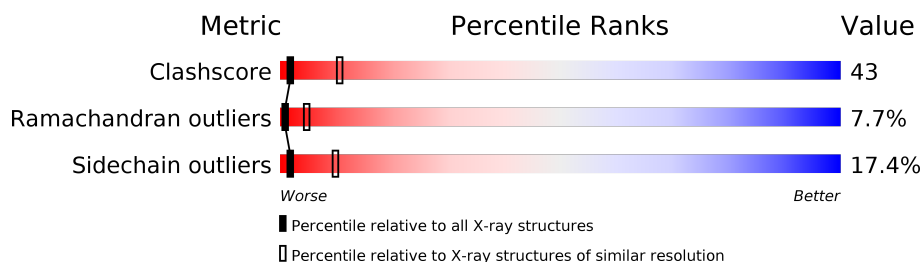
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	
1	C	164	
1	D	164	
2	X	81	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5030 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 PROTEIN (SIV INTEGRASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1169	733	213	214	9			
1	B	142	Total	C	N	O	S	0	0	0
			1111	697	203	202	9			
1	C	143	Total	C	N	O	S	0	0	0
			1118	702	204	203	9			
1	D	142	Total	C	N	O	S	0	0	0
			1111	697	203	202	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	HIS	PHE	ENGINEERED MUTATION	UNP Q88016
B	185	HIS	PHE	ENGINEERED MUTATION	UNP Q88016
C	185	HIS	PHE	ENGINEERED MUTATION	UNP Q88016
D	185	HIS	PHE	ENGINEERED MUTATION	UNP Q88016

- Molecule 2 is a protein called PROTEIN (SIU89134).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	55	Total	C	N	O	0	0	0
			455	296	85	74			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	250	LEU	ILE	CONFLICT	UNP Q87706

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	10	Total 10	O 10	0	0
3	C	24	Total 24	O 24	0	0
3	D	12	Total 12	O 12	0	0
3	X	4	Total 4	O 4	0	0

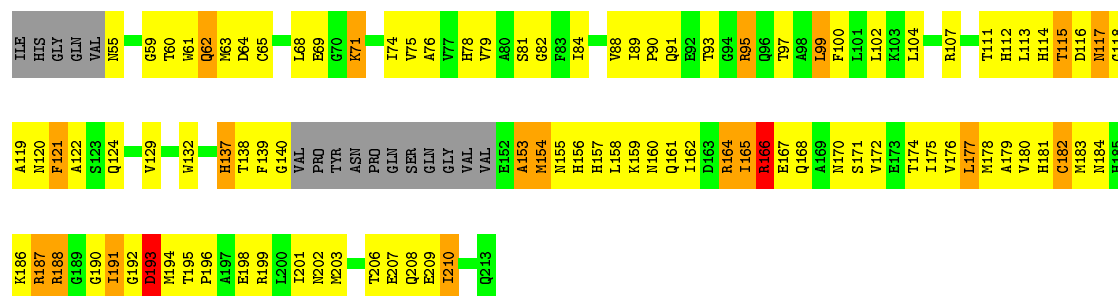
3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

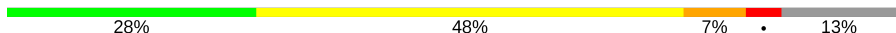
Note EDS was not executed.

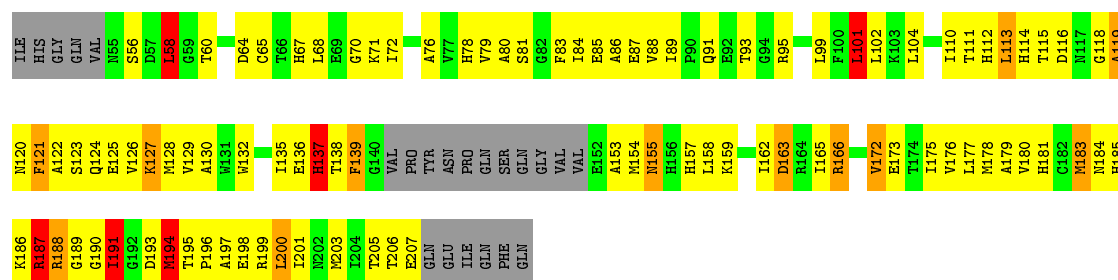
• Molecule 1: PROTEIN (SIV INTEGRASE)

Chain A: 



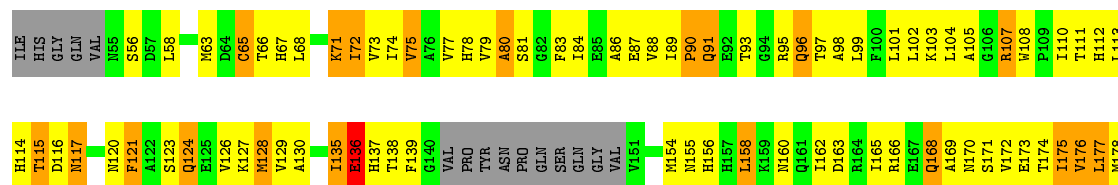
• Molecule 1: PROTEIN (SIV INTEGRASE)

Chain B: 



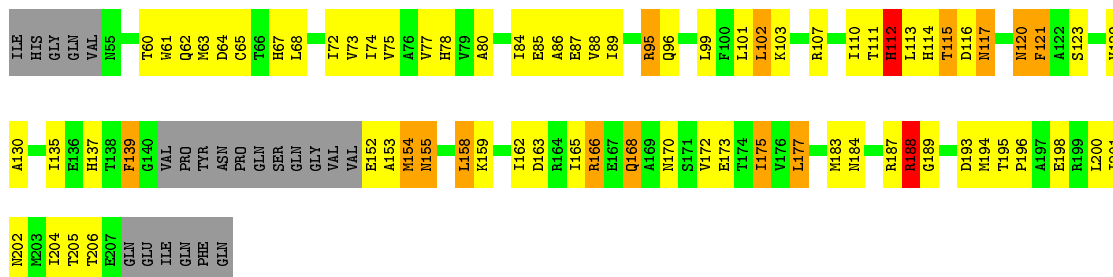
• Molecule 1: PROTEIN (SIV INTEGRASE)

Chain C: 

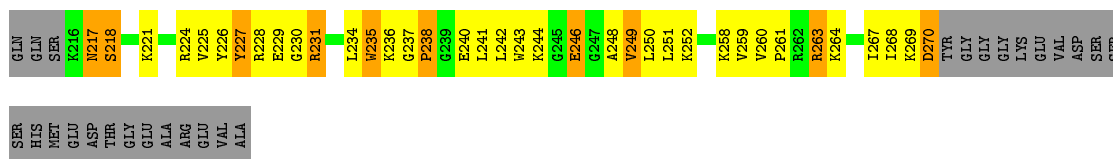
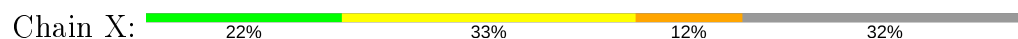




• Molecule 1: PROTEIN (SIV INTEGRASE)



• Molecule 2: PROTEIN (SIU89134)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.57 Å 100.00 Å 150.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5030	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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	0.52	0/1192	0.81	0/1612
1	B	0.48	0/1133	0.84	2/1533 (0.1%)
1	C	0.51	0/1140	0.85	4/1543 (0.3%)
1	D	0.46	0/1133	0.74	0/1533
2	X	0.49	0/464	0.77	0/618
All	All	0.49	0/5062	0.80	6/6839 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	GLY	N-CA-C	-6.53	96.76	113.10
1	C	121	PHE	N-CA-C	5.49	125.81	111.00
1	B	101	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	187	ARG	N-CA-C	5.41	125.59	111.00
1	C	104	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	194	MET	N-CA-C	5.11	124.81	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1169	0	1146	118	0
1	B	1111	0	1092	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1118	0	1101	115	0
1	D	1111	0	1092	78	0
2	X	455	0	487	44	0
3	A	16	0	0	2	0
3	B	10	0	0	0	0
3	C	24	0	0	1	0
3	D	12	0	0	0	0
3	X	4	0	0	0	0
All	All	5030	0	4918	423	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 43.

All (423) 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:B:119:ALA:HA	1:B:122:ALA:HB3	1.22	1.11
1:B:71:LYS:HG3	1:B:172:VAL:HG21	1.44	1.00
1:A:165:ILE:HD11	1:A:182:CYS:SG	2.03	0.98
1:B:158:LEU:HA	1:B:183:MET:HE1	1.46	0.95
1:B:81:SER:HA	1:B:199:ARG:HD2	1.46	0.94
1:B:172:VAL:HA	1:B:175:ILE:HG22	1.49	0.93
1:C:177:LEU:HB3	1:D:102:LEU:HD12	1.48	0.93
1:C:165:ILE:HG12	1:C:168:GLN:HG3	1.50	0.91
2:X:260:VAL:HG13	2:X:264:LYS:HE2	1.53	0.90
1:B:60:THR:HG23	1:B:112:HIS:HB2	1.54	0.88
2:X:249:VAL:HG23	2:X:260:VAL:HB	1.54	0.87
1:D:159:LYS:O	1:D:162:ILE:HG13	1.75	0.86
1:A:194:MET:HG2	1:A:198:GLU:HG3	1.59	0.85
1:D:165:ILE:HG13	1:D:168:GLN:HG3	1.58	0.85
1:C:96:GLN:HA	1:C:96:GLN:HE21	1.40	0.84
1:B:191:ILE:HG23	1:C:199:ARG:NH2	1.92	0.84
1:A:172:VAL:O	1:A:176:VAL:HG23	1.78	0.83
1:B:191:ILE:HG23	1:C:199:ARG:HH22	1.40	0.83
1:C:95:ARG:HH22	1:D:173:GLU:HB3	1.44	0.83
1:D:95:ARG:HH21	1:D:95:ARG:HG2	1.43	0.83
1:A:95:ARG:HD2	1:A:95:ARG:H	1.40	0.82
1:C:135:ILE:HG22	1:C:136:GLU:H	1.43	0.81
1:C:75:VAL:HG21	1:C:155:ASN:ND2	1.97	0.80
1:D:115:THR:HG21	1:D:120:ASN:HD21	1.47	0.80
1:D:130:ALA:HB1	1:D:135:ILE:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:HA	1:B:196:PRO:HG2	1.64	0.78
1:B:190:GLY:O	1:B:191:ILE:HD12	1.84	0.78
1:C:169:ALA:HB3	1:C:175:ILE:HD13	1.66	0.78
1:D:84:ILE:HD11	1:D:154:MET:SD	2.24	0.78
1:B:187:ARG:HD2	1:B:193:ASP:HB2	1.64	0.78
1:A:203:MET:O	1:A:206:THR:HG22	1.82	0.77
1:A:194:MET:HB3	1:A:199:ARG:HB2	1.66	0.77
1:B:84:ILE:HG23	1:B:180:VAL:HG13	1.65	0.77
1:B:101:LEU:HD21	1:B:135:ILE:HD13	1.66	0.76
1:B:125:GLU:O	1:B:129:VAL:HG23	1.86	0.76
1:A:137:HIS:CE1	1:A:139:PHE:HE1	2.03	0.75
1:B:56:SER:HB2	1:B:80:ALA:HB2	1.67	0.75
1:D:78:HIS:CE1	1:D:80:ALA:HB3	2.22	0.75
1:A:115:THR:HG21	1:A:121:PHE:HB2	1.68	0.75
1:C:205:THR:HG21	1:D:205:THR:HG21	1.68	0.74
1:A:195:THR:HG22	1:A:198:GLU:HG2	1.68	0.74
1:D:163:ASP:HA	1:D:166:ARG:HG3	1.67	0.74
1:B:165:ILE:HG13	1:B:175:ILE:HD11	1.69	0.74
1:B:88:VAL:HG21	1:B:173:GLU:HA	1.69	0.74
1:C:96:GLN:HA	1:C:96:GLN:NE2	2.04	0.73
1:C:205:THR:OG1	1:D:201:ILE:HG22	1.88	0.72
1:C:187:ARG:N	1:C:195:THR:HG22	2.05	0.72
1:A:165:ILE:CD1	1:A:182:CYS:SG	2.78	0.71
1:D:115:THR:HG21	1:D:120:ASN:ND2	2.05	0.71
1:B:188:ARG:NE	1:B:188:ARG:HA	2.05	0.71
1:B:123:SER:HB2	1:B:126:VAL:HG23	1.73	0.71
2:X:227:TYR:H	2:X:227:TYR:HD2	1.38	0.71
2:X:225:VAL:HB	2:X:267:ILE:HG23	1.73	0.70
1:D:101:LEU:HD21	1:D:135:ILE:HD13	1.73	0.70
1:D:163:ASP:HA	1:D:166:ARG:CG	2.21	0.70
1:C:171:SER:OG	1:C:174:THR:HB	1.91	0.70
1:D:78:HIS:ND1	1:D:200:LEU:HD13	2.07	0.69
2:X:234:LEU:HD12	2:X:235:TRP:HD1	1.58	0.69
1:B:187:ARG:HA	1:B:195:THR:HG22	1.75	0.69
1:C:187:ARG:H	1:C:195:THR:HG22	1.59	0.68
1:A:62:GLN:O	1:A:76:ALA:HA	1.94	0.67
1:C:187:ARG:HB2	1:C:193:ASP:O	1.93	0.67
1:D:77:VAL:HG12	1:D:84:ILE:HA	1.76	0.67
1:A:158:LEU:O	1:A:162:ILE:HG13	1.94	0.67
1:B:130:ALA:HA	1:B:135:ILE:HG12	1.76	0.66
1:B:187:ARG:O	1:B:187:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ILE:CG1	1:C:168:GLN:HG3	2.23	0.65
1:A:207:GLU:O	1:A:210:ILE:HB	1.96	0.65
1:C:188:ARG:HD2	3:C:415:HOH:O	1.96	0.65
1:A:71:LYS:HE3	1:A:71:LYS:HA	1.77	0.65
1:B:176:VAL:O	1:B:180:VAL:HG23	1.96	0.64
1:B:188:ARG:HE	1:B:188:ARG:HA	1.62	0.64
1:B:153:ALA:HB1	1:B:157:HIS:NE2	2.11	0.64
1:C:179:ALA:O	1:C:183:MET:HG3	1.98	0.64
1:A:84:ILE:HD13	1:A:183:MET:HG2	1.80	0.64
1:C:121:PHE:HE2	1:C:137:HIS:HB3	1.63	0.64
1:A:104:LEU:HD22	3:A:445:HOH:O	1.97	0.63
1:D:95:ARG:NH2	1:D:95:ARG:HG2	2.08	0.63
1:C:97:THR:HG21	1:C:120:ASN:HA	1.81	0.63
2:X:226:TYR:CD1	2:X:238:PRO:HG3	2.34	0.62
1:A:84:ILE:HD11	1:A:154:MET:HG3	1.81	0.62
1:B:58:LEU:HD21	1:B:207:GLU:HG3	1.82	0.62
1:C:67:HIS:HA	1:C:71:LYS:O	2.00	0.62
1:D:188:ARG:HA	1:D:188:ARG:CZ	2.29	0.62
1:B:186:LYS:HG3	1:B:186:LYS:O	1.99	0.61
1:C:107:ARG:HD3	1:D:107:ARG:HD3	1.81	0.61
2:X:224:ARG:HB3	2:X:238:PRO:HB3	1.82	0.61
2:X:231:ARG:HE	2:X:231:ARG:N	1.99	0.61
1:C:126:VAL:HA	1:C:129:VAL:HG12	1.81	0.61
1:B:189:GLY:HA2	1:B:199:ARG:HH22	1.66	0.61
1:C:174:THR:OG1	1:D:99:LEU:HD11	2.00	0.61
1:B:113:LEU:HD23	1:B:115:THR:OG1	2.00	0.60
1:D:65:CYS:SG	1:D:74:ILE:HG13	2.41	0.60
1:A:180:VAL:HG12	1:A:184:ASN:ND2	2.16	0.60
1:A:183:MET:O	1:A:196:PRO:HG2	2.01	0.60
1:C:75:VAL:HG12	1:C:86:ALA:HB2	1.84	0.60
1:A:65:CYS:HB2	1:A:121:PHE:HZ	1.65	0.60
1:D:77:VAL:HG12	1:D:84:ILE:HG12	1.83	0.60
1:A:63:MET:HE2	1:A:121:PHE:HE1	1.67	0.60
1:A:132:TRP:CZ2	1:B:178:MET:HG2	2.35	0.60
1:C:102:LEU:HB2	1:C:129:VAL:HG21	1.82	0.60
1:A:117:ASN:HB3	1:A:139:PHE:HB3	1.83	0.60
1:D:162:ILE:HD12	1:D:163:ASP:N	2.17	0.60
2:X:229:GLU:HA	2:X:264:LYS:CB	2.31	0.60
1:C:124:GLN:HA	1:C:127:LYS:HB2	1.84	0.60
1:A:172:VAL:HA	1:A:175:ILE:HG22	1.83	0.60
1:D:84:ILE:HD12	1:D:183:MET:SD	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:CE2	1:C:137:HIS:HB3	2.37	0.59
1:D:172:VAL:HA	1:D:175:ILE:HG22	1.83	0.59
2:X:229:GLU:HA	2:X:264:LYS:HB2	1.85	0.59
1:A:202:ASN:ND2	2:X:268:ILE:HG12	2.17	0.59
1:B:183:MET:O	1:B:186:LYS:HG2	2.02	0.59
1:C:88:VAL:HG21	1:C:173:GLU:HA	1.83	0.59
1:A:115:THR:CG2	1:A:116:ASP:N	2.66	0.59
1:C:102:LEU:HD13	1:C:129:VAL:CG2	2.33	0.58
1:B:191:ILE:HG23	1:C:199:ARG:CZ	2.33	0.58
1:C:77:VAL:HG21	1:C:154:MET:HG3	1.85	0.58
1:A:102:LEU:HD13	1:A:129:VAL:HG13	1.85	0.58
1:B:76:ALA:HB3	1:B:85:GLU:HB2	1.84	0.58
1:A:188:ARG:HA	1:A:188:ARG:NE	2.19	0.58
1:C:75:VAL:HG21	1:C:155:ASN:HD21	1.66	0.58
1:C:101:LEU:HD21	1:C:135:ILE:HG13	1.86	0.58
1:B:127:LYS:HB2	1:B:127:LYS:NZ	2.19	0.58
1:B:71:LYS:HG3	1:B:172:VAL:CG2	2.28	0.58
1:B:180:VAL:HG12	1:B:184:ASN:ND2	2.19	0.58
1:C:205:THR:HG1	1:D:201:ILE:HG22	1.67	0.57
2:X:251:LEU:O	2:X:251:LEU:HD12	2.05	0.57
2:X:241:LEU:HD22	2:X:267:ILE:HG21	1.85	0.56
1:A:59:GLY:HA3	1:A:111:THR:OG1	2.05	0.56
1:B:195:THR:HB	1:B:196:PRO:HD2	1.87	0.56
1:C:66:THR:HG21	1:C:155:ASN:HB3	1.87	0.56
1:B:124:GLN:O	1:B:128:MET:HG2	2.05	0.56
2:X:248:ALA:O	2:X:249:VAL:HG13	2.06	0.56
1:B:71:LYS:CG	1:B:172:VAL:HG21	2.29	0.56
1:B:111:THR:HG22	1:B:112:HIS:CE1	2.41	0.56
1:C:95:ARG:NH2	1:D:173:GLU:HB3	2.17	0.56
1:D:84:ILE:CD1	1:D:154:MET:SD	2.94	0.56
2:X:269:LYS:NZ	2:X:270:ASP:HB3	2.21	0.56
1:B:83:PHE:HA	1:B:196:PRO:HB2	1.88	0.55
1:B:86:ALA:O	1:B:87:GLU:HG3	2.05	0.55
1:B:81:SER:CA	1:B:199:ARG:HD2	2.30	0.55
1:C:156:HIS:CE1	1:C:160:ASN:HD21	2.24	0.55
1:B:118:GLY:C	1:B:120:ASN:H	2.10	0.55
1:D:202:ASN:O	1:D:205:THR:HG22	2.06	0.55
1:B:181:HIS:O	1:B:185:HIS:HD2	1.90	0.55
1:C:86:ALA:O	1:C:87:GLU:HG3	2.06	0.55
1:A:84:ILE:HD13	1:A:183:MET:CG	2.37	0.55
1:A:117:ASN:HA	1:A:139:PHE:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD12	1:B:183:MET:HE1	1.90	0.54
1:C:184:ASN:O	1:C:196:PRO:HD2	2.07	0.54
1:A:208:GLN:NE2	1:C:191:ILE:HD13	2.23	0.54
1:B:83:PHE:CD1	1:B:197:ALA:HA	2.42	0.54
1:A:190:GLY:HA2	1:A:193:ASP:HB3	1.89	0.54
1:A:82:GLY:O	1:A:84:ILE:HD12	2.07	0.54
1:B:83:PHE:HD1	1:B:197:ALA:HA	1.73	0.54
1:C:172:VAL:O	1:C:176:VAL:HG23	2.07	0.54
1:A:61:TRP:CE3	1:A:104:LEU:HD21	2.43	0.54
1:C:184:ASN:O	1:C:195:THR:HB	2.07	0.54
1:A:181:HIS:CD2	1:B:132:TRP:HZ3	2.26	0.54
1:C:91:GLN:CD	1:C:93:THR:HG23	2.28	0.53
1:A:162:ILE:HG12	1:A:179:ALA:HB2	1.88	0.53
1:A:208:GLN:NE2	1:C:191:ILE:CD1	2.71	0.53
1:C:178:MET:HG2	1:D:102:LEU:HD11	1.90	0.53
1:A:132:TRP:CZ3	1:B:181:HIS:HD2	2.26	0.53
1:D:77:VAL:CG1	1:D:84:ILE:HG12	2.39	0.53
1:D:194:MET:HA	1:D:198:GLU:OE1	2.09	0.52
1:A:202:ASN:HD21	2:X:269:LYS:H	1.55	0.52
1:A:186:LYS:N	1:A:195:THR:OG1	2.42	0.52
1:A:182:CYS:O	1:A:186:LYS:HG3	2.10	0.52
1:B:189:GLY:HA2	1:B:199:ARG:NH2	2.24	0.52
1:C:124:GLN:HG3	1:C:124:GLN:O	2.10	0.52
1:C:128:MET:HE3	1:C:129:VAL:HA	1.91	0.52
1:B:205:THR:C	1:B:207:GLU:H	2.13	0.52
2:X:243:TRP:CD1	2:X:244:LYS:N	2.77	0.52
1:C:177:LEU:CB	1:D:102:LEU:HD12	2.32	0.52
1:D:110:ILE:HG13	1:D:135:ILE:HG12	1.91	0.52
1:A:122:ALA:HB2	1:A:139:PHE:HE2	1.75	0.52
1:B:78:HIS:HE1	1:B:203:MET:SD	2.33	0.52
2:X:227:TYR:CD2	2:X:236:LYS:HB3	2.45	0.52
1:B:189:GLY:CA	1:B:199:ARG:HH22	2.22	0.52
1:A:161:GLN:HE21	1:A:165:ILE:HD12	1.74	0.51
1:A:137:HIS:HD1	1:A:137:HIS:C	2.14	0.51
1:A:81:SER:HB3	1:A:203:MET:HE2	1.92	0.51
1:B:58:LEU:CD2	1:B:207:GLU:HG3	2.39	0.51
2:X:269:LYS:HZ3	2:X:270:ASP:HB3	1.75	0.51
1:A:157:HIS:HA	1:A:160:ASN:OD1	2.10	0.51
1:A:161:GLN:HA	1:A:164:ARG:HG3	1.91	0.51
1:C:99:LEU:HD22	1:D:177:LEU:HD23	1.91	0.51
1:A:164:ARG:O	1:A:165:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:O	1:C:191:ILE:HG22	2.10	0.51
2:X:226:TYR:HD1	2:X:238:PRO:HG3	1.75	0.51
2:X:260:VAL:CG1	2:X:264:LYS:HE2	2.36	0.51
2:X:251:LEU:HD12	2:X:258:LYS:HB2	1.91	0.51
1:D:158:LEU:O	1:D:162:ILE:HG23	2.11	0.51
1:D:162:ILE:O	1:D:166:ARG:HG2	2.11	0.51
1:B:172:VAL:O	1:B:176:VAL:HG23	2.11	0.51
1:B:111:THR:O	1:B:135:ILE:HA	2.11	0.51
1:C:83:PHE:CD1	1:C:200:LEU:HD22	2.46	0.51
1:C:98:ALA:HB1	1:C:129:VAL:HG11	1.93	0.50
1:A:161:GLN:HE21	1:A:165:ILE:CD1	2.24	0.50
1:A:188:ARG:HA	1:A:188:ARG:CZ	2.42	0.50
1:D:73:VAL:HG23	1:D:88:VAL:HG13	1.94	0.50
2:X:249:VAL:HG22	2:X:260:VAL:O	2.12	0.50
1:C:115:THR:OG1	1:C:116:ASP:N	2.45	0.50
1:C:162:ILE:HD11	1:C:176:VAL:HG13	1.93	0.50
2:X:249:VAL:CG2	2:X:260:VAL:HB	2.34	0.50
1:B:200:LEU:HD12	1:B:201:ILE:H	1.76	0.50
1:B:81:SER:HB2	1:B:199:ARG:HB3	1.93	0.50
1:C:162:ILE:HD11	1:C:176:VAL:HA	1.94	0.50
1:D:162:ILE:HB	1:D:175:ILE:HD12	1.94	0.50
1:A:68:LEU:HB2	1:A:159:LYS:HE3	1.92	0.50
1:A:179:ALA:O	1:A:183:MET:HB2	2.12	0.49
1:A:184:ASN:O	1:A:196:PRO:HD2	2.12	0.49
1:D:67:HIS:NE2	1:D:72:ILE:HG12	2.28	0.49
1:A:166:ARG:NH2	1:A:170:ASN:O	2.44	0.49
2:X:227:TYR:CE2	2:X:236:LYS:HB3	2.47	0.49
2:X:269:LYS:HG2	2:X:270:ASP:N	2.27	0.49
1:A:97:THR:HG21	1:A:121:PHE:CD1	2.48	0.49
1:B:180:VAL:HG12	1:B:184:ASN:HD21	1.77	0.49
1:B:121:PHE:CE1	1:B:136:GLU:O	2.65	0.49
1:C:165:ILE:HG12	1:C:168:GLN:CG	2.35	0.49
1:A:201:ILE:HG23	1:B:201:ILE:HG23	1.95	0.49
1:A:137:HIS:NE2	1:A:139:PHE:HE1	2.11	0.49
1:A:81:SER:OG	1:A:82:GLY:N	2.45	0.49
2:X:229:GLU:HG2	2:X:231:ARG:CZ	2.43	0.49
1:A:84:ILE:HD11	1:A:154:MET:CG	2.42	0.49
1:B:188:ARG:HH12	1:C:80:ALA:HB2	1.78	0.49
1:A:177:LEU:HD23	1:B:99:LEU:HD11	1.95	0.48
1:A:165:ILE:O	1:A:167:GLU:N	2.47	0.48
1:A:202:ASN:HD22	2:X:268:ILE:HG12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:HA	1:B:196:PRO:CG	2.41	0.48
1:B:200:LEU:HD12	1:B:201:ILE:N	2.28	0.48
1:C:162:ILE:O	1:C:166:ARG:N	2.46	0.48
1:D:86:ALA:O	1:D:87:GLU:HG3	2.13	0.48
1:B:72:ILE:HB	1:B:89:ILE:O	2.13	0.48
1:C:135:ILE:HG22	1:C:136:GLU:N	2.19	0.48
1:A:162:ILE:O	1:A:165:ILE:HB	2.14	0.48
2:X:243:TRP:HD1	2:X:244:LYS:N	2.12	0.48
1:C:112:HIS:CE1	1:C:137:HIS:HA	2.49	0.48
1:D:78:HIS:NE2	1:D:80:ALA:HB3	2.29	0.48
1:B:121:PHE:CZ	1:B:136:GLU:O	2.67	0.48
2:X:221:LYS:HE3	2:X:240:GLU:OE1	2.14	0.48
1:A:63:MET:HE2	1:A:121:PHE:CE1	2.48	0.48
1:B:130:ALA:HA	1:B:135:ILE:CG1	2.44	0.48
1:B:137:HIS:ND1	1:B:137:HIS:C	2.67	0.47
1:C:81:SER:HA	1:C:199:ARG:HD2	1.96	0.47
1:A:194:MET:SD	1:A:199:ARG:HA	2.55	0.47
1:C:102:LEU:HD13	1:C:129:VAL:HG23	1.96	0.47
1:C:56:SER:OG	1:C:111:THR:HG21	2.13	0.47
1:C:163:ASP:HA	1:C:166:ARG:HD3	1.96	0.47
1:C:74:ILE:HB	1:C:89:ILE:HD13	1.95	0.47
1:C:201:ILE:HG12	1:D:204:ILE:HG21	1.96	0.47
1:A:74:ILE:HB	1:A:89:ILE:HD13	1.96	0.47
1:B:191:ILE:HG23	1:C:199:ARG:NH1	2.28	0.47
1:A:117:ASN:CA	1:A:139:PHE:HD2	2.27	0.47
1:D:188:ARG:HB3	1:D:189:GLY:H	1.57	0.47
1:D:112:HIS:ND1	1:D:112:HIS:C	2.68	0.47
1:A:180:VAL:HG12	1:A:184:ASN:HD22	1.80	0.47
1:B:195:THR:O	1:B:199:ARG:HB2	2.15	0.47
1:C:113:LEU:HG	1:C:114:HIS:N	2.30	0.47
1:C:58:LEU:O	1:C:78:HIS:NE2	2.48	0.47
1:D:102:LEU:CD2	1:D:129:VAL:HG13	2.45	0.47
1:B:162:ILE:O	1:B:166:ARG:HB2	2.15	0.47
1:A:95:ARG:O	1:A:99:LEU:HB2	2.15	0.47
1:D:202:ASN:HA	1:D:205:THR:HG22	1.96	0.47
1:A:153:ALA:C	1:A:155:ASN:H	2.18	0.46
1:C:135:ILE:O	1:C:136:GLU:HB2	2.14	0.46
1:D:61:TRP:HB2	1:D:110:ILE:HD13	1.97	0.46
1:D:74:ILE:HB	1:D:89:ILE:HD13	1.97	0.46
1:B:158:LEU:HD12	1:B:183:MET:CE	2.45	0.46
1:C:88:VAL:CG2	1:C:173:GLU:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:MET:HG3	1:C:113:LEU:HD11	1.98	0.46
1:A:139:PHE:N	1:A:139:PHE:CD1	2.83	0.46
1:B:111:THR:HG22	1:B:112:HIS:ND1	2.30	0.46
1:B:84:ILE:HD13	1:B:158:LEU:HD13	1.97	0.46
1:C:116:ASP:CG	1:C:117:ASN:H	2.18	0.46
1:C:203:MET:HG2	1:C:203:MET:H	1.50	0.46
1:D:63:MET:HG3	1:D:115:THR:HG23	1.98	0.46
2:X:269:LYS:HG2	2:X:270:ASP:H	1.80	0.46
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.79	0.46
1:C:175:ILE:HA	1:C:175:ILE:HD12	1.58	0.46
1:C:67:HIS:CD2	1:C:72:ILE:HD13	2.49	0.46
1:A:115:THR:HG23	1:A:116:ASP:H	1.80	0.46
1:A:195:THR:HG22	1:A:198:GLU:CG	2.40	0.46
1:D:84:ILE:CG1	1:D:154:MET:SD	3.04	0.46
1:A:165:ILE:HG22	1:A:175:ILE:HD11	1.98	0.46
1:A:178:MET:O	1:A:182:CYS:SG	2.74	0.46
1:C:138:THR:OG1	1:C:139:PHE:N	2.49	0.46
1:A:118:GLY:O	1:A:120:ASN:N	2.48	0.45
1:D:130:ALA:HB2	1:D:137:HIS:HE1	1.81	0.45
1:B:95:ARG:HH21	1:B:95:ARG:HG3	1.82	0.45
1:C:194:MET:HB2	1:C:198:GLU:HB2	1.97	0.45
1:A:176:VAL:O	1:A:180:VAL:HG23	2.16	0.45
1:C:107:ARG:HD3	1:D:107:ARG:CD	2.46	0.45
1:C:199:ARG:O	1:C:203:MET:HG2	2.16	0.45
1:C:114:HIS:CE1	1:C:138:THR:O	2.69	0.45
2:X:261:PRO:O	2:X:264:LYS:HG3	2.16	0.45
1:A:63:MET:HA	1:A:75:VAL:O	2.17	0.45
1:A:178:MET:HE2	1:B:102:LEU:HD21	1.99	0.45
1:A:172:VAL:O	1:A:175:ILE:HG22	2.17	0.45
1:A:190:GLY:O	1:A:191:ILE:HG22	2.17	0.45
1:B:125:GLU:O	1:B:128:MET:HB2	2.17	0.45
1:A:160:ASN:N	1:A:160:ASN:ND2	2.65	0.45
1:C:105:ALA:HA	1:C:110:ILE:HG22	1.99	0.45
1:C:84:ILE:CG2	1:C:180:VAL:HG22	2.47	0.45
1:B:162:ILE:O	1:B:166:ARG:N	2.50	0.45
1:A:171:SER:O	1:A:175:ILE:HB	2.17	0.44
1:B:188:ARG:CZ	1:B:189:GLY:H	2.29	0.44
1:D:172:VAL:HA	1:D:175:ILE:CG2	2.47	0.44
1:B:191:ILE:HG22	1:B:191:ILE:O	2.17	0.44
2:X:261:PRO:HD2	2:X:264:LYS:CE	2.47	0.44
1:A:115:THR:HG23	1:A:116:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HG12	1:D:204:ILE:CG2	2.48	0.44
1:C:87:GLU:CD	1:D:103:LYS:HD3	2.38	0.44
1:C:105:ALA:HA	1:C:110:ILE:CG2	2.48	0.44
1:D:183:MET:O	1:D:196:PRO:HG2	2.17	0.44
2:X:227:TYR:N	2:X:227:TYR:CD2	2.82	0.44
1:B:183:MET:O	1:B:196:PRO:HG3	2.18	0.44
1:D:84:ILE:HG12	1:D:154:MET:SD	2.57	0.44
2:X:250:LEU:HG	2:X:259:VAL:HG22	2.00	0.44
1:B:186:LYS:O	1:B:188:ARG:N	2.51	0.44
1:C:204:ILE:HA	1:C:204:ILE:HD12	1.83	0.44
1:D:78:HIS:CE1	1:D:200:LEU:HD13	2.52	0.44
1:B:114:HIS:CD2	1:B:139:PHE:O	2.71	0.44
1:D:102:LEU:HD23	1:D:129:VAL:HG13	1.99	0.43
2:X:250:LEU:HA	2:X:259:VAL:HA	2.00	0.43
1:A:69:GLU:HB2	1:A:172:VAL:HG21	1.99	0.43
1:B:205:THR:O	1:B:207:GLU:N	2.50	0.43
1:C:114:HIS:CD2	1:C:115:THR:N	2.86	0.43
1:D:65:CYS:HA	1:D:73:VAL:O	2.18	0.43
2:X:242:LEU:HD21	2:X:252:LYS:HB2	2.01	0.43
1:A:114:HIS:CD2	1:A:138:THR:OG1	2.72	0.43
1:A:78:HIS:HE1	1:A:203:MET:HE3	1.83	0.43
1:C:89:ILE:O	1:C:89:ILE:HG13	2.19	0.43
1:D:115:THR:CG2	1:D:120:ASN:HD21	2.24	0.43
1:C:107:ARG:HD2	1:C:108:TRP:CD1	2.53	0.43
1:C:162:ILE:HG23	1:C:175:ILE:CG2	2.49	0.43
1:C:206:THR:O	1:C:207:GLU:HB2	2.18	0.43
2:X:243:TRP:HD1	2:X:244:LYS:H	1.67	0.43
1:A:179:ALA:HA	1:A:182:CYS:SG	2.59	0.43
1:B:119:ALA:HA	1:B:122:ALA:CB	2.16	0.43
1:B:194:MET:HA	1:B:198:GLU:CD	2.39	0.43
1:C:99:LEU:CD1	1:D:173:GLU:HG2	2.49	0.43
1:A:116:ASP:HA	1:A:140:GLY:H	1.83	0.43
2:X:251:LEU:CD1	2:X:258:LYS:HB2	2.49	0.43
1:A:187:ARG:HA	1:A:195:THR:HA	2.00	0.43
1:D:102:LEU:HD23	1:D:129:VAL:HG22	1.99	0.43
1:B:158:LEU:HA	1:B:183:MET:CE	2.31	0.43
1:A:63:MET:HG3	1:A:113:LEU:HD11	2.00	0.42
1:A:99:LEU:HD12	1:B:177:LEU:CD2	2.49	0.42
1:B:118:GLY:O	1:B:120:ASN:N	2.51	0.42
1:C:160:ASN:O	1:C:163:ASP:HB2	2.19	0.42
1:D:155:ASN:O	1:D:159:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:HB2	1:C:135:ILE:CG2	2.49	0.42
1:D:62:GLN:HG2	1:D:114:HIS:HB3	2.01	0.42
1:A:60:THR:HA	1:A:112:HIS:O	2.20	0.42
1:B:115:THR:HG22	1:B:116:ASP:N	2.34	0.42
1:B:162:ILE:HG23	1:B:166:ARG:HD3	2.01	0.42
1:C:103:LYS:HD3	1:D:87:GLU:OE1	2.19	0.42
1:C:201:ILE:HG21	1:D:204:ILE:HG22	2.01	0.42
1:B:155:ASN:O	1:B:159:LYS:HG3	2.19	0.42
1:C:65:CYS:SG	1:C:74:ILE:HA	2.59	0.42
1:D:111:THR:O	1:D:112:HIS:HB2	2.20	0.42
1:A:201:ILE:N	1:A:201:ILE:HD12	2.35	0.42
1:C:102:LEU:HD22	1:C:129:VAL:CG2	2.49	0.42
1:D:117:ASN:ND2	1:D:121:PHE:CD1	2.87	0.42
1:C:126:VAL:HA	1:C:129:VAL:CG1	2.46	0.42
1:C:84:ILE:HG23	1:C:180:VAL:HG22	2.02	0.42
1:D:187:ARG:HG2	1:D:195:THR:HG22	2.02	0.42
1:A:137:HIS:ND1	1:A:137:HIS:C	2.73	0.42
1:A:74:ILE:HG21	1:A:100:PHE:CD2	2.54	0.42
1:D:113:LEU:HG	1:D:114:HIS:H	1.83	0.42
1:A:157:HIS:O	1:A:161:GLN:HB3	2.19	0.42
1:D:96:GLN:HA	1:D:96:GLN:OE1	2.20	0.42
1:A:117:ASN:HB3	1:A:139:PHE:CD2	2.55	0.41
1:A:81:SER:HB3	1:A:203:MET:CE	2.49	0.41
1:B:84:ILE:HG12	1:B:85:GLU:N	2.34	0.41
1:C:102:LEU:HD22	1:C:129:VAL:HG23	2.02	0.41
2:X:235:TRP:N	2:X:235:TRP:CD1	2.87	0.41
1:C:87:GLU:OE1	1:D:103:LYS:HD3	2.20	0.41
1:C:90:PRO:HD2	1:C:96:GLN:OE1	2.19	0.41
1:C:89:ILE:HB	1:C:96:GLN:HB3	2.03	0.41
1:A:90:PRO:O	1:A:91:GLN:HG3	2.20	0.41
1:A:187:ARG:HH21	1:A:198:GLU:CD	2.24	0.41
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.84	0.41
1:A:195:THR:HG22	1:A:198:GLU:H	1.86	0.41
1:A:55:ASN:HA	3:A:462:HOH:O	2.20	0.41
1:A:62:GLN:HA	1:A:114:HIS:O	2.21	0.41
1:B:165:ILE:HD11	1:B:179:ALA:HA	2.03	0.41
1:B:84:ILE:HD12	1:B:154:MET:HG3	2.02	0.41
1:B:91:GLN:HB2	1:B:93:THR:HG23	2.03	0.41
1:A:172:VAL:HA	1:A:175:ILE:CG2	2.48	0.41
1:C:187:ARG:NH2	1:C:198:GLU:OE2	2.54	0.41
2:X:229:GLU:HA	2:X:264:LYS:HB3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:229:GLU:OE1	2:X:231:ARG:NH1	2.54	0.41
1:C:124:GLN:HE21	1:C:124:GLN:HB2	1.66	0.41
2:X:261:PRO:HB3	2:X:263:ARG:NH2	2.36	0.41
1:A:139:PHE:H	1:A:139:PHE:HD1	1.67	0.41
1:C:181:HIS:ND1	1:C:181:HIS:C	2.73	0.41
1:A:95:ARG:HD2	1:A:95:ARG:N	2.21	0.41
1:C:130:ALA:HA	1:C:135:ILE:HG12	2.03	0.41
1:C:162:ILE:HG23	1:C:175:ILE:HG21	2.02	0.41
1:A:186:LYS:N	1:A:195:THR:HG1	2.18	0.41
1:B:84:ILE:CG2	1:B:180:VAL:HG13	2.45	0.41
1:A:181:HIS:C	1:A:181:HIS:ND1	2.74	0.41
1:B:58:LEU:HD12	1:B:203:MET:HG2	2.02	0.41
1:D:184:ASN:HA	1:D:196:PRO:HB2	2.02	0.41
1:C:113:LEU:HG	1:C:114:HIS:H	1.86	0.40
1:D:63:MET:HB2	1:D:75:VAL:O	2.21	0.40
1:A:195:THR:H	1:A:198:GLU:HG2	1.85	0.40
1:A:156:HIS:C	1:A:158:LEU:H	2.25	0.40
1:A:71:LYS:HD3	1:A:88:VAL:HG11	2.04	0.40
1:B:114:HIS:CE1	1:B:138:THR:HG1	2.39	0.40
2:X:263:ARG:HH21	2:X:263:ARG:HG2	1.86	0.40
1:A:71:LYS:HG3	1:A:172:VAL:HB	2.02	0.40
1:B:68:LEU:C	1:B:70:GLY:H	2.25	0.40
1:B:56:SER:CB	1:B:80:ALA:HB2	2.43	0.40
1:C:158:LEU:HD23	1:C:183:MET:SD	2.62	0.40
1:D:60:THR:HA	1:D:112:HIS:O	2.21	0.40
1:A:162:ILE:O	1:A:166:ARG:N	2.53	0.40
1:A:89:ILE:O	1:A:89:ILE:HG13	2.21	0.40
1:B:188:ARG:NE	1:B:189:GLY:H	2.20	0.40
1:C:169:ALA:HB2	1:C:178:MET:CE	2.52	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	144/164 (88%)	107 (74%)	25 (17%)	12 (8%)	1	4
1	B	138/164 (84%)	109 (79%)	18 (13%)	11 (8%)	1	4
1	C	139/164 (85%)	105 (76%)	25 (18%)	9 (6%)	1	7
1	D	138/164 (84%)	115 (83%)	15 (11%)	8 (6%)	1	10
2	X	53/81 (65%)	33 (62%)	13 (24%)	7 (13%)	0	1
All	All	612/737 (83%)	469 (77%)	96 (16%)	47 (8%)	1	5

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	117	ASN
1	A	153	ALA
1	A	166	ARG
1	B	139	PHE
1	B	187	ARG
1	C	79	VAL
1	D	121	PHE
2	X	218	SER
2	X	237	GLY
1	A	165	ILE
1	B	166	ARG
1	B	191	ILE
1	B	194	MET
1	C	136	GLU
1	D	112	HIS
1	D	123	SER
2	X	217	ASN
2	X	249	VAL
1	A	119	ALA
1	A	192	GLY
1	B	58	LEU
1	B	119	ALA
1	B	206	THR
1	C	80	ALA
1	C	90	PRO
1	C	135	ILE
1	C	187	ARG
1	D	116	ASP
1	D	170	ASN
1	D	188	ARG

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Mol	Chain	Res	Type
2	X	230	GLY
2	X	238	PRO
2	X	246	GLU
1	A	107	ARG
1	A	168	GLN
1	A	193	ASP
1	A	209	GLU
1	B	79	VAL
1	B	163	ASP
1	C	107	ARG
1	C	190	GLY
1	D	139	PHE
1	D	153	ALA
1	B	137	HIS
1	C	123	SER
1	A	191	ILE

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	124/138 (90%)	104 (84%)	20 (16%)	2	12
1	B	117/138 (85%)	98 (84%)	19 (16%)	2	12
1	C	118/138 (86%)	96 (81%)	22 (19%)	1	8
1	D	117/138 (85%)	96 (82%)	21 (18%)	2	9
2	X	47/67 (70%)	38 (81%)	9 (19%)	1	8
All	All	523/619 (84%)	432 (83%)	91 (17%)	2	10

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	64	ASP
1	A	71	LYS

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Mol	Chain	Res	Type
1	A	93	THR
1	A	95	ARG
1	A	99	LEU
1	A	115	THR
1	A	121	PHE
1	A	124	GLN
1	A	137	HIS
1	A	154	MET
1	A	164	ARG
1	A	166	ARG
1	A	174	THR
1	A	177	LEU
1	A	182	CYS
1	A	187	ARG
1	A	188	ARG
1	A	193	ASP
1	A	210	ILE
1	B	58	LEU
1	B	64	ASP
1	B	65	CYS
1	B	67	HIS
1	B	101	LEU
1	B	104	LEU
1	B	110	ILE
1	B	113	LEU
1	B	121	PHE
1	B	127	LYS
1	B	137	HIS
1	B	155	ASN
1	B	163	ASP
1	B	172	VAL
1	B	183	MET
1	B	188	ARG
1	B	191	ILE
1	B	194	MET
1	B	200	LEU
1	C	65	CYS
1	C	68	LEU
1	C	71	LYS
1	C	72	ILE
1	C	73	VAL
1	C	75	VAL

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Mol	Chain	Res	Type
1	C	91	GLN
1	C	96	GLN
1	C	115	THR
1	C	117	ASN
1	C	124	GLN
1	C	128	MET
1	C	136	GLU
1	C	158	LEU
1	C	168	GLN
1	C	170	ASN
1	C	175	ILE
1	C	176	VAL
1	C	177	LEU
1	C	181	HIS
1	C	203	MET
1	C	204	ILE
1	D	64	ASP
1	D	68	LEU
1	D	85	GLU
1	D	95	ARG
1	D	102	LEU
1	D	112	HIS
1	D	115	THR
1	D	117	ASN
1	D	120	ASN
1	D	139	PHE
1	D	152	GLU
1	D	154	MET
1	D	155	ASN
1	D	158	LEU
1	D	166	ARG
1	D	168	GLN
1	D	175	ILE
1	D	177	LEU
1	D	188	ARG
1	D	193	ASP
1	D	206	THR
2	X	217	ASN
2	X	218	SER
2	X	227	TYR
2	X	228	ARG
2	X	231	ARG

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Mol	Chain	Res	Type
2	X	235	TRP
2	X	246	GLU
2	X	263	ARG
2	X	270	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	114	HIS
1	A	120	ASN
1	A	161	GLN
1	A	184	ASN
1	A	202	ASN
1	A	208	GLN
1	A	211	GLN
1	B	96	GLN
1	B	124	GLN
1	B	181	HIS
1	B	185	HIS
1	C	67	HIS
1	C	114	HIS
1	C	120	ASN
1	C	124	GLN
1	C	137	HIS
1	C	155	ASN
1	C	156	HIS
1	C	161	GLN
1	C	168	GLN
1	C	170	ASN
1	D	62	GLN
1	D	120	ASN
1	D	160	ASN
1	D	168	GLN
2	X	217	ASN

5.3.3 RNA ⓘ

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.