



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:42 am BST

PDB ID : 5C8U
Title : Crystal structure of the SARS coronavirus nsp14-nsp10 complex
Authors : Ma, Y.Y.; Wu, L.J.; Zhang, R.G.; Rao, Z.H.
Deposited on : 2015-06-26
Resolution : 3.40 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) : 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

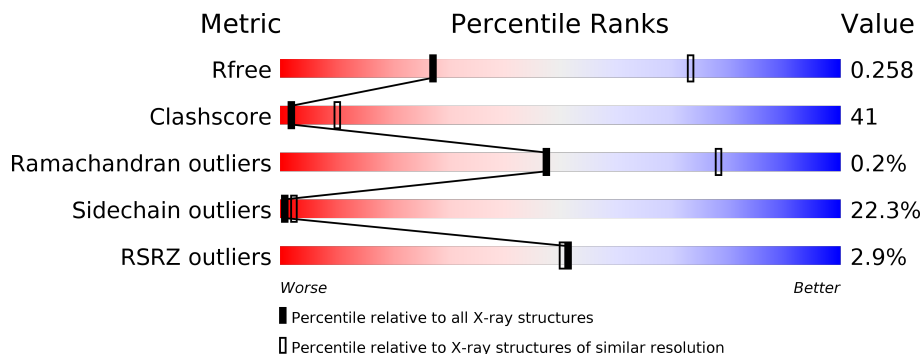
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 $\leq 5\%$. 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	144	
1	C	144	
2	B	528	
2	D	528	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10172 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 Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	969	600	164	189	16	0	0	0
1	C	133	969	600	164	189	16	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P0C6X7
A	-3	PRO	-	expression tag	UNP P0C6X7
A	-2	LEU	-	expression tag	UNP P0C6X7
A	-1	GLY	-	expression tag	UNP P0C6X7
A	0	SER	-	expression tag	UNP P0C6X7
C	-4	GLY	-	expression tag	UNP P0C6X7
C	-3	PRO	-	expression tag	UNP P0C6X7
C	-2	LEU	-	expression tag	UNP P0C6X7
C	-1	GLY	-	expression tag	UNP P0C6X7
C	0	SER	-	expression tag	UNP P0C6X7

- Molecule 2 is a protein called Guanine-N7 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	514	4111	2632	704	739	36	0	0	0
2	D	514	4111	2632	704	739	36	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P0C6X7
D	0	MET	-	expression tag	UNP P0C6X7

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	A	2	Total 2	Zn 2	0	0
3	D	3	Total 3	Zn 3	0	0
3	C	2	Total 2	Zn 2	0	0

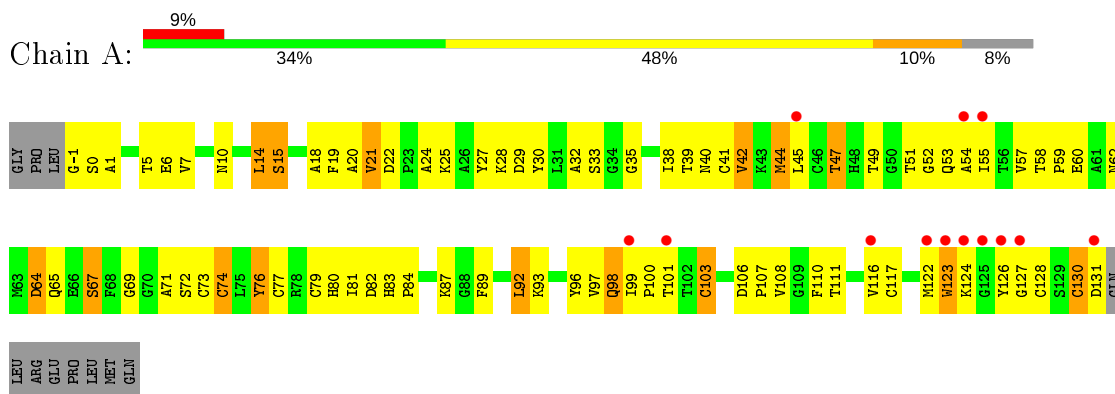
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0

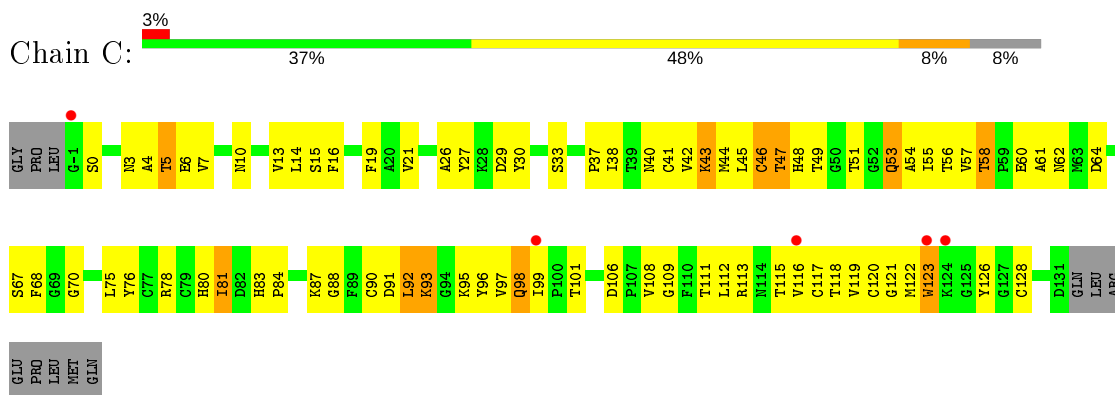
3 Residue-property plots [i](#)

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.

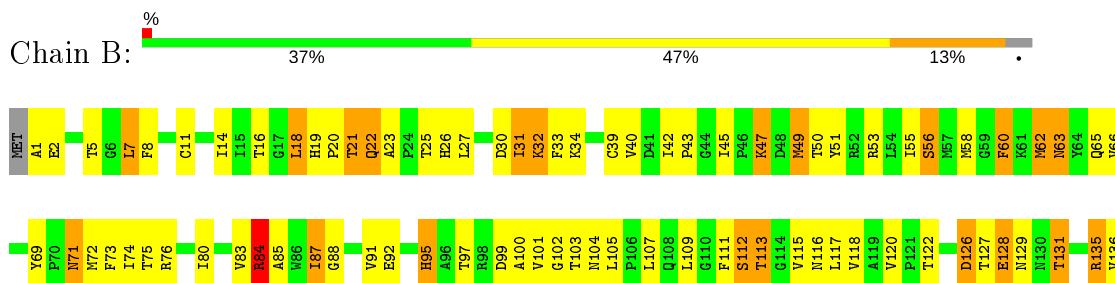
- Molecule 1: Non-structural protein 10

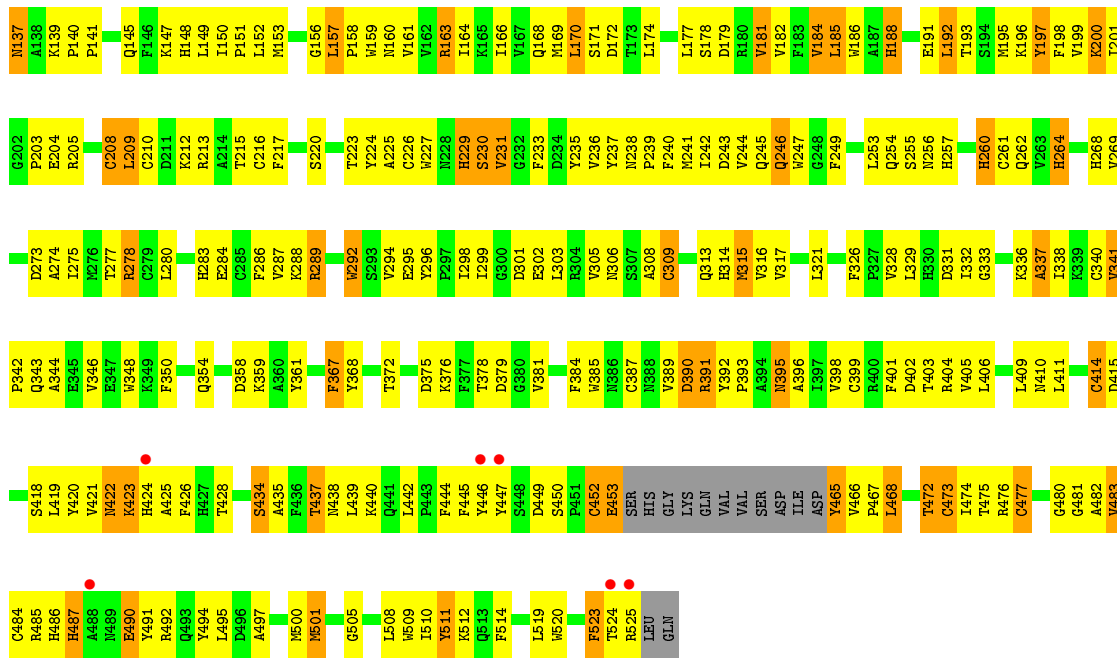


- Molecule 1: Non-structural protein 10

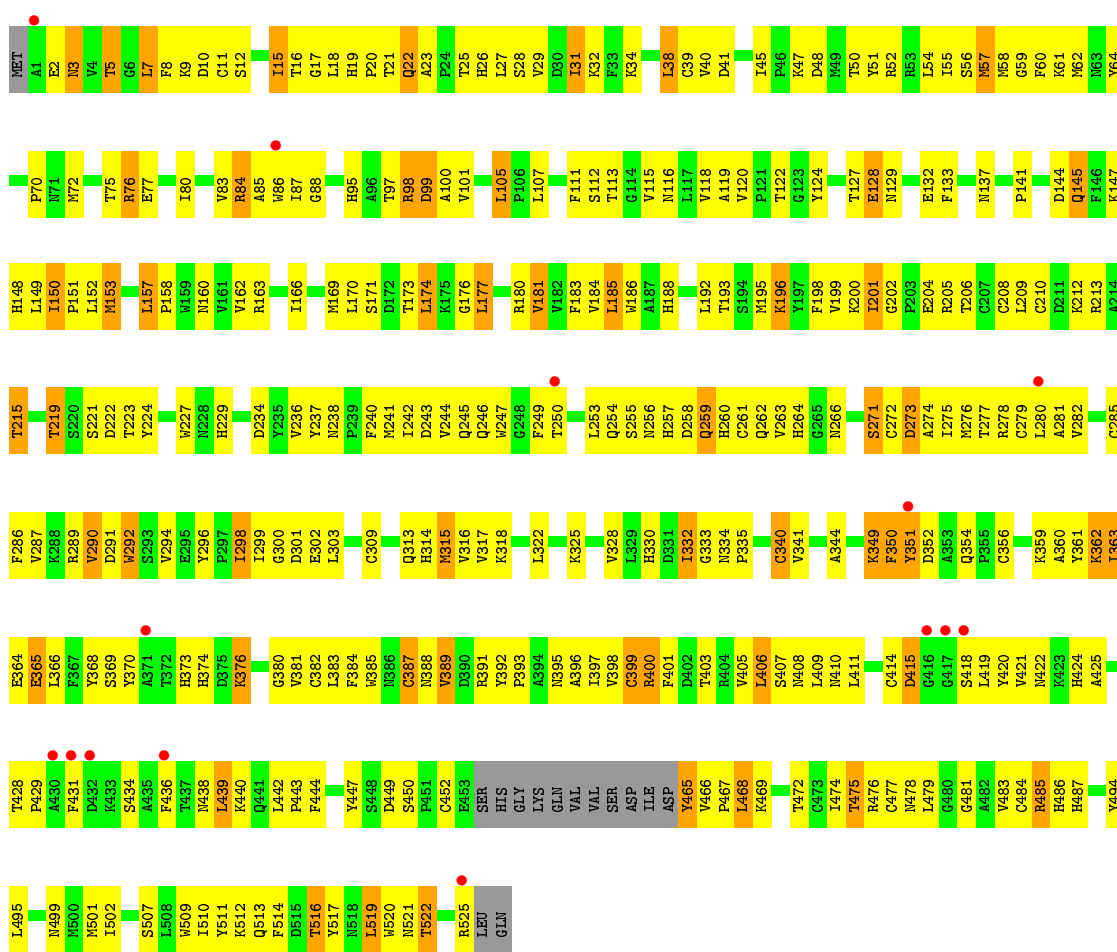


- Molecule 2: Guanine-N7 methyltransferase





• Molecule 2: Guanine-N7 methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	189.93Å 194.98Å 179.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.35 – 3.40 45.35 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.35-3.40) 99.9 (45.35-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.218 , 0.266 0.210 , 0.258	Depositor DCC
R_{free} test set	2327 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	109.9	Xtrriage
Anisotropy	0.690	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 103.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10172	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.32	0/991	0.58	0/1348
1	C	0.37	0/991	0.58	0/1348
2	B	0.41	0/4228	0.63	0/5745
2	D	0.41	0/4228	0.62	0/5745
All	All	0.40	0/10438	0.62	0/14186

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	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	LYS	Peptide
2	B	84	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	969	0	920	93	0
1	C	969	0	920	99	0
2	B	4111	0	3981	361	1
2	D	4111	0	3981	320	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	10172	0	9802	818	1

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 41.

All (818) 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)
2:B:476:ARG:HB2	2:B:487:HIS:CE1	1.86	1.09
2:B:452:CYS:SG	2:B:484:CYS:HB3	1.92	1.08
2:D:440:LYS:HD2	2:D:512:LYS:HA	1.37	1.04
2:D:397:ILE:HG12	2:D:510:ILE:HG13	1.40	1.04
2:B:476:ARG:HH11	2:B:487:HIS:CD2	1.79	1.00
2:B:296:TYR:H	2:B:423:LYS:HE3	1.25	0.99
2:B:205:ARG:HD2	2:B:224:TYR:HE2	1.29	0.98
2:B:302:GLU:HG3	2:B:422:ASN:HB3	1.43	0.96
2:D:421:VAL:HG13	2:D:425:ALA:HB2	1.46	0.94
2:D:384:PHE:HB2	2:D:398:VAL:HG23	1.49	0.94
2:B:296:TYR:N	2:B:423:LYS:HE3	1.83	0.94
2:B:205:ARG:HD2	2:B:224:TYR:CE2	2.02	0.93
1:A:21:VAL:HG13	2:B:200:LYS:HG2	1.48	0.93
1:C:55:ILE:HG22	1:C:97:VAL:HA	1.51	0.93
2:B:120:VAL:O	2:B:122:THR:HG23	1.68	0.91
2:D:15:ILE:H	2:D:15:ILE:HD13	1.34	0.90
2:B:163:ARG:NH2	2:B:235:TYR:OH	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:ASN:O	2:B:395:ASN:ND2	2.05	0.90
1:C:68:PHE:HD2	1:C:99:ILE:HD13	1.33	0.89
2:B:450:SER:HB2	2:B:476:ARG:HE	1.35	0.89
2:B:249:PHE:HB3	2:B:256:ASN:ND2	1.86	0.89
2:D:118:VAL:HG11	2:D:152:LEU:HD22	1.56	0.87
1:C:117:CYS:SG	1:C:119:VAL:HB	2.14	0.87
2:D:257:HIS:CE1	2:D:261:CYS:HB3	2.09	0.86
2:D:173:THR:HG22	2:D:174:LEU:HD13	1.57	0.86
1:A:93:LYS:HD3	2:B:128:GLU:O	1.75	0.86
1:C:76:TYR:HB2	1:C:83:HIS:CE1	2.11	0.86
2:B:55:ILE:HG12	2:B:126:ASP:OD1	1.75	0.85
2:B:450:SER:HB2	2:B:476:ARG:NE	1.92	0.85
2:B:442:LEU:HD23	2:B:510:ILE:HB	1.58	0.85
1:C:64:ASP:O	1:C:101:THR:OG1	1.95	0.85
2:D:144:ASP:OD1	2:D:145:GLN:NE2	2.09	0.85
2:B:317:VAL:HG11	2:B:340:CYS:SG	2.16	0.85
2:D:181:VAL:HG22	2:D:227:TRP:HZ2	1.43	0.84
2:B:157:LEU:HD23	2:B:161:VAL:HG11	1.60	0.84
2:B:49:MET:SD	2:B:49:MET:N	2.51	0.84
1:A:80:HIS:HD2	2:B:55:ILE:HG21	1.42	0.83
2:B:200:LYS:HD2	2:B:235:TYR:CE2	2.13	0.83
1:A:44:MET:CE	1:A:96:TYR:HE2	1.92	0.82
2:B:249:PHE:HB3	2:B:256:ASN:HD21	1.41	0.82
2:B:476:ARG:NH1	2:B:487:HIS:CD2	2.47	0.82
2:B:294:VAL:HG23	2:B:423:LYS:NZ	1.95	0.81
1:C:56:THR:HG21	1:C:60:GLU:HB2	1.62	0.81
1:C:13:VAL:HG13	1:C:30:TYR:CD2	2.15	0.81
2:D:181:VAL:HG22	2:D:227:TRP:CZ2	2.16	0.81
2:B:302:GLU:CG	2:B:422:ASN:HB3	2.11	0.80
2:B:447:TYR:CD2	2:B:519:LEU:HD13	2.16	0.80
2:D:19:HIS:ND1	2:D:47:LYS:HB3	1.96	0.80
2:B:475:THR:O	2:B:523:PHE:HE2	1.65	0.80
1:A:5:THR:O	2:B:25:THR:HG21	1.81	0.79
1:A:38:ILE:HB	1:A:108:VAL:HG21	1.65	0.79
2:B:423:LYS:CE	2:B:424:HIS:H	1.96	0.79
2:B:474:ILE:HD12	2:B:474:ILE:O	1.82	0.79
2:B:160:ASN:HA	2:B:163:ARG:HD3	1.65	0.79
2:D:359:LYS:HA	2:D:360:ALA:HB2	1.62	0.79
2:B:191:GLU:O	2:B:195:MET:HG3	1.81	0.79
2:D:519:LEU:O	2:D:522:THR:OG1	2.01	0.79
2:D:313:GLN:OE1	2:D:385:TRP:NE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:VAL:HG21	2:B:505:GLY:HA3	1.65	0.79
1:C:13:VAL:HG22	1:C:30:TYR:CE2	2.18	0.79
2:B:476:ARG:HD3	2:B:487:HIS:CG	2.18	0.78
2:D:83:VAL:HG11	2:D:286:PHE:HE2	1.45	0.78
1:C:44:MET:HE1	2:D:41:ASP:H	1.48	0.78
2:D:72:MET:HB3	2:D:241:MET:HE3	1.64	0.78
2:B:476:ARG:HD3	2:B:487:HIS:CD2	2.18	0.78
2:D:149:LEU:HA	2:D:152:LEU:HD12	1.65	0.78
2:D:511:TYR:CE1	2:D:514:PHE:HB2	2.18	0.78
1:A:44:MET:HE2	1:A:96:TYR:HE2	1.48	0.77
1:A:80:HIS:CD2	2:B:55:ILE:HG21	2.18	0.77
2:D:147:LYS:O	2:D:150:ILE:HG23	1.83	0.77
2:B:88:GLY:N	2:B:112:SER:OG	2.16	0.76
2:D:32:LYS:HD3	2:D:45:ILE:HD11	1.67	0.76
1:C:67:SER:HB2	1:C:98:GLN:HE22	1.51	0.76
1:C:55:ILE:HG21	1:C:97:VAL:HG22	1.66	0.76
2:B:309:CYS:SG	2:B:501:MET:HE1	2.25	0.75
2:D:83:VAL:HG21	2:D:286:PHE:CZ	2.20	0.75
2:B:249:PHE:CE2	2:B:280:LEU:HD21	2.21	0.75
2:D:405:VAL:O	2:D:410:ASN:ND2	2.19	0.75
2:D:185:LEU:N	2:D:185:LEU:HD22	2.02	0.75
2:D:351:TYR:HB3	2:D:365:GLU:H	1.51	0.74
2:D:83:VAL:HG21	2:D:286:PHE:HZ	1.52	0.74
2:B:302:GLU:OE2	2:B:422:ASN:ND2	2.20	0.74
2:D:391:ARG:HD2	2:D:434:SER:O	1.88	0.73
2:B:283:HIS:HB2	2:B:414:CYS:SG	2.27	0.73
2:B:171:SER:HA	2:B:227:TRP:CE3	2.23	0.73
2:D:396:ALA:HB3	2:D:439:LEU:HD11	1.69	0.73
1:A:27:TYR:OH	1:A:106:ASP:OD2	2.03	0.73
2:B:135:ARG:HH11	2:B:135:ARG:HG2	1.51	0.73
2:B:447:TYR:HD2	2:B:519:LEU:HD13	1.52	0.73
2:D:309:CYS:HA	2:D:501:MET:HE3	1.71	0.73
2:B:156:GLY:HA3	2:B:157:LEU:HD12	1.69	0.72
2:B:69:TYR:CE1	2:B:203:PRO:HD3	2.23	0.72
1:C:120:CYS:HB2	1:C:122:MET:N	2.04	0.72
2:B:249:PHE:HD2	2:B:256:ASN:HD22	1.36	0.72
1:A:47:THR:OG1	1:A:49:THR:HG22	1.90	0.72
2:B:169:MET:SD	2:B:170:LEU:HD23	2.30	0.72
2:B:115:VAL:HG21	2:B:169:MET:CE	2.20	0.72
2:B:163:ARG:HE	2:B:235:TYR:HE1	1.34	0.72
1:A:93:LYS:NZ	2:B:127:THR:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:OE2	2:D:128:GLU:N	2.21	0.71
2:B:84:ARG:HB2	2:B:411:LEU:HD13	1.72	0.71
2:B:264:HIS:CD2	2:B:275:ILE:HG22	2.23	0.71
2:B:476:ARG:HA	2:B:523:PHE:CZ	2.25	0.71
2:D:80:ILE:O	2:D:83:VAL:HG23	1.89	0.71
1:A:44:MET:HB2	1:A:67:SER:HB3	1.71	0.71
2:B:76:ARG:O	2:B:80:ILE:HG12	1.90	0.71
1:A:126:TYR:N	1:A:127:GLY:HA2	2.05	0.71
2:B:313:GLN:O	2:B:317:VAL:HG12	1.91	0.71
1:A:107:PRO:O	1:A:111:THR:HG23	1.90	0.71
2:B:247:TRP:HB2	2:B:249:PHE:HE1	1.56	0.70
2:B:309:CYS:HA	2:B:501:MET:HE3	1.73	0.70
2:D:185:LEU:H	2:D:185:LEU:HD22	1.55	0.70
2:D:313:GLN:HA	2:D:385:TRP:CZ2	2.26	0.70
1:A:93:LYS:HE2	2:B:22:GLN:HA	1.72	0.70
2:D:495:LEU:HD12	2:D:495:LEU:O	1.92	0.70
1:A:76:TYR:CD2	1:A:84:PRO:HD3	2.26	0.70
1:C:10:ASN:HD21	1:C:38:ILE:HG23	1.57	0.70
2:B:135:ARG:CG	2:B:135:ARG:HH11	2.05	0.70
2:B:487:HIS:CD2	2:B:487:HIS:H	2.08	0.69
2:D:83:VAL:HG11	2:D:286:PHE:CE2	2.26	0.69
2:B:150:ILE:HB	2:B:151:PRO:HD3	1.73	0.69
1:C:21:VAL:HG23	2:D:201:ILE:O	1.93	0.69
1:A:40:ASN:OD1	2:B:25:THR:OG1	2.10	0.69
2:B:200:LYS:HD2	2:B:235:TYR:CD2	2.28	0.69
2:B:287:VAL:O	2:B:289:ARG:NE	2.26	0.69
2:B:215:THR:HG22	2:B:216:CYS:SG	2.33	0.69
2:B:476:ARG:HH22	2:B:486:HIS:CE1	2.09	0.69
2:B:260:HIS:CD2	2:B:283:HIS:CE1	2.82	0.68
1:A:19:PHE:CE1	2:B:196:LYS:HA	2.28	0.68
2:D:313:GLN:CD	2:D:385:TRP:CE2	2.67	0.68
2:D:368:TYR:OH	2:D:393:PRO:HD3	1.94	0.68
2:B:88:GLY:C	2:B:274:ALA:HB1	2.14	0.68
2:B:476:ARG:HD3	2:B:487:HIS:CE1	2.29	0.67
2:B:226:CYS:O	2:B:230:SER:HB3	1.93	0.67
2:B:230:SER:O	2:B:230:SER:OG	2.12	0.67
2:B:476:ARG:HA	2:B:523:PHE:HZ	1.58	0.67
1:C:37:PRO:HB3	1:C:106:ASP:OD1	1.94	0.67
2:B:56:SER:HB2	2:B:103:THR:HB	1.75	0.67
2:D:166:ILE:O	2:D:170:LEU:HB2	1.94	0.67
2:B:11:CYS:HB3	2:B:101:VAL:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:447:TYR:CD2	2:B:474:ILE:HG12	2.30	0.67
1:C:68:PHE:CD2	1:C:99:ILE:HD13	2.24	0.67
1:C:92:LEU:HD13	1:C:97:VAL:HG21	1.74	0.67
2:B:19:HIS:CD2	2:B:47:LYS:HG2	2.30	0.66
1:C:6:GLU:OE1	1:C:78:ARG:NH2	2.25	0.66
2:D:485:ARG:HG3	2:D:486:HIS:N	2.10	0.66
2:B:66:VAL:HG11	2:B:69:TYR:HD2	1.61	0.66
2:D:144:ASP:H	2:D:147:LYS:HE3	1.60	0.66
2:D:210:CYS:SG	2:D:229:HIS:HE1	2.13	0.66
2:B:237:TYR:CE1	2:B:238:ASN:ND2	2.64	0.66
2:B:421:VAL:HG22	2:B:425:ALA:CB	2.26	0.66
1:C:48:HIS:HB3	1:C:61:ALA:HB3	1.77	0.66
1:C:120:CYS:HB2	1:C:121:GLY:C	2.15	0.66
2:D:31:ILE:HD12	2:D:32:LYS:HG3	1.78	0.66
1:C:76:TYR:HB2	1:C:83:HIS:ND1	2.11	0.65
1:C:57:VAL:HG22	1:C:95:LYS:HE3	1.78	0.65
2:B:298:ILE:HD11	2:B:302:GLU:HB2	1.78	0.65
2:B:368:TYR:HD2	2:B:389:VAL:HG11	1.61	0.65
1:A:124:LYS:HD2	1:A:128:CYS:SG	2.37	0.65
2:B:31:ILE:H	2:B:31:ILE:HD13	1.61	0.65
1:C:13:VAL:HG13	1:C:30:TYR:CE2	2.31	0.65
2:B:391:ARG:HA	2:B:435:ALA:HA	1.79	0.65
2:D:180:ARG:C	2:D:227:TRP:HH2	1.99	0.65
2:D:292:TRP:HZ2	2:D:335:PRO:HG2	1.62	0.65
1:C:47:THR:N	1:C:48:HIS:HA	2.12	0.65
2:B:423:LYS:HE2	2:B:424:HIS:H	1.61	0.64
2:D:80:ILE:HD11	2:D:285:CYS:HB3	1.79	0.64
2:D:398:VAL:HG12	2:D:509:TRP:HB2	1.79	0.64
1:A:54:ALA:O	1:A:97:VAL:HA	1.98	0.64
2:D:328:VAL:HG22	2:D:380:GLY:HA3	1.80	0.64
2:D:26:HIS:CE1	2:D:34:LYS:HE3	2.33	0.64
2:D:127:THR:HB	2:D:128:GLU:OE2	1.97	0.64
2:B:145:GLN:OE1	2:B:145:GLN:N	2.23	0.64
1:C:67:SER:HB2	1:C:98:GLN:NE2	2.11	0.64
1:A:15:SER:HB3	2:B:60:PHE:HD1	1.62	0.63
2:D:150:ILE:N	2:D:151:PRO:HD2	2.13	0.63
1:A:44:MET:HA	2:B:39:CYS:O	1.99	0.63
1:A:108:VAL:O	1:A:111:THR:OG1	2.16	0.63
2:B:181:VAL:HG22	2:B:227:TRP:HZ2	1.63	0.63
2:B:342:PRO:HG2	2:B:343:GLN:HG2	1.79	0.63
1:C:40:ASN:HD21	2:D:27:LEU:HD23	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:THR:O	2:D:25:THR:HG21	1.98	0.63
2:D:7:LEU:HD12	2:D:8:PHE:CD2	2.33	0.63
1:C:67:SER:CB	1:C:98:GLN:HE22	2.11	0.62
2:B:309:CYS:HA	2:B:501:MET:CE	2.29	0.62
2:B:361:TYR:H	2:B:361:TYR:HD1	1.46	0.62
2:B:440:LYS:HE3	2:B:512:LYS:HD3	1.80	0.62
2:B:487:HIS:CD2	2:B:487:HIS:N	2.66	0.62
2:D:88:GLY:HA2	2:D:184:VAL:HG23	1.82	0.62
2:B:361:TYR:CE2	2:D:314:HIS:ND1	2.68	0.62
2:D:199:VAL:HG22	2:D:236:VAL:HB	1.80	0.62
1:A:44:MET:CE	1:A:96:TYR:CE2	2.81	0.62
2:D:313:GLN:HG2	2:D:385:TRP:CZ2	2.34	0.62
2:D:272:CYS:O	2:D:276:MET:HG3	2.00	0.62
2:D:84:ARG:NE	2:D:299:ILE:HD11	2.15	0.62
2:B:30:ASP:OD2	2:B:32:LYS:HE3	2.00	0.62
2:B:84:ARG:HG3	2:B:411:LEU:HD22	1.80	0.62
2:D:186:TRP:CH2	2:D:245:GLN:HG3	2.35	0.62
2:B:42:ILE:CG2	2:B:45:ILE:HG22	2.30	0.61
2:D:381:VAL:HA	2:D:395:ASN:HD21	1.65	0.61
2:B:375:ASP:HB2	2:B:376:LYS:HE3	1.81	0.61
2:B:116:ASN:ND2	2:B:269:VAL:HG12	2.16	0.61
2:D:335:PRO:HG3	2:D:352:ASP:OD2	2.01	0.61
2:B:184:VAL:HG21	2:B:278:ARG:HG3	1.83	0.61
1:C:70:GLY:HA2	1:C:97:VAL:HG23	1.82	0.61
2:D:105:LEU:HD13	2:D:105:LEU:N	2.16	0.61
1:A:10:ASN:O	1:A:14:LEU:HG	2.00	0.60
1:C:53:GLN:HA	1:C:122:MET:HG3	1.82	0.60
2:B:171:SER:HA	2:B:227:TRP:HE3	1.66	0.60
2:B:200:LYS:HD2	2:B:235:TYR:HE2	1.65	0.60
2:D:334:ASN:ND2	2:D:350:PHE:HD2	1.99	0.60
2:D:11:CYS:O	2:D:100:ALA:HB1	2.02	0.60
1:A:74:CYS:SG	1:A:77:CYS:HB2	2.42	0.60
2:D:313:GLN:HA	2:D:385:TRP:HZ2	1.64	0.60
2:B:229:HIS:H	2:B:229:HIS:HD1	1.49	0.60
2:B:309:CYS:SG	2:B:501:MET:CE	2.90	0.60
2:B:473:CYS:SG	2:B:475:THR:HG22	2.42	0.60
1:C:44:MET:SD	1:C:96:TYR:CE1	2.95	0.59
2:B:31:ILE:N	2:B:31:ILE:HD13	2.17	0.59
2:B:389:VAL:HG12	2:B:390:ASP:OD2	2.02	0.59
2:B:475:THR:O	2:B:523:PHE:CE2	2.52	0.59
2:D:243:ASP:OD2	2:D:246:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:447:TYR:HD1	2:D:474:ILE:CG2	2.15	0.59
2:D:181:VAL:CG2	2:D:227:TRP:HZ2	2.14	0.59
2:B:465:TYR:CD2	2:B:466:VAL:HG13	2.37	0.59
1:C:44:MET:HE1	2:D:41:ASP:N	2.17	0.59
2:D:278:ARG:O	2:D:281:ALA:N	2.35	0.59
2:D:298:ILE:HG22	2:D:302:GLU:OE2	2.03	0.59
2:D:447:TYR:HD1	2:D:474:ILE:HG22	1.68	0.59
2:B:158:PRO:O	2:B:161:VAL:HB	2.02	0.59
2:B:446:TYR:OH	2:B:490:GLU:OE1	2.20	0.59
2:B:128:GLU:CD	2:B:128:GLU:H	2.06	0.59
2:B:337:ALA:HB3	2:B:359:LYS:HE3	1.85	0.59
2:D:485:ARG:HG3	2:D:486:HIS:H	1.67	0.59
2:D:15:ILE:N	2:D:15:ILE:HD13	2.13	0.58
2:B:80:ILE:HG23	2:B:286:PHE:CE1	2.39	0.58
2:D:309:CYS:HA	2:D:501:MET:CE	2.33	0.58
2:B:115:VAL:HG21	2:B:169:MET:HE3	1.84	0.58
2:D:88:GLY:C	2:D:274:ALA:HB1	2.24	0.58
2:D:31:ILE:CD1	2:D:32:LYS:HG3	2.34	0.58
1:A:44:MET:HE3	1:A:96:TYR:HE2	1.69	0.58
2:B:66:VAL:CG1	2:B:69:TYR:HD2	2.16	0.58
1:C:15:SER:HB3	2:D:60:PHE:HD1	1.68	0.58
1:C:67:SER:CB	1:C:98:GLN:NE2	2.67	0.58
2:D:384:PHE:HB2	2:D:398:VAL:CG2	2.26	0.58
2:B:185:LEU:HD22	2:B:185:LEU:H	1.67	0.57
2:B:260:HIS:CD2	2:B:283:HIS:ND1	2.72	0.57
2:D:401:PHE:HB3	2:D:428:THR:HG21	1.85	0.57
2:B:185:LEU:HD22	2:B:185:LEU:N	2.19	0.57
2:D:400:ARG:NH2	2:D:429:PRO:HD2	2.18	0.57
1:A:21:VAL:HG22	2:B:201:ILE:O	2.05	0.57
2:B:69:TYR:HE1	2:B:203:PRO:HD3	1.66	0.57
2:D:393:PRO:O	2:D:439:LEU:HD13	2.03	0.57
1:A:76:TYR:CZ	1:A:84:PRO:HG3	2.39	0.57
2:B:465:TYR:HD2	2:B:466:VAL:HG13	1.69	0.57
2:D:264:HIS:CE1	2:D:279:CYS:HB2	2.40	0.57
1:C:44:MET:SD	1:C:96:TYR:HE1	2.28	0.57
2:D:19:HIS:CG	2:D:47:LYS:HB3	2.39	0.57
2:B:510:ILE:HG23	2:B:511:TYR:O	2.04	0.57
2:B:139:LYS:C	2:B:153:MET:HE1	2.25	0.57
2:B:445:PHE:CE2	2:B:514:PHE:CZ	2.93	0.57
2:B:208:CYS:O	2:B:209:LEU:HB3	2.05	0.57
2:B:209:LEU:O	2:B:209:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:PHE:HB3	2:D:256:ASN:HD21	1.69	0.57
2:D:290:VAL:HG23	2:D:291:ASP:N	2.19	0.57
2:D:315:MET:HE1	2:D:447:TYR:O	2.05	0.57
2:B:481:GLY:N	2:B:482:ALA:HA	2.19	0.56
1:A:10:ASN:HB3	1:A:14:LEU:HD11	1.87	0.56
1:A:42:VAL:HG12	1:A:72:SER:HB3	1.85	0.56
2:B:215:THR:HG21	2:B:227:TRP:CZ3	2.39	0.56
2:D:396:ALA:HB3	2:D:439:LEU:CD1	2.33	0.56
2:B:361:TYR:CE2	2:D:314:HIS:CE1	2.94	0.56
2:D:144:ASP:N	2:D:147:LYS:HE3	2.20	0.56
1:A:93:LYS:HG2	2:B:22:GLN:HA	1.87	0.56
2:B:215:THR:HG21	2:B:227:TRP:CE3	2.41	0.56
2:B:113:THR:HB	2:B:115:VAL:HG13	1.87	0.56
2:B:326:PHE:CD2	2:B:381:VAL:HB	2.40	0.56
2:B:440:LYS:HE3	2:B:512:LYS:CD	2.36	0.56
2:D:273:ASP:O	2:D:277:THR:OG1	2.23	0.56
2:D:424:HIS:CD2	2:D:424:HIS:N	2.72	0.56
2:B:476:ARG:CD	2:B:487:HIS:CG	2.88	0.56
1:A:44:MET:HE3	1:A:96:TYR:CE2	2.40	0.56
1:A:18:ALA:HB1	2:B:196:LYS:NZ	2.20	0.56
2:B:95:HIS:ND1	2:B:104:ASN:OD1	2.39	0.56
2:D:313:GLN:OE1	2:D:385:TRP:CD1	2.58	0.56
1:C:123:TRP:CE3	1:C:123:TRP:HA	2.40	0.56
2:D:313:GLN:CG	2:D:385:TRP:CZ2	2.89	0.56
2:B:84:ARG:CG	2:B:411:LEU:HD22	2.36	0.56
2:B:476:ARG:HH11	2:B:487:HIS:CG	2.22	0.56
2:D:25:THR:HG23	2:D:28:SER:H	1.70	0.56
2:D:450:SER:OG	2:D:487:HIS:NE2	2.39	0.56
2:D:215:THR:HG21	2:D:227:TRP:CZ2	2.41	0.55
2:D:70:PRO:HG3	2:D:238:ASN:ND2	2.21	0.55
2:B:186:TRP:HZ3	2:B:244:VAL:HG12	1.71	0.55
2:B:249:PHE:H	2:B:249:PHE:HD1	1.52	0.55
2:B:316:VAL:HG13	2:B:317:VAL:N	2.22	0.55
2:B:434:SER:O	2:B:437:THR:HG22	2.06	0.55
1:C:106:ASP:OD2	1:C:109:GLY:N	2.37	0.55
2:D:332:ILE:HG13	2:D:384:PHE:CE1	2.41	0.55
1:A:38:ILE:HD12	1:A:108:VAL:HG11	1.89	0.55
2:B:26:HIS:CE1	2:B:34:LYS:HD3	2.42	0.55
2:B:392:TYR:O	2:B:438:ASN:ND2	2.39	0.55
1:C:54:ALA:HB1	1:C:55:ILE:HG23	1.89	0.55
1:A:73:CYS:SG	1:A:107:PRO:HB2	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:HG13	1:A:58:THR:HG23	1.89	0.55
2:B:256:ASN:HB3	2:B:280:LEU:HD11	1.89	0.55
2:B:66:VAL:HB	2:B:69:TYR:HB2	1.88	0.55
1:C:10:ASN:ND2	1:C:38:ILE:HG23	2.21	0.55
2:D:373:HIS:CE1	2:D:376:LYS:HE2	2.41	0.55
2:B:315:MET:HE3	2:B:494:TYR:CE2	2.42	0.55
2:B:136:VAL:HG12	2:B:137:ASN:N	2.21	0.55
2:B:264:HIS:CD2	2:B:275:ILE:CG2	2.90	0.55
1:C:117:CYS:HB3	1:C:122:MET:H	1.72	0.55
2:D:26:HIS:ND1	2:D:34:LYS:HE3	2.22	0.55
2:B:182:VAL:HA	2:B:240:PHE:O	2.07	0.55
2:D:88:GLY:H	2:D:112:SER:HB2	1.69	0.54
2:B:148:HIS:CE1	2:B:149:LEU:HD12	2.42	0.54
2:B:186:TRP:CD2	2:B:253:LEU:HB2	2.42	0.54
1:C:43:LYS:HG3	1:C:68:PHE:CE1	2.41	0.54
2:D:387:CYS:O	2:D:392:TYR:OH	2.25	0.54
2:B:33:PHE:O	2:B:40:VAL:HG12	2.06	0.54
2:D:334:ASN:HD22	2:D:350:PHE:HD2	1.54	0.54
2:D:333:GLY:HA3	2:D:387:CYS:SG	2.48	0.54
1:A:76:TYR:HD2	1:A:82:ASP:O	1.90	0.54
2:B:168:GLN:HG3	2:B:169:MET:N	2.23	0.54
2:B:476:ARG:HD3	2:B:487:HIS:NE2	2.23	0.54
2:D:292:TRP:CZ2	2:D:335:PRO:HG2	2.42	0.54
2:D:64:TYR:OH	2:D:72:MET:HG3	2.07	0.54
2:D:97:THR:HG23	2:D:98:ARG:H	1.72	0.54
1:C:117:CYS:SG	1:C:119:VAL:CB	2.94	0.54
2:D:149:LEU:HA	2:D:152:LEU:CD1	2.37	0.54
2:D:84:ARG:NH2	2:D:296:TYR:HB3	2.22	0.54
2:D:249:PHE:HB3	2:D:256:ASN:ND2	2.23	0.54
1:A:19:PHE:HE1	2:B:196:LYS:HA	1.70	0.54
2:D:185:LEU:CD2	2:D:185:LEU:N	2.70	0.54
1:A:79:CYS:HB2	1:A:81:ILE:HD13	1.88	0.54
2:B:74:ILE:O	2:B:242:ILE:HD13	2.06	0.54
2:B:66:VAL:HG11	2:B:69:TYR:CD2	2.42	0.54
2:D:111:PHE:O	2:D:113:THR:O	2.26	0.54
2:D:149:LEU:CA	2:D:152:LEU:HD12	2.37	0.54
2:D:205:ARG:HD3	2:D:224:TYR:CE2	2.43	0.54
2:D:171:SER:HA	2:D:227:TRP:CD1	2.42	0.54
2:D:330:HIS:HB2	2:D:382:CYS:HB3	1.90	0.54
1:A:38:ILE:CB	1:A:108:VAL:HG21	2.37	0.53
2:B:63:ASN:ND2	2:B:63:ASN:O	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:VAL:O	2:D:166:ILE:HG13	2.07	0.53
2:D:99:ASP:OD1	2:D:137:ASN:ND2	2.41	0.53
2:B:249:PHE:HE2	2:B:280:LEU:HD21	1.73	0.53
1:C:75:LEU:HD22	1:C:112:LEU:HD11	1.91	0.53
2:D:145:GLN:O	2:D:148:HIS:HD2	1.91	0.53
2:D:388:ASN:OD1	2:D:400:ARG:NH2	2.41	0.53
2:B:423:LYS:HA	2:B:423:LYS:HE2	1.89	0.53
2:D:521:ASN:O	2:D:525:ARG:HG3	2.07	0.53
1:A:103:CYS:HB3	1:A:110:PHE:CE2	2.43	0.53
2:D:263:VAL:HG23	2:D:415:ASP:HB2	1.89	0.53
2:D:95:HIS:CD2	2:D:141:PRO:HG3	2.43	0.53
2:B:421:VAL:HG22	2:B:425:ALA:HB2	1.90	0.53
2:D:119:ALA:HB2	2:D:162:VAL:HG21	1.91	0.53
2:B:197:TYR:N	2:B:197:TYR:CD1	2.76	0.53
2:D:222:ASP:O	2:D:223:THR:HG23	2.09	0.53
2:D:403:THR:HB	2:D:418:SER:CB	2.38	0.53
1:A:15:SER:HB3	2:B:60:PHE:CD1	2.43	0.53
2:D:124:TYR:CE2	2:D:133:PHE:HD1	2.26	0.53
2:D:442:LEU:HD23	2:D:443:PRO:O	2.09	0.53
1:C:47:THR:HB	1:C:49:THR:OG1	2.08	0.53
2:B:18:LEU:HB3	2:B:23:ALA:HB2	1.90	0.53
2:B:26:HIS:ND1	2:B:26:HIS:O	2.42	0.53
1:C:53:GLN:HG3	1:C:121:GLY:O	2.09	0.53
2:D:356:CYS:O	2:D:362:LYS:HG2	2.09	0.53
2:B:440:LYS:HG3	2:B:512:LYS:HG2	1.91	0.52
2:D:392:TYR:HE2	2:D:436:PHE:HE1	1.57	0.52
2:D:475:THR:HG21	2:D:487:HIS:HB3	1.92	0.52
2:D:257:HIS:ND1	2:D:279:CYS:SG	2.77	0.52
2:B:181:VAL:HG22	2:B:227:TRP:CZ2	2.45	0.52
2:B:444:PHE:CE2	2:B:495:LEU:HD12	2.45	0.52
1:C:44:MET:SD	2:D:39:CYS:O	2.68	0.52
2:D:160:ASN:HA	2:D:163:ARG:HH11	1.75	0.52
2:D:385:TRP:CZ3	2:D:399:CYS:HB3	2.44	0.52
2:B:328:VAL:HG11	2:B:379:ASP:OD1	2.10	0.52
2:B:476:ARG:HD3	2:B:487:HIS:ND1	2.24	0.52
2:B:389:VAL:HG12	2:B:390:ASP:H	1.75	0.52
2:B:403:THR:HG22	2:B:418:SER:OG	2.10	0.52
2:B:474:ILE:HA	2:B:520:TRP:CH2	2.45	0.52
1:C:10:ASN:O	1:C:14:LEU:HD12	2.10	0.52
2:D:11:CYS:HB3	2:D:101:VAL:O	2.09	0.52
1:C:42:VAL:HG12	2:D:26:HIS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:TRP:O	2:D:87:ILE:HD13	2.10	0.52
1:A:0:SER:HA	1:A:1:ALA:C	2.30	0.51
2:B:186:TRP:CE3	2:B:245:GLN:HB2	2.45	0.51
2:B:510:ILE:HG12	2:B:511:TYR:CD1	2.45	0.51
2:D:116:ASN:CG	2:D:271:SER:HG	2.12	0.51
1:A:126:TYR:N	1:A:127:GLY:CA	2.73	0.51
2:B:476:ARG:NH1	2:B:487:HIS:HD2	2.01	0.51
2:D:196:LYS:HG3	2:D:196:LYS:O	2.09	0.51
2:D:198:PHE:CD1	2:D:199:VAL:HG23	2.45	0.51
2:D:266:ASN:N	2:D:276:MET:HE1	2.25	0.51
2:D:403:THR:HB	2:D:418:SER:HB3	1.92	0.51
2:B:445:PHE:CE2	2:B:514:PHE:HZ	2.28	0.51
2:D:398:VAL:CG1	2:D:509:TRP:HB2	2.41	0.51
2:B:217:PHE:HD2	2:B:224:TYR:CE1	2.27	0.51
1:C:76:TYR:CD1	1:C:81:ILE:HD11	2.46	0.51
2:D:31:ILE:HD12	2:D:32:LYS:H	1.75	0.51
1:C:42:VAL:O	1:C:42:VAL:HG23	2.11	0.51
2:D:85:ALA:HB1	2:D:180:ARG:O	2.11	0.51
1:A:76:TYR:CD1	1:A:76:TYR:N	2.78	0.51
2:B:510:ILE:HG12	2:B:511:TYR:CE1	2.46	0.51
2:B:101:VAL:CG1	2:B:102:GLY:N	2.74	0.51
2:B:83:VAL:HG21	2:B:286:PHE:CE2	2.46	0.51
2:B:292:TRP:HA	2:B:424:HIS:HD2	1.76	0.51
2:D:97:THR:HG23	2:D:98:ARG:N	2.26	0.51
2:B:421:VAL:HG22	2:B:425:ALA:HB1	1.93	0.51
2:D:317:VAL:HG11	2:D:340:CYS:SG	2.51	0.51
2:B:186:TRP:CE2	2:B:253:LEU:HB2	2.45	0.51
2:D:289:ARG:HG3	2:D:354:GLN:HG3	1.93	0.51
2:D:442:LEU:C	2:D:442:LEU:HD23	2.30	0.51
2:D:204:GLU:OE2	2:D:213:ARG:NH1	2.44	0.50
1:A:5:THR:HG23	1:A:6:GLU:HG2	1.93	0.50
2:B:447:TYR:C	2:B:447:TYR:CD1	2.85	0.50
2:B:80:ILE:O	2:B:83:VAL:HG23	2.11	0.50
2:D:72:MET:O	2:D:241:MET:HG2	2.12	0.50
2:B:249:PHE:N	2:B:249:PHE:CD1	2.79	0.50
2:B:260:HIS:N	2:B:260:HIS:ND1	2.59	0.50
2:D:56:SER:OG	2:D:58:MET:HG3	2.11	0.50
2:B:87:ILE:HA	2:B:112:SER:HG	1.77	0.50
2:D:291:ASP:OD1	2:D:292:TRP:N	2.45	0.50
2:D:373:HIS:ND1	2:D:376:LYS:HE2	2.25	0.50
2:D:313:GLN:OE1	2:D:385:TRP:CE2	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:VAL:O	2:B:423:LYS:NZ	2.37	0.50
2:B:511:TYR:N	2:B:511:TYR:CD1	2.76	0.50
1:C:13:VAL:HG22	1:C:30:TYR:HE2	1.72	0.50
2:D:177:LEU:HD12	2:D:177:LEU:N	2.25	0.50
1:A:116:VAL:HG12	1:A:123:TRP:CE3	2.46	0.50
2:B:308:ALA:HB1	2:B:497:ALA:O	2.12	0.50
2:D:333:GLY:O	2:D:335:PRO:HD3	2.12	0.50
2:D:466:VAL:N	2:D:467:PRO:HD2	2.26	0.50
1:A:39:THR:O	1:A:40:ASN:HB3	2.12	0.50
2:B:182:VAL:HG12	2:B:240:PHE:HB2	1.94	0.50
2:B:389:VAL:HG12	2:B:390:ASP:N	2.27	0.50
1:A:18:ALA:HB1	2:B:196:LYS:HZ1	1.76	0.49
2:D:208:CYS:SG	2:D:209:LEU:HD13	2.52	0.49
2:D:420:TYR:CE2	2:D:422:ASN:HB2	2.47	0.49
2:B:475:THR:OG1	2:B:477:CYS:C	2.49	0.49
1:C:54:ALA:HB1	1:C:55:ILE:CG2	2.42	0.49
2:D:18:LEU:O	2:D:29:VAL:HA	2.13	0.49
2:B:396:ALA:HB3	2:B:439:LEU:HD21	1.94	0.49
1:C:46:CYS:HB3	1:C:48:HIS:ND1	2.28	0.49
2:D:369:SER:H	2:D:373:HIS:HD2	1.60	0.49
2:B:88:GLY:HA3	2:B:274:ALA:O	2.11	0.49
2:B:260:HIS:CD2	2:B:283:HIS:CG	3.01	0.49
1:C:76:TYR:CE1	1:C:84:PRO:HG3	2.48	0.49
1:C:80:HIS:CE1	2:D:55:ILE:HG12	2.47	0.49
2:D:392:TYR:O	2:D:438:ASN:ND2	2.43	0.49
2:D:289:ARG:O	2:D:290:VAL:HG22	2.11	0.49
1:C:15:SER:CB	2:D:60:PHE:HD1	2.26	0.49
1:A:10:ASN:HD21	1:A:39:THR:H	1.61	0.49
2:B:148:HIS:CE1	2:B:149:LEU:CD1	2.95	0.49
2:B:225:ALA:CB	2:B:230:SER:HB2	2.43	0.49
2:B:302:GLU:CD	2:B:422:ASN:HB3	2.32	0.49
1:C:83:HIS:NE2	1:C:90:CYS:HB2	2.27	0.49
2:B:442:LEU:HD23	2:B:510:ILE:CB	2.38	0.49
1:C:21:VAL:HG21	2:D:237:TYR:HE1	1.77	0.49
2:D:195:MET:HE1	2:D:241:MET:SD	2.53	0.49
2:B:257:HIS:NE2	2:B:264:HIS:HB2	2.27	0.49
2:B:200:LYS:HB2	2:B:235:TYR:HD2	1.78	0.49
2:B:73:PHE:CZ	2:B:241:MET:HG3	2.47	0.49
2:B:423:LYS:CD	2:B:424:HIS:H	2.26	0.49
1:C:56:THR:OG1	1:C:58:THR:O	2.25	0.49
2:D:313:GLN:HG2	2:D:385:TRP:CH2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:421:VAL:HA	2:D:425:ALA:HA	1.94	0.49
2:B:391:ARG:HB2	2:B:435:ALA:HA	1.94	0.48
1:A:44:MET:CB	1:A:67:SER:HB3	2.42	0.48
2:B:333:GLY:HA3	2:B:387:CYS:HB2	1.95	0.48
1:C:83:HIS:CD2	1:C:90:CYS:HB2	2.48	0.48
2:D:177:LEU:CD1	2:D:177:LEU:N	2.76	0.48
2:D:314:HIS:CD2	2:D:314:HIS:O	2.66	0.48
1:C:44:MET:HE3	2:D:40:VAL:HA	1.96	0.48
2:B:344:ALA:HB3	2:B:346:VAL:HG12	1.94	0.48
2:B:465:TYR:HD2	2:B:466:VAL:H	1.60	0.48
2:B:511:TYR:HD1	2:B:511:TYR:H	1.53	0.48
2:B:247:TRP:HB2	2:B:249:PHE:CE1	2.44	0.48
1:A:93:LYS:NZ	2:B:51:TYR:OH	2.25	0.48
2:D:150:ILE:HG13	2:D:151:PRO:N	2.27	0.48
2:B:88:GLY:O	2:B:274:ALA:HB1	2.14	0.48
1:C:45:LEU:HD12	1:C:46:CYS:N	2.28	0.48
2:D:124:TYR:CZ	2:D:196:LYS:HE3	2.48	0.48
2:D:224:TYR:HE2	2:D:237:TYR:CZ	2.32	0.48
1:A:42:VAL:HG12	1:A:72:SER:CB	2.43	0.48
1:A:44:MET:HE2	1:A:96:TYR:CE2	2.37	0.48
2:B:331:ASP:HB2	2:B:348:TRP:HE1	1.78	0.48
2:B:358:ASP:O	2:B:359:LYS:HB2	2.14	0.48
2:D:516:THR:O	2:D:519:LEU:HB2	2.13	0.48
2:B:186:TRP:CZ3	2:B:244:VAL:HG12	2.49	0.48
2:B:284:GLU:O	2:B:288:LYS:HE3	2.13	0.48
2:D:84:ARG:CZ	2:D:299:ILE:HD11	2.43	0.48
2:B:107:LEU:HD23	2:B:149:LEU:HD23	1.96	0.48
2:B:314:HIS:CD2	2:B:341:VAL:HG13	2.48	0.48
1:C:43:LYS:O	2:D:38:LEU:HD13	2.14	0.48
2:D:452:CYS:HB3	2:D:477:CYS:SG	2.53	0.48
2:D:447:TYR:CD1	2:D:474:ILE:HG22	2.48	0.48
2:D:50:THR:HA	2:D:128:GLU:CG	2.43	0.48
2:B:109:LEU:N	2:B:109:LEU:HD12	2.29	0.48
2:B:21:THR:O	2:B:22:GLN:CB	2.62	0.48
1:C:16:PHE:CD2	2:D:64:TYR:CD2	3.01	0.48
2:D:257:HIS:CE1	2:D:261:CYS:CB	2.85	0.48
2:D:384:PHE:HB3	2:D:387:CYS:HB3	1.95	0.48
1:A:76:TYR:CE2	1:A:84:PRO:HG3	2.49	0.48
2:B:135:ARG:NH1	2:B:135:ARG:CG	2.72	0.48
2:B:476:ARG:NH1	2:B:486:HIS:ND1	2.57	0.48
2:D:144:ASP:O	2:D:147:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:392:TYR:CE2	2:D:436:PHE:HE1	2.32	0.48
2:D:469:LYS:HG3	2:D:481:GLY:HA2	1.96	0.48
1:C:93:LYS:HD3	2:D:22:GLN:HA	1.96	0.47
2:D:384:PHE:HB3	2:D:387:CYS:CB	2.43	0.47
1:A:123:TRP:HA	1:A:123:TRP:CE3	2.49	0.47
2:D:213:ARG:NH2	2:D:240:PHE:HE1	2.12	0.47
2:D:444:PHE:HE1	2:D:494:TYR:CE1	2.33	0.47
2:D:72:MET:HB3	2:D:72:MET:HE2	1.63	0.47
2:B:260:HIS:HD2	2:B:283:HIS:CG	2.33	0.47
2:B:302:GLU:CD	2:B:422:ASN:CB	2.82	0.47
2:B:18:LEU:HD21	2:B:53:ARG:NE	2.29	0.47
2:B:286:PHE:CD2	2:B:419:LEU:HD11	2.49	0.47
2:D:148:HIS:CE1	2:D:149:LEU:HD12	2.50	0.47
2:D:363:ILE:HD13	2:D:363:ILE:N	2.29	0.47
1:C:13:VAL:HG22	1:C:30:TYR:CZ	2.48	0.47
2:D:438:ASN:C	2:D:512:LYS:HE2	2.35	0.47
1:A:76:TYR:H	1:A:76:TYR:HD1	1.62	0.47
2:B:181:VAL:O	2:B:240:PHE:HB2	2.15	0.47
2:B:208:CYS:HB3	2:B:224:TYR:O	2.14	0.47
2:B:215:THR:H	2:B:226:CYS:HA	1.80	0.47
1:A:5:THR:HG22	2:B:8:PHE:O	2.14	0.47
2:D:350:PHE:N	2:D:350:PHE:CD1	2.82	0.47
2:B:188:HIS:NE2	2:B:192:LEU:HD12	2.29	0.47
2:B:384:PHE:O	2:B:398:VAL:HG23	2.15	0.47
2:B:445:PHE:HE2	2:B:514:PHE:CZ	2.33	0.47
2:D:397:ILE:CG1	2:D:510:ILE:HG13	2.27	0.47
2:B:185:LEU:CD2	2:B:185:LEU:N	2.78	0.47
2:D:314:HIS:C	2:D:314:HIS:CD2	2.88	0.47
2:B:197:TYR:N	2:B:197:TYR:HD1	2.13	0.47
1:A:21:VAL:CG1	2:B:200:LYS:HG2	2.34	0.47
2:B:475:THR:HG1	2:B:477:CYS:C	2.18	0.47
1:A:25:LYS:HG2	2:B:69:TYR:HH	1.80	0.47
1:C:120:CYS:HB3	1:C:122:MET:CE	2.45	0.47
1:C:16:PHE:CE1	1:C:26:ALA:HB1	2.50	0.47
1:A:80:HIS:HA	2:B:131:THR:HG21	1.97	0.46
2:B:401:PHE:CE2	2:B:420:TYR:CD2	3.04	0.46
2:B:62:MET:SD	2:B:192:LEU:HD21	2.55	0.46
1:C:76:TYR:CD1	1:C:84:PRO:HD3	2.50	0.46
2:D:315:MET:HG3	2:D:316:VAL:N	2.29	0.46
2:D:349:LYS:HZ2	2:D:351:TYR:HE1	1.63	0.46
2:D:330:HIS:HB2	2:D:382:CYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:LEU:C	2:B:329:LEU:HD23	2.36	0.46
2:D:19:HIS:CD2	2:D:20:PRO:HD2	2.50	0.46
2:B:168:GLN:HG3	2:B:169:MET:H	1.81	0.46
2:B:255:SER:OG	2:B:256:ASN:N	2.48	0.46
2:B:450:SER:CB	2:B:476:ARG:HE	2.17	0.46
2:D:107:LEU:O	2:D:118:VAL:HA	2.15	0.46
2:D:174:LEU:HA	2:D:174:LEU:HD12	1.74	0.46
2:B:361:TYR:CD2	2:D:314:HIS:ND1	2.83	0.46
2:D:364:GLU:O	2:D:365:GLU:CB	2.63	0.46
2:D:517:TYR:HA	2:D:520:TRP:HD1	1.81	0.46
2:B:188:HIS:CD2	2:B:188:HIS:C	2.89	0.46
2:B:231:VAL:C	2:B:233:PHE:H	2.17	0.46
2:D:221:SER:O	2:D:222:ASP:C	2.53	0.46
2:D:332:ILE:HB	2:D:384:PHE:CD1	2.50	0.46
2:D:420:TYR:O	2:D:425:ALA:HA	2.15	0.46
2:D:439:LEU:HB2	2:D:510:ILE:O	2.16	0.46
2:D:444:PHE:HE1	2:D:494:TYR:HE1	1.63	0.46
2:B:243:ASP:HB3	2:B:246:GLN:HB2	1.98	0.46
2:B:358:ASP:OD1	2:B:358:ASP:N	2.45	0.46
1:C:27:TYR:O	1:C:30:TYR:N	2.46	0.46
2:D:332:ILE:HB	2:D:384:PHE:HD1	1.80	0.46
2:D:351:TYR:HB3	2:D:364:GLU:HB3	1.97	0.46
2:D:368:TYR:HD1	2:D:389:VAL:HB	1.80	0.46
1:A:98:GLN:C	1:A:99:ILE:HD12	2.36	0.46
2:B:49:MET:O	2:B:128:GLU:HG2	2.16	0.46
2:B:198:PHE:CD1	2:B:199:VAL:HG23	2.50	0.46
2:B:31:ILE:CD1	2:B:31:ILE:H	2.17	0.46
1:C:123:TRP:HA	1:C:123:TRP:HE3	1.80	0.46
1:C:55:ILE:CG2	1:C:97:VAL:HG22	2.39	0.46
2:B:261:CYS:HA	2:B:415:ASP:HB3	1.96	0.46
2:B:375:ASP:O	2:B:378:THR:HG23	2.15	0.46
2:B:472:THR:O	2:B:473:CYS:HB3	2.16	0.46
1:C:93:LYS:HG2	2:D:128:GLU:O	2.15	0.46
1:C:4:ALA:HA	2:D:9:LYS:CB	2.46	0.46
1:A:53:GLN:HG2	1:A:122:MET:HE2	1.97	0.46
2:B:159:TRP:CE2	2:B:197:TYR:CD2	3.04	0.46
1:C:40:ASN:ND2	2:D:25:THR:OG1	2.49	0.46
2:B:393:PRO:O	2:B:439:LEU:HD21	2.16	0.46
2:D:145:GLN:O	2:D:148:HIS:CD2	2.69	0.46
2:D:368:TYR:HA	2:D:373:HIS:CD2	2.51	0.46
2:D:401:PHE:CE1	2:D:420:TYR:CD1	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:GLY:O	1:A:1:ALA:HB3	2.14	0.46
2:B:204:GLU:OE2	2:B:213:ARG:NH1	2.49	0.46
2:B:423:LYS:HE2	2:B:424:HIS:N	2.29	0.46
1:C:43:LYS:HA	1:C:68:PHE:CD1	2.51	0.46
2:D:150:ILE:N	2:D:151:PRO:CD	2.78	0.46
2:D:264:HIS:CE1	2:D:279:CYS:CB	2.99	0.46
2:D:72:MET:HB3	2:D:241:MET:CE	2.41	0.46
2:B:83:VAL:HG21	2:B:286:PHE:CZ	2.51	0.45
2:B:447:TYR:HA	2:B:474:ILE:HG13	1.98	0.45
2:D:17:GLY:HA2	2:D:18:LEU:HA	1.74	0.45
2:D:259:GLN:NE2	2:D:260:HIS:NE2	2.64	0.45
1:A:99:ILE:HG22	1:A:100:PRO:O	2.16	0.45
1:A:30:TYR:CE2	1:A:35:GLY:HA3	2.52	0.45
2:B:208:CYS:O	2:B:209:LEU:CB	2.64	0.45
2:B:261:CYS:SG	2:B:415:ASP:CB	3.04	0.45
2:B:261:CYS:SG	2:B:415:ASP:HB3	2.56	0.45
2:D:128:GLU:CD	2:D:128:GLU:H	2.10	0.45
2:D:170:LEU:HD12	2:D:170:LEU:HA	1.80	0.45
1:A:21:VAL:HG21	2:B:237:TYR:HE2	1.81	0.45
2:B:292:TRP:CD1	2:B:424:HIS:CD2	3.04	0.45
2:B:71:ASN:OD1	2:B:71:ASN:N	2.50	0.45
1:A:5:THR:CG2	2:B:8:PHE:O	2.64	0.45
2:D:183:PHE:HB2	2:D:241:MET:HB3	1.97	0.45
2:D:264:HIS:NE2	2:D:279:CYS:CB	2.80	0.45
2:D:414:CYS:HA	2:D:415:ASP:HA	1.63	0.45
2:D:84:ARG:CG	2:D:177:LEU:HB3	2.47	0.45
2:B:117:LEU:CD1	2:B:166:ILE:HG13	2.46	0.45
2:B:257:HIS:CE1	2:B:261:CYS:HB3	2.50	0.45
2:B:390:ASP:OD2	2:B:390:ASP:N	2.43	0.45
2:B:467:PRO:HB2	2:B:483:VAL:HG21	1.97	0.45
2:D:57:MET:HB3	2:D:193:THR:HG23	1.98	0.45
2:D:255:SER:OG	2:D:256:ASN:OD1	2.35	0.45
2:B:474:ILE:CD1	2:B:474:ILE:O	2.59	0.45
2:D:177:LEU:HA	2:D:299:ILE:HD13	1.98	0.45
2:D:384:PHE:CE2	2:D:392:TYR:CD1	3.04	0.45
1:A:89:PHE:N	1:A:89:PHE:CD1	2.81	0.45
2:B:484:CYS:O	2:B:486:HIS:N	2.50	0.45
2:D:406:LEU:HD22	2:D:406:LEU:H	1.81	0.45
2:D:411:LEU:O	2:D:419:LEU:N	2.35	0.45
2:D:80:ILE:HD13	2:D:80:ILE:HA	1.79	0.45
1:A:24:ALA:O	1:A:28:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:CYS:CB	2:B:101:VAL:O	2.63	0.44
1:C:115:THR:HG22	1:C:116:VAL:N	2.31	0.44
2:B:301:ASP:O	2:B:305:VAL:HG23	2.16	0.44
2:D:158:PRO:O	2:D:162:VAL:HG23	2.17	0.44
2:D:2:GLU:HA	2:D:3:ASN:HA	1.61	0.44
1:A:93:LYS:HE2	2:B:22:GLN:CA	2.45	0.44
2:D:210:CYS:SG	2:D:212:LYS:HB2	2.57	0.44
2:B:217:PHE:HD2	2:B:224:TYR:HE1	1.65	0.44
2:B:84:ARG:HD3	2:B:84:ARG:HA	1.68	0.44
2:D:52:ARG:NH1	2:D:132:GLU:OE1	2.46	0.44
2:D:7:LEU:HD12	2:D:8:PHE:CG	2.52	0.44
1:A:25:LYS:HG2	2:B:69:TYR:OH	2.17	0.44
2:B:115:VAL:HG21	2:B:169:MET:HE2	1.96	0.44
2:B:414:CYS:HA	2:B:415:ASP:HA	1.69	0.44
2:B:481:GLY:N	2:B:482:ALA:CA	2.80	0.44
1:C:120:CYS:HB2	1:C:121:GLY:CA	2.48	0.44
1:C:19:PHE:CE1	2:D:196:LYS:HA	2.52	0.44
2:D:360:ALA:O	2:D:361:TYR:C	2.56	0.44
2:B:95:HIS:NE2	2:B:141:PRO:HA	2.32	0.44
2:B:294:VAL:HG23	2:B:423:LYS:HZ3	1.80	0.44
2:B:313:GLN:O	2:B:316:VAL:HG12	2.17	0.44
2:B:91:VAL:HG12	2:B:92:GLU:O	2.17	0.44
1:C:120:CYS:CB	1:C:122:MET:HB2	2.48	0.44
2:D:384:PHE:CD2	2:D:392:TYR:CE1	3.06	0.44
2:D:84:ARG:HG3	2:D:177:LEU:HB3	2.00	0.44
2:D:5:THR:OG1	2:D:7:LEU:HB2	2.18	0.44
2:D:88:GLY:H	2:D:112:SER:CB	2.30	0.44
2:D:349:LYS:HB3	2:D:351:TYR:CE1	2.53	0.44
1:A:64:ASP:O	1:A:101:THR:OG1	2.24	0.44
2:B:111:PHE:HB2	2:B:115:VAL:HG22	2.00	0.43
2:B:186:TRP:CZ3	2:B:245:GLN:HB2	2.53	0.43
2:B:294:VAL:HG23	2:B:423:LYS:HZ2	1.77	0.43
2:D:57:MET:HG3	2:D:60:PHE:CE2	2.53	0.43
2:D:83:VAL:HG12	2:D:83:VAL:O	2.18	0.43
2:D:145:GLN:H	2:D:145:GLN:HG3	1.54	0.43
1:A:20:ALA:HA	2:B:201:ILE:HG22	1.99	0.43
2:B:298:ILE:CD1	2:B:302:GLU:HB2	2.46	0.43
1:C:19:PHE:C	2:D:201:ILE:HG22	2.38	0.43
1:C:91:ASP:N	1:C:91:ASP:OD1	2.48	0.43
2:D:298:ILE:HG22	2:D:300:GLY:O	2.18	0.43
1:A:38:ILE:HB	1:A:108:VAL:CG2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:VAL:O	2:B:233:PHE:HD1	2.02	0.43
1:C:76:TYR:CZ	1:C:84:PRO:HG3	2.53	0.43
2:D:341:VAL:HG12	2:D:344:ALA:H	1.82	0.43
2:D:349:LYS:HB3	2:D:351:TYR:HE1	1.84	0.43
2:D:466:VAL:N	2:D:467:PRO:CD	2.82	0.43
1:A:76:TYR:HB2	1:A:83:HIS:CD2	2.53	0.43
2:B:468:LEU:HB2	2:B:492:ARG:NH1	2.33	0.43
1:C:44:MET:HA	2:D:39:CYS:O	2.19	0.43
2:D:50:THR:HB	2:D:128:GLU:OE1	2.19	0.43
2:D:289:ARG:O	2:D:354:GLN:NE2	2.51	0.43
1:A:100:PRO:HG2	1:A:126:TYR:CD2	2.53	0.43
2:B:174:LEU:CD2	2:B:181:VAL:HG13	2.48	0.43
1:A:71:ALA:CB	2:B:22:GLN:H	2.32	0.43
2:B:391:ARG:HA	2:B:435:ALA:CA	2.47	0.43
2:B:491:TYR:C	2:B:491:TYR:CD1	2.92	0.43
2:D:315:MET:HE1	2:D:447:TYR:H	1.82	0.43
2:D:54:LEU:C	2:D:55:ILE:HD12	2.39	0.43
2:B:14:ILE:HG21	2:B:53:ARG:NH2	2.34	0.43
2:B:178:SER:OG	2:B:179:ASP:N	2.52	0.43
2:D:25:THR:CG2	2:D:28:SER:H	2.31	0.43
2:D:298:ILE:HG23	2:D:302:GLU:HB2	2.01	0.43
2:B:140:PRO:HG3	2:B:150:ILE:HG12	2.01	0.43
2:B:185:LEU:CD2	2:B:185:LEU:H	2.30	0.43
2:B:296:TYR:HD2	2:B:421:VAL:HG13	1.84	0.43
2:B:487:HIS:HD2	2:B:487:HIS:N	2.15	0.43
2:D:325:LYS:CE	2:D:525:ARG:HH12	2.31	0.43
2:D:328:VAL:CG2	2:D:380:GLY:HA3	2.46	0.43
2:B:337:ALA:HA	2:B:350:PHE:CE2	2.54	0.42
1:C:92:LEU:HD11	1:C:111:THR:HG21	2.00	0.42
2:D:318:LYS:O	2:D:322:LEU:HD13	2.19	0.42
2:D:407:SER:OG	2:D:410:ASN:HB2	2.18	0.42
2:D:88:GLY:O	2:D:111:PHE:HA	2.19	0.42
1:A:58:THR:O	1:A:60:GLU:HG2	2.19	0.42
2:B:480:GLY:C	2:B:482:ALA:HB2	2.40	0.42
1:C:117:CYS:O	1:C:121:GLY:CA	2.67	0.42
1:A:130:CYS:O	1:A:131:ASP:HB2	2.20	0.42
1:A:22:ASP:OD1	1:A:25:LYS:HB3	2.19	0.42
2:B:11:CYS:O	2:B:100:ALA:HB1	2.19	0.42
2:B:137:ASN:N	2:B:137:ASN:OD1	2.52	0.42
2:B:445:PHE:C	2:B:445:PHE:CD1	2.93	0.42
2:B:465:TYR:HD2	2:B:466:VAL:N	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:HB3	2:B:65:GLN:O	2.19	0.42
2:D:10:ASP:C	2:D:10:ASP:OD1	2.58	0.42
2:D:32:LYS:HD3	2:D:45:ILE:CD1	2.41	0.42
2:B:198:PHE:CE1	2:B:199:VAL:HG23	2.54	0.42
1:C:83:HIS:HB2	1:C:88:GLY:O	2.19	0.42
2:D:294:VAL:HG22	2:D:296:TYR:CE1	2.55	0.42
2:D:7:LEU:HD22	2:D:59:GLY:O	2.19	0.42
2:B:197:TYR:H	2:B:197:TYR:HD1	1.67	0.42
2:B:201:ILE:HD12	2:B:201:ILE:HA	1.96	0.42
1:A:42:VAL:CG1	1:A:69:GLY:HA3	2.49	0.42
2:B:296:TYR:CD2	2:B:421:VAL:HG13	2.55	0.42
2:B:62:MET:HB2	2:B:62:MET:HE2	1.82	0.42
2:D:301:ASP:OD1	2:D:301:ASP:N	2.52	0.42
2:D:51:TYR:O	2:D:127:THR:HA	2.20	0.42
2:B:21:THR:O	2:B:22:GLN:HB3	2.19	0.42
2:B:289:ARG:HD2	2:B:289:ARG:N	2.35	0.42
2:B:80:ILE:HG23	2:B:286:PHE:HE1	1.81	0.42
2:B:88:GLY:O	2:B:111:PHE:HA	2.20	0.42
2:D:31:ILE:HD12	2:D:32:LYS:N	2.34	0.42
2:B:101:VAL:HG12	2:B:102:GLY:N	2.33	0.42
2:B:264:HIS:HD2	2:B:275:ILE:HG22	1.83	0.42
2:B:337:ALA:H	2:B:359:LYS:HD3	1.85	0.42
2:D:364:GLU:O	2:D:365:GLU:HB3	2.20	0.42
2:D:406:LEU:HD13	2:D:406:LEU:N	2.34	0.42
1:C:123:TRP:O	1:C:126:TYR:O	2.38	0.42
1:C:38:ILE:HG21	1:C:78:ARG:NH1	2.35	0.42
2:D:359:LYS:N	2:D:360:ALA:HA	2.34	0.42
2:D:385:TRP:HZ3	2:D:399:CYS:HB3	1.84	0.42
1:A:52:GLY:HA2	1:A:62:ASN:OD1	2.19	0.42
2:B:215:THR:O	2:B:237:TYR:N	2.43	0.42
1:C:13:VAL:CG2	1:C:30:TYR:CE2	2.96	0.42
2:D:289:ARG:N	2:D:289:ARG:HD2	2.35	0.42
2:B:84:ARG:HG3	2:B:177:LEU:CD1	2.49	0.41
2:B:402:ASP:OD1	2:B:404:ARG:HG3	2.20	0.41
2:B:73:PHE:CE2	2:B:241:MET:HG3	2.54	0.41
1:C:54:ALA:HA	1:C:55:ILE:HA	1.77	0.41
2:D:478:ASN:OD1	2:D:478:ASN:C	2.59	0.41
2:B:260:HIS:HD2	2:B:283:HIS:ND1	2.18	0.41
2:B:83:VAL:C	2:B:85:ALA:H	2.23	0.41
2:D:153:MET:HE3	2:D:153:MET:HB2	1.76	0.41
2:D:271:SER:O	2:D:275:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:370:TYR:CE1	2:D:374:HIS:HB3	2.54	0.41
1:A:76:TYR:CE2	1:A:84:PRO:HD3	2.55	0.41
2:B:195:MET:O	2:B:199:VAL:HB	2.20	0.41
2:B:116:ASN:HD21	2:B:269:VAL:HG12	1.84	0.41
2:B:302:GLU:HG3	2:B:422:ASN:CB	2.30	0.41
2:B:326:PHE:CG	2:B:381:VAL:HB	2.55	0.41
1:C:47:THR:HG1	1:C:48:HIS:C	2.24	0.41
2:D:21:THR:O	2:D:22:GLN:CB	2.68	0.41
2:D:224:TYR:HE2	2:D:237:TYR:CE1	2.37	0.41
2:D:219:THR:OG1	2:D:234:ASP:OD2	2.36	0.41
2:D:349:LYS:NZ	2:D:351:TYR:HE1	2.17	0.41
2:D:55:ILE:N	2:D:55:ILE:HD12	2.35	0.41
1:A:92:LEU:CD1	1:A:97:VAL:HG21	2.50	0.41
2:B:398:VAL:HG13	2:B:509:TRP:HB2	2.02	0.41
1:A:80:HIS:CD2	2:B:55:ILE:HG13	2.55	0.41
2:D:465:TYR:HB3	2:D:466:VAL:H	1.69	0.41
1:A:62:ASN:HB2	1:A:65:GLN:HG3	2.02	0.41
2:B:33:PHE:HB3	2:B:40:VAL:O	2.19	0.41
1:C:120:CYS:N	1:C:121:GLY:HA2	2.36	0.41
2:D:157:LEU:HD13	2:D:157:LEU:HA	1.79	0.41
1:A:59:PRO:HD3	1:A:96:TYR:CE1	2.55	0.41
1:A:99:ILE:HG23	1:A:110:PHE:CE2	2.56	0.41
2:B:163:ARG:NE	2:B:235:TYR:HE1	2.10	0.41
2:B:321:LEU:HA	2:B:321:LEU:HD23	1.68	0.41
1:C:10:ASN:OD1	1:C:38:ILE:HA	2.20	0.41
2:D:210:CYS:SG	2:D:229:HIS:CE1	3.03	0.41
2:D:468:LEU:O	2:D:483:VAL:HG23	2.20	0.41
2:D:56:SER:HG	2:D:58:MET:HG3	1.85	0.41
1:A:29:ASP:O	1:A:32:ALA:HB3	2.19	0.41
2:B:7:LEU:HD23	2:B:58:MET:O	2.19	0.41
2:D:201:ILE:HD13	2:D:202:GLY:N	2.36	0.41
2:D:254:GLN:O	2:D:258:ASP:HB2	2.21	0.41
2:D:411:LEU:HB2	2:D:419:LEU:HB3	2.02	0.41
2:D:215:THR:HG21	2:D:227:TRP:CH2	2.56	0.41
2:D:397:ILE:HG12	2:D:510:ILE:CG1	2.29	0.41
2:B:92:GLU:HB3	2:B:149:LEU:HD21	2.03	0.41
1:C:83:HIS:HA	1:C:84:PRO:HD3	1.94	0.41
1:C:87:LYS:HA	1:C:87:LYS:HD2	1.84	0.41
2:D:359:LYS:HG3	2:D:359:LYS:O	2.21	0.41
2:B:192:LEU:O	2:B:195:MET:HB2	2.21	0.41
2:B:229:HIS:N	2:B:229:HIS:ND1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:PHE:HD1	2:B:368:TYR:N	2.19	0.41
2:B:385:TRP:CZ3	2:B:399:CYS:HB2	2.56	0.41
2:B:42:ILE:O	2:B:43:PRO:C	2.59	0.41
2:D:18:LEU:HB3	2:D:23:ALA:HB2	2.03	0.41
1:A:103:CYS:HB3	1:A:110:PHE:CD2	2.56	0.40
2:B:19:HIS:CG	2:B:20:PRO:HD2	2.56	0.40
2:B:236:VAL:HG12	2:B:239:PRO:HD3	2.02	0.40
1:C:55:ILE:O	1:C:55:ILE:HD12	2.20	0.40
1:C:80:HIS:CD2	2:D:8:PHE:CD1	3.09	0.40
2:D:12:SER:HA	2:D:100:ALA:HB2	2.02	0.40
2:D:299:ILE:O	2:D:299:ILE:HG22	2.21	0.40
2:D:516:THR:HA	2:D:519:LEU:HD23	2.03	0.40
2:D:76:ARG:HB3	2:D:247:TRP:HE1	1.86	0.40
2:D:8:PHE:O	2:D:55:ILE:HG23	2.22	0.40
2:B:423:LYS:O	2:B:424:HIS:C	2.59	0.40
2:D:176:GLY:O	2:D:299:ILE:HG23	2.22	0.40
2:D:511:TYR:CD1	2:D:513:GLN:HB2	2.57	0.40
2:B:423:LYS:HD3	2:B:424:HIS:CE1	2.57	0.40
1:C:120:CYS:HB3	1:C:122:MET:HE3	2.03	0.40
2:B:1:ALA:HA	2:B:2:GLU:HA	1.52	0.40
2:D:315:MET:HG2	2:D:494:TYR:OH	2.21	0.40
2:D:76:ARG:HB3	2:D:247:TRP:NE1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:GLU:O	2:B:453:GLU:O[3_555]	2.14	0.06

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	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	C	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
2	B	510/528 (97%)	490 (96%)	18 (4%)	2 (0%)	34	67
2	D	510/528 (97%)	490 (96%)	19 (4%)	1 (0%)	47	78
All	All	1282/1344 (95%)	1231 (96%)	48 (4%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	290	VAL
2	B	337	ALA
2	B	338	ILE

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	107/117 (92%)	86 (80%)	21 (20%)	1	4
1	C	107/117 (92%)	84 (78%)	23 (22%)	1	3
2	B	451/464 (97%)	338 (75%)	113 (25%)	0	2
2	D	451/464 (97%)	359 (80%)	92 (20%)	1	3
All	All	1116/1162 (96%)	867 (78%)	249 (22%)	1	2

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	14	LEU
1	A	15	SER
1	A	21	VAL
1	A	41	CYS
1	A	42	VAL
1	A	44	MET
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	47	THR
1	A	51	THR
1	A	55	ILE
1	A	64	ASP
1	A	67	SER
1	A	74	CYS
1	A	76	TYR
1	A	92	LEU
1	A	98	GLN
1	A	103	CYS
1	A	117	CYS
1	A	123	TRP
1	A	130	CYS
2	B	5	THR
2	B	7	LEU
2	B	16	THR
2	B	18	LEU
2	B	21	THR
2	B	22	GLN
2	B	27	LEU
2	B	31	ILE
2	B	32	LYS
2	B	47	LYS
2	B	49	MET
2	B	50	THR
2	B	56	SER
2	B	60	PHE
2	B	62	MET
2	B	63	ASN
2	B	71	ASN
2	B	72	MET
2	B	75	THR
2	B	84	ARG
2	B	87	ILE
2	B	95	HIS
2	B	97	THR
2	B	99	ASP
2	B	105	LEU
2	B	112	SER
2	B	113	THR
2	B	118	VAL
2	B	126	ASP

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Mol	Chain	Res	Type
2	B	128	GLU
2	B	129	ASN
2	B	131	THR
2	B	135	ARG
2	B	137	ASN
2	B	147	LYS
2	B	152	LEU
2	B	157	LEU
2	B	163	ARG
2	B	164	ILE
2	B	170	LEU
2	B	172	ASP
2	B	181	VAL
2	B	184	VAL
2	B	185	LEU
2	B	188	HIS
2	B	192	LEU
2	B	193	THR
2	B	197	TYR
2	B	200	LYS
2	B	208	CYS
2	B	209	LEU
2	B	210	CYS
2	B	212	LYS
2	B	220	SER
2	B	223	THR
2	B	229	HIS
2	B	230	SER
2	B	231	VAL
2	B	246	GLN
2	B	254	GLN
2	B	260	HIS
2	B	262	GLN
2	B	264	HIS
2	B	268	HIS
2	B	273	ASP
2	B	277	THR
2	B	278	ARG
2	B	289	ARG
2	B	292	TRP
2	B	295	GLU
2	B	299	ILE

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Mol	Chain	Res	Type
2	B	303	LEU
2	B	306	ASN
2	B	309	CYS
2	B	315	MET
2	B	332	ILE
2	B	336	LYS
2	B	341	VAL
2	B	354	GLN
2	B	367	PHE
2	B	372	THR
2	B	390	ASP
2	B	391	ARG
2	B	395	ASN
2	B	406	LEU
2	B	409	LEU
2	B	410	ASN
2	B	414	CYS
2	B	422	ASN
2	B	423	LYS
2	B	426	PHE
2	B	428	THR
2	B	434	SER
2	B	437	THR
2	B	449	ASP
2	B	452	CYS
2	B	453	GLU
2	B	465	TYR
2	B	468	LEU
2	B	472	THR
2	B	473	CYS
2	B	477	CYS
2	B	483	VAL
2	B	485	ARG
2	B	487	HIS
2	B	490	GLU
2	B	500	MET
2	B	501	MET
2	B	508	LEU
2	B	511	TYR
2	B	523	PHE
2	B	524	THR
2	B	525	ARG

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Mol	Chain	Res	Type
1	C	0	SER
1	C	3	ASN
1	C	5	THR
1	C	7	VAL
1	C	29	ASP
1	C	33	SER
1	C	41	CYS
1	C	43	LYS
1	C	46	CYS
1	C	47	THR
1	C	51	THR
1	C	53	GLN
1	C	58	THR
1	C	62	ASN
1	C	81	ILE
1	C	92	LEU
1	C	93	LYS
1	C	98	GLN
1	C	108	VAL
1	C	113	ARG
1	C	118	THR
1	C	123	TRP
1	C	128	CYS
2	D	3	ASN
2	D	5	THR
2	D	7	LEU
2	D	15	ILE
2	D	16	THR
2	D	22	GLN
2	D	31	ILE
2	D	38	LEU
2	D	48	ASP
2	D	57	MET
2	D	61	LYS
2	D	62	MET
2	D	75	THR
2	D	76	ARG
2	D	77	GLU
2	D	84	ARG
2	D	98	ARG
2	D	99	ASP
2	D	105	LEU

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Mol	Chain	Res	Type
2	D	115	VAL
2	D	120	VAL
2	D	122	THR
2	D	128	GLU
2	D	129	ASN
2	D	145	GLN
2	D	150	ILE
2	D	153	MET
2	D	157	LEU
2	D	169	MET
2	D	174	LEU
2	D	177	LEU
2	D	181	VAL
2	D	185	LEU
2	D	188	HIS
2	D	192	LEU
2	D	196	LYS
2	D	200	LYS
2	D	201	ILE
2	D	206	THR
2	D	215	THR
2	D	219	THR
2	D	242	ILE
2	D	244	VAL
2	D	250	THR
2	D	253	LEU
2	D	259	GLN
2	D	262	GLN
2	D	271	SER
2	D	273	ASP
2	D	280	LEU
2	D	282	VAL
2	D	287	VAL
2	D	292	TRP
2	D	298	ILE
2	D	303	LEU
2	D	315	MET
2	D	332	ILE
2	D	340	CYS
2	D	349	LYS
2	D	350	PHE
2	D	351	TYR

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Mol	Chain	Res	Type
2	D	362	LYS
2	D	363	ILE
2	D	365	GLU
2	D	366	LEU
2	D	376	LYS
2	D	383	LEU
2	D	387	CYS
2	D	389	VAL
2	D	399	CYS
2	D	400	ARG
2	D	406	LEU
2	D	408	ASN
2	D	409	LEU
2	D	415	ASP
2	D	431	PHE
2	D	439	LEU
2	D	449	ASP
2	D	465	TYR
2	D	468	LEU
2	D	472	THR
2	D	475	THR
2	D	476	ARG
2	D	479	LEU
2	D	484	CYS
2	D	485	ARG
2	D	499	ASN
2	D	502	ILE
2	D	507	SER
2	D	516	THR
2	D	519	LEU
2	D	522	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
2	B	256	ASN
2	B	257	HIS
2	B	260	HIS
2	B	314	HIS
2	B	424	HIS
2	B	487	HIS

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Mol	Chain	Res	Type
1	C	40	ASN
1	C	83	HIS
2	D	148	HIS
2	D	229	HIS
2	D	257	HIS
2	D	334	ASN
2	D	354	GLN
2	D	424	HIS

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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	133/144 (92%)	0.40	13 (9%) 7 9	117, 183, 230, 256	0
1	C	133/144 (92%)	0.06	5 (3%) 40 39	106, 158, 206, 226	0
2	B	514/528 (97%)	0.06	6 (1%) 79 77	91, 142, 194, 231	0
2	D	514/528 (97%)	0.18	14 (2%) 54 53	93, 138, 209, 310	0
All	All	1294/1344 (96%)	0.14	38 (2%) 51 50	91, 146, 209, 310	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TRP	5.2
1	A	126	TYR	4.6
1	A	125	GLY	4.6
2	D	525	ARG	3.9
2	B	525	ARG	3.8
2	D	436	PHE	3.6
1	A	122	MET	3.5
2	B	524	THR	3.3
1	C	123	TRP	3.2
1	A	131	ASP	3.2
1	A	54	ALA	3.0
2	B	446	TYR	3.0
1	A	116	VAL	2.8
1	A	45	LEU	2.8
2	B	488	ALA	2.8
2	D	417	GLY	2.7
2	D	430	ALA	2.6
2	D	431	PHE	2.5
1	C	116	VAL	2.5
1	A	101	THR	2.4
2	D	250	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	432	ASP	2.3
2	D	1	ALA	2.3
1	A	99	ILE	2.3
1	C	124	LYS	2.2
2	B	447	TYR	2.2
2	D	371	ALA	2.2
2	D	418	SER	2.2
1	C	99	ILE	2.2
1	A	127	GLY	2.1
1	C	-1	GLY	2.1
2	D	86	TRP	2.1
1	A	55	ILE	2.1
2	B	424	HIS	2.1
2	D	351	TYR	2.1
1	A	124	LYS	2.0
2	D	280	LEU	2.0
2	D	416	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	604	1/1	0.83	0.39	132,132,132,132	0
4	MG	D	604	1/1	0.87	0.15	151,151,151,151	0
3	ZN	B	603	1/1	0.95	0.10	147,147,147,147	0
3	ZN	B	601	1/1	0.96	0.13	225,225,225,225	0
3	ZN	C	202	1/1	0.97	0.06	184,184,184,184	0
3	ZN	A	202	1/1	0.97	0.05	261,261,261,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	ZN	D	602	1/1	0.98	0.06	183,183,183,183	0
3	ZN	A	201	1/1	0.99	0.14	215,215,215,215	0
3	ZN	C	201	1/1	0.99	0.15	132,132,132,132	0
3	ZN	D	603	1/1	0.99	0.09	117,117,117,117	0
3	ZN	B	602	1/1	0.99	0.11	160,160,160,160	0
3	ZN	D	601	1/1	0.99	0.18	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.