Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 02:59 PM EST

PDB ID	:	3IWM
Title	:	The octameric SARS-CoV main protease
Authors	:	Zhong, N.; Zhang, S.; Xue, F.; Lou, Z.; Rao, Z.; Xia, B.
Deposited on	:	2009-09-02
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

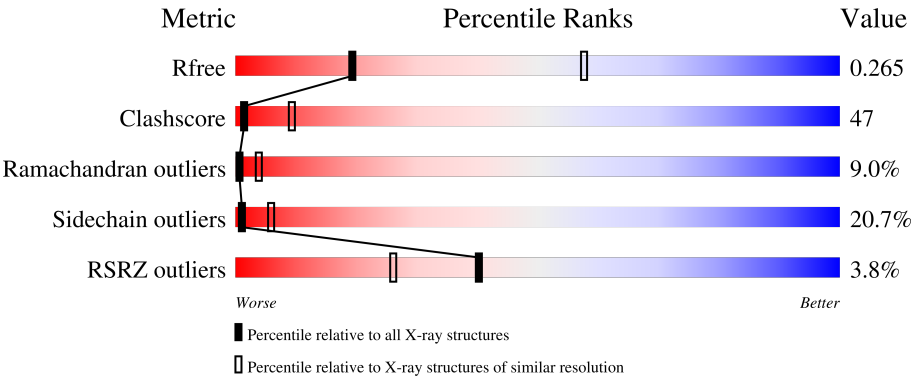
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 of 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	306	2% 34% 50% 12%
1	B	306	2% 36% 46% 14%
1	C	306	34% 47% 14%
1	D	306	11% 31% 47% 19%
2	E	6	17% 17% 50% 33%

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Mol	Chain	Length	Quality of chain
2	F	6	17% 67% 17%
2	G	6	50% 33% 17%
2	H	6	17% 67% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	02J	E	1	-	-	-	X
2	PJE	E	5	X	X	-	-
2	PJE	G	5	X	-	-	-
2	02J	H	1	-	-	-	X
2	PJE	H	5	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9512 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2332	1474	399	437	22			
1	B	301	Total	C	N	O	S	0	0	0
			2332	1474	399	437	22			
1	C	300	Total	C	N	O	S	0	0	0
			2326	1471	398	435	22			
1	D	300	Total	C	N	O	S	0	0	0
			2326	1471	398	435	22			

- Molecule 2 is a protein called N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE.

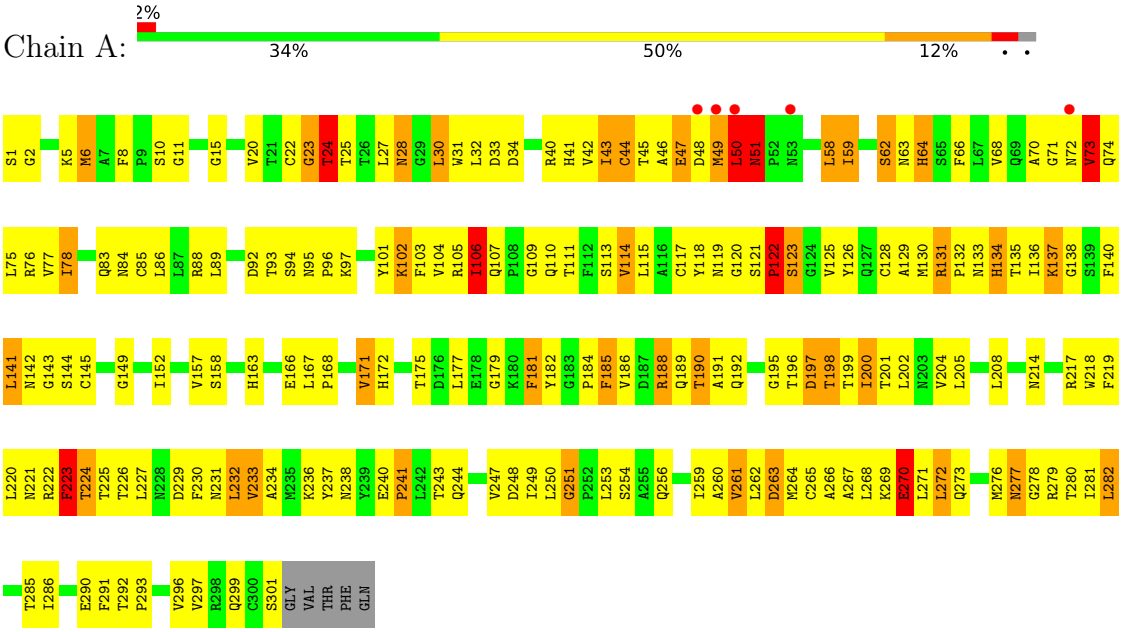
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	F	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	G	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	E	6	Total	C	N	O	0	0	0
			49	35	6	8			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

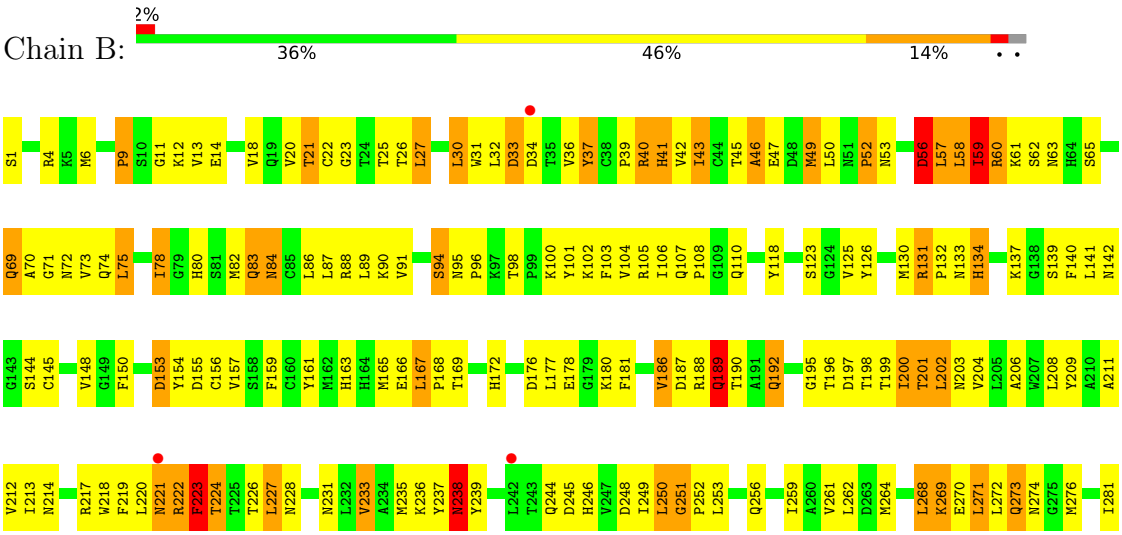
• Molecule 1: 3C-like proteinase

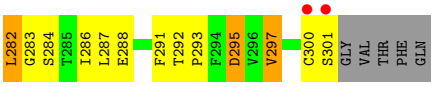
Chain A:



• Molecule 1: 3C-like proteinase

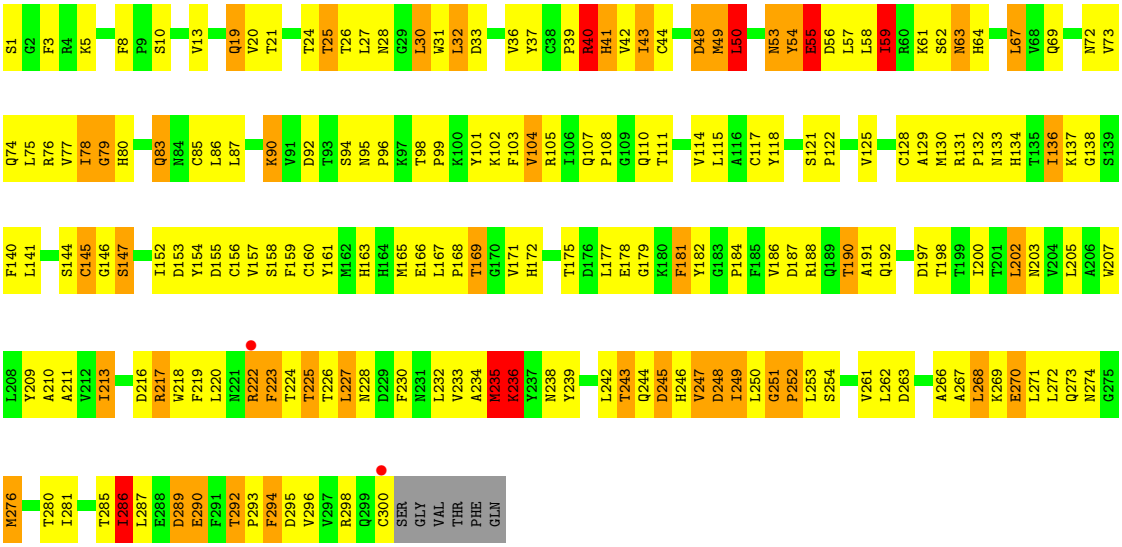
Chain B:





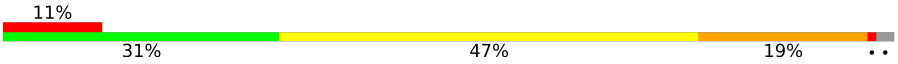
• Molecule 1: 3C-like proteinase

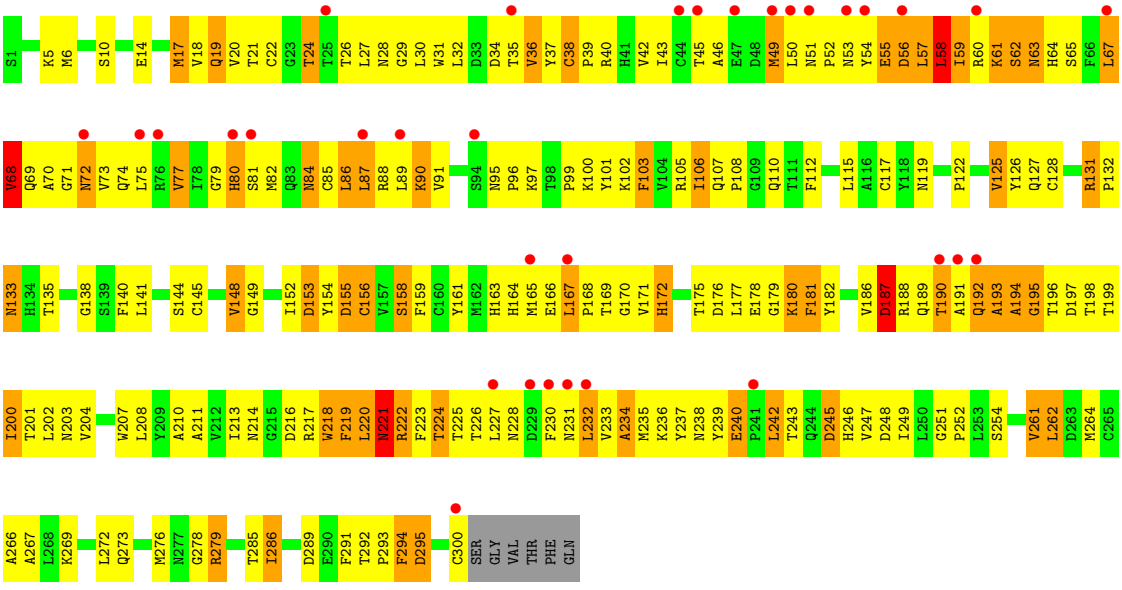
Chain C:



• Molecule 1: 3C-like proteinase

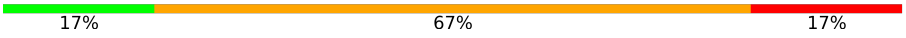
Chain D:

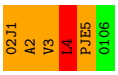




• Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE

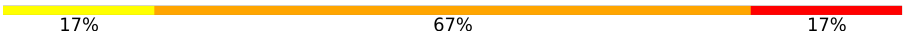
Chain H:





• Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE

Chain F:

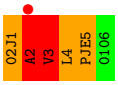


• Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE

Chain G:

• Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	161.93Å 161.93Å 166.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 3.20 48.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.94-3.20) 80.8 (48.94-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.220 , 0.272 0.214 , 0.265	Depositor DCC
R_{free} test set	1849 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	99.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 77.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.006 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9512	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 010, PJE, 02J

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	0.47	0/2384	0.70	0/3239
1	B	0.46	0/2384	0.72	0/3239
1	C	0.50	1/2378 (0.0%)	0.71	1/3231 (0.0%)
1	D	0.42	0/2378	0.69	1/3231 (0.0%)
2	E	2.21	2/19 (10.5%)	2.17	0/25
2	F	2.10	2/19 (10.5%)	1.85	0/25
2	G	2.19	2/19 (10.5%)	1.62	0/25
2	H	2.13	2/19 (10.5%)	1.83	0/25
All	All	0.50	9/9600 (0.1%)	0.72	2/13040 (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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	1
2	E	1	1
2	F	0	2
2	G	1	3
2	H	1	1
All	All	3	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	VAL	C-N	6.08	1.48	1.34
2	E	3	VAL	C-N	5.94	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	ALA	C-N	5.87	1.47	1.34
2	F	2	ALA	C-N	5.73	1.47	1.34
2	G	2	ALA	C-N	5.66	1.47	1.34
2	H	2	ALA	C-N	5.65	1.47	1.34
2	F	3	VAL	C-N	5.64	1.47	1.34
2	H	3	VAL	C-N	5.61	1.47	1.34
1	C	145	CYS	CB-SG	-5.30	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	59	ILE	N-CA-C	-6.30	94.00	111.00
1	C	217	ARG	N-CA-C	5.09	124.73	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	5	PJE	C26
2	G	5	PJE	CA
2	E	5	PJE	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	PHE	Peptide
1	A	71	GLY	Peptide
1	B	222	ARG	Peptide
1	B	59	ILE	Peptide
1	C	50	LEU	Peptide
1	C	59	ILE	Peptide
1	D	58	LEU	Peptide
2	E	2	ALA	Mainchain
2	F	2	ALA	Mainchain
2	F	3	VAL	Mainchain
2	G	3	VAL	Peptide
2	G	4	LEU	Peptide,Mainchain
2	H	2	ALA	Mainchain

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	2332	0	2286	260	0
1	B	2332	0	2286	236	0
1	C	2326	0	2281	225	0
1	D	2326	0	2281	259	0
2	E	49	0	41	10	0
2	F	49	0	40	13	0
2	G	49	0	40	7	0
2	H	49	0	40	13	0
All	All	9512	0	9295	888	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (888) 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:D:191:ALA:HA	2:E:2:ALA:HB3	1.26	1.14
1:D:106:ILE:HD11	1:D:110:GLN:HB2	1.31	1.09
1:B:83:GLN:HG3	1:B:88:ARG:HH12	0.93	1.07
1:D:50:LEU:HA	1:D:189:GLN:HB3	1.37	1.05
1:A:270:GLU:HA	1:A:273:GLN:H	1.27	1.00
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.44	1.00
1:A:122:PRO:O	1:A:123:SER:HB3	1.61	0.97
1:B:83:GLN:HG3	1:B:88:ARG:NH1	1.79	0.96
1:C:166:GLU:HG3	1:C:172:HIS:CD2	2.00	0.96
1:C:40:ARG:O	1:C:42:VAL:N	2.00	0.94
1:C:166:GLU:HG3	1:C:172:HIS:HD2	1.30	0.92
1:D:161:TYR:HE1	1:D:163:HIS:HB2	1.35	0.91
1:D:166:GLU:HB2	2:E:5:PJE:O8	1.72	0.90
1:A:279:ARG:HG2	1:A:280:THR:H	1.37	0.89
1:B:145:CYS:SG	2:F:5:PJE:C20	2.61	0.89
1:B:33:ASP:O	1:B:94:SER:HA	1.74	0.88
1:C:40:ARG:HD3	1:C:85:CYS:HA	1.56	0.86
1:A:167:LEU:HD11	1:A:185:PHE:CE1	2.10	0.86
1:B:83:GLN:O	1:B:84:ASN:HB2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:LEU:HB3	1:D:168:PRO:HD2	1.58	0.85
1:A:201:THR:HG22	1:C:239:TYR:HD2	1.42	0.85
1:D:18:VAL:HG12	1:D:70:ALA:HB2	1.58	0.84
1:B:63:ASN:OD1	1:B:80:HIS:HD2	1.60	0.84
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.59	0.84
1:C:230:PHE:HZ	1:C:268:LEU:HD12	1.41	0.84
1:C:59:ILE:HD12	1:C:61:LYS:O	1.76	0.84
1:B:282:LEU:HD21	1:D:211:ALA:HA	1.58	0.84
1:B:203:ASN:HB3	1:D:291:PHE:O	1.77	0.83
1:B:221:ASN:OD1	1:D:267:ALA:HA	1.78	0.83
1:C:31:TRP:HB2	1:C:36:VAL:HG22	1.61	0.82
1:A:222:ARG:HD2	1:C:270:GLU:HG2	1.61	0.82
1:D:154:TYR:O	1:D:156:CYS:N	2.12	0.82
1:C:63:ASN:HD21	1:C:79:GLY:N	1.76	0.82
1:A:129:ALA:CB	1:C:290:GLU:HG3	2.10	0.81
1:A:107:GLN:O	1:A:110:GLN:HG3	1.80	0.81
1:A:201:THR:HG22	1:C:239:TYR:CD2	2.15	0.81
1:D:145:CYS:HB2	2:E:5:PJE:O	1.80	0.81
1:C:230:PHE:CZ	1:C:268:LEU:HD12	2.16	0.81
1:B:145:CYS:SG	2:F:5:PJE:C21	2.68	0.81
1:C:178:GLU:OE1	1:C:178:GLU:HA	1.80	0.80
1:B:189:GLN:HE21	2:F:3:VAL:HA	1.47	0.80
1:A:291:PHE:CZ	1:C:5:LYS:HG3	2.15	0.80
1:A:254:SER:OG	1:A:260:ALA:HA	1.82	0.79
1:A:41:HIS:CD2	2:H:4:LEU:HD23	2.17	0.79
1:D:67:LEU:HD11	1:D:69:GLN:HB2	1.62	0.79
1:C:145:CYS:SG	2:G:5:PJE:C20	2.72	0.78
1:D:21:THR:HB	1:D:67:LEU:HB3	1.66	0.78
1:D:279:ARG:HH11	1:D:279:ARG:CG	1.97	0.78
1:A:276:MET:SD	1:A:281:ILE:HD12	2.24	0.77
1:D:279:ARG:HH11	1:D:279:ARG:HG3	1.49	0.77
1:D:168:PRO:HD3	2:E:2:ALA:HB2	1.67	0.77
1:A:102:LYS:NZ	1:A:102:LYS:HA	1.99	0.77
1:B:268:LEU:CD2	1:B:272:LEU:HG	2.15	0.77
1:A:145:CYS:SG	2:H:5:PJE:C25	2.73	0.77
1:D:87:LEU:HD12	1:D:89:LEU:HD21	1.67	0.76
1:A:201:THR:CG2	1:C:239:TYR:HB3	2.15	0.76
1:B:25:THR:HA	2:F:6:010:H4	1.65	0.76
1:A:102:LYS:HA	1:A:102:LYS:CE	2.15	0.76
1:C:103:PHE:CE1	1:C:177:LEU:HB3	2.21	0.76
1:B:202:LEU:HD11	1:D:249:ILE:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASN:ND2	1:A:188:ARG:HE	1.84	0.75
1:B:198:THR:HA	1:D:238:ASN:ND2	2.02	0.75
1:D:145:CYS:SG	2:E:5:PJE:C20	2.75	0.75
1:D:217:ARG:O	1:D:217:ARG:HG2	1.85	0.74
1:B:221:ASN:HB2	1:D:223:PHE:CG	2.22	0.74
1:A:247:VAL:CG1	1:A:261:VAL:HG21	2.17	0.74
1:D:58:LEU:HB2	1:D:61:LYS:H	1.52	0.74
1:C:243:THR:HG23	1:C:246:HIS:CD2	2.23	0.74
1:B:78:ILE:HG12	1:B:78:ILE:O	1.88	0.74
1:B:223:PHE:O	1:B:224:THR:OG1	2.05	0.74
1:A:129:ALA:HB3	1:C:290:GLU:HG3	1.67	0.73
1:D:50:LEU:HD23	1:D:189:GLN:O	1.88	0.73
1:C:108:PRO:HB3	1:C:132:PRO:HA	1.69	0.73
1:D:103:PHE:CE1	1:D:177:LEU:HB3	2.23	0.73
1:B:238:ASN:HB2	1:D:198:THR:HG22	1.71	0.73
1:C:246:HIS:O	1:C:250:LEU:HD12	1.88	0.72
1:D:22:CYS:SG	1:D:43:ILE:HA	2.29	0.72
1:A:200:ILE:HG13	1:C:289:ASP:OD2	1.90	0.72
1:D:40:ARG:O	1:D:40:ARG:HG2	1.87	0.72
2:H:3:VAL:HG12	2:H:3:VAL:O	1.88	0.72
1:B:246:HIS:HB3	1:D:202:LEU:HD13	1.71	0.72
1:D:221:ASN:O	1:D:223:PHE:N	2.22	0.72
1:A:225:THR:HG22	1:A:262:LEU:O	1.90	0.72
1:C:138:GLY:O	1:C:172:HIS:HE1	1.73	0.71
1:A:290:GLU:HG3	1:C:129:ALA:HB2	1.72	0.71
1:C:10:SER:HB2	1:C:115:LEU:HD13	1.73	0.71
1:C:186:VAL:HG22	1:C:188:ARG:NH1	2.06	0.71
1:C:13:VAL:HG12	1:C:115:LEU:HD22	1.73	0.71
1:D:245:ASP:O	1:D:249:ILE:HG23	1.90	0.71
1:B:59:ILE:O	1:B:60:ARG:HB3	1.88	0.70
1:A:23:GLY:O	1:A:24:THR:HB	1.88	0.70
1:B:37:TYR:HB3	1:B:86:LEU:HD13	1.72	0.70
1:B:237:TYR:OH	1:B:273:GLN:HB3	1.89	0.70
1:C:90:LYS:NZ	1:C:90:LYS:HB3	2.06	0.70
1:B:40:ARG:O	1:B:42:VAL:N	2.23	0.70
1:B:118:TYR:OH	1:B:141:LEU:HB2	1.91	0.70
1:D:20:VAL:HG12	1:D:42:VAL:HG21	1.73	0.70
1:D:86:LEU:HD21	1:D:179:GLY:HA2	1.73	0.70
1:D:108:PRO:HB3	1:D:132:PRO:HA	1.72	0.70
1:D:106:ILE:HD11	1:D:110:GLN:CB	2.16	0.70
1:B:189:GLN:NE2	2:F:3:VAL:HA	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:TRP:CE2	1:C:95:ASN:HB2	2.27	0.70
1:C:247:VAL:HG12	1:C:261:VAL:HG21	1.73	0.70
1:A:223:PHE:CE2	1:C:270:GLU:CB	2.75	0.69
1:B:231:ASN:O	1:B:235:MET:HG2	1.91	0.69
1:D:63:ASN:H	1:D:80:HIS:CE1	2.10	0.69
1:B:25:THR:HA	2:F:6:010:C4	2.22	0.69
1:B:30:LEU:HG	1:B:148:VAL:HG11	1.75	0.69
1:A:27:LEU:HG	1:A:42:VAL:HG23	1.74	0.69
1:B:203:ASN:OD1	1:D:292:THR:HA	1.92	0.69
1:B:281:ILE:CD1	1:D:219:PHE:CE2	2.76	0.69
1:B:200:ILE:HD12	1:D:289:ASP:OD2	1.93	0.69
1:C:21:THR:HB	1:C:67:LEU:HB3	1.74	0.69
1:C:32:LEU:HD12	1:C:37:TYR:HE2	1.56	0.69
1:A:223:PHE:CE2	1:C:270:GLU:HB2	2.28	0.68
1:B:131:ARG:HD3	1:B:137:LYS:NZ	2.09	0.68
1:D:58:LEU:HA	1:D:60:ARG:H	1.56	0.68
1:A:43:ILE:HD13	1:A:58:LEU:HD23	1.75	0.68
1:D:294:PHE:HD2	1:D:294:PHE:C	1.96	0.68
1:A:220:LEU:O	1:C:222:ARG:HD3	1.93	0.68
1:C:244:GLN:O	1:C:247:VAL:HG23	1.94	0.68
1:A:200:ILE:O	1:A:204:VAL:HG23	1.94	0.68
1:D:191:ALA:HA	2:E:2:ALA:CB	2.14	0.68
1:D:279:ARG:NH1	1:D:279:ARG:HB2	2.08	0.68
1:C:253:LEU:HD12	1:C:253:LEU:H	1.58	0.68
2:E:3:VAL:HG13	2:E:4:LEU:O	1.93	0.68
1:B:239:TYR:CD1	1:D:199:THR:HB	2.29	0.67
1:B:43:ILE:HG12	1:B:43:ILE:O	1.94	0.67
1:C:243:THR:HG23	1:C:246:HIS:CG	2.28	0.67
2:H:3:VAL:O	2:H:4:LEU:C	2.32	0.67
1:A:118:TYR:CE1	1:A:144:SER:HB3	2.29	0.67
1:D:58:LEU:HD23	1:D:61:LYS:HE2	1.76	0.67
1:B:78:ILE:HD13	1:B:90:LYS:O	1.95	0.67
1:A:101:TYR:O	1:A:102:LYS:HE2	1.93	0.67
1:C:175:THR:HG22	1:C:181:PHE:HA	1.75	0.67
1:D:58:LEU:HD12	1:D:58:LEU:O	1.95	0.67
2:H:1:02J:O	2:H:3:VAL:HG23	1.95	0.67
1:A:202:LEU:HD12	1:A:202:LEU:O	1.93	0.67
1:B:86:LEU:O	1:B:87:LEU:HD23	1.95	0.67
1:C:292:THR:HG23	1:C:295:ASP:CG	2.15	0.67
1:A:270:GLU:CA	1:A:273:GLN:H	2.06	0.66
1:D:21:THR:OG1	1:D:67:LEU:HD23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD13	1:A:51:ASN:N	2.10	0.66
1:D:58:LEU:HB3	1:D:61:LYS:HD3	1.76	0.66
1:A:49:MET:HG2	1:A:50:LEU:N	2.09	0.66
1:D:186:VAL:HB	1:D:188:ARG:HG3	1.78	0.66
1:B:250:LEU:HD13	1:D:202:LEU:HD11	1.78	0.66
1:A:269:LYS:O	1:A:269:LYS:HG2	1.95	0.66
1:B:227:LEU:HD13	1:B:228:ASN:N	2.11	0.66
1:B:271:LEU:HD21	1:B:287:LEU:HD21	1.77	0.66
1:D:140:PHE:HB3	1:D:144:SER:OG	1.95	0.66
1:A:41:HIS:O	1:A:44:CYS:HB2	1.96	0.65
1:B:223:PHE:CZ	1:B:269:LYS:HD3	2.31	0.65
1:D:231:ASN:O	1:D:234:ALA:HB3	1.96	0.65
1:C:245:ASP:HA	1:C:248:ASP:OD1	1.96	0.65
1:D:57:LEU:O	1:D:60:ARG:HB2	1.96	0.65
1:A:140:PHE:CZ	1:A:163:HIS:HD2	2.15	0.65
1:C:247:VAL:CG1	1:C:261:VAL:HG21	2.27	0.64
1:C:251:GLY:O	1:C:254:SER:HB3	1.97	0.64
1:D:193:ALA:O	1:D:194:ALA:HB2	1.98	0.64
1:A:102:LYS:HZ2	1:A:103:PHE:H	1.45	0.64
1:B:281:ILE:CD1	1:D:219:PHE:HE2	2.11	0.64
1:D:246:HIS:O	1:D:249:ILE:HG13	1.98	0.64
1:A:259:ILE:HG21	1:C:220:LEU:HD11	1.80	0.64
1:D:27:LEU:CD1	1:D:39:PRO:HD2	2.28	0.64
1:B:288:GLU:HB2	1:D:207:TRP:CE2	2.33	0.63
1:C:118:TYR:CE1	1:C:141:LEU:HB2	2.34	0.63
1:A:63:ASN:ND2	1:A:77:VAL:O	2.32	0.63
1:C:181:PHE:HE1	1:C:187:ASP:HB3	1.63	0.63
1:B:166:GLU:HB2	2:F:5:PJE:O8	1.98	0.63
1:A:28:ASN:H	1:A:28:ASN:ND2	1.96	0.63
1:B:107:GLN:HB2	1:B:110:GLN:NE2	2.13	0.63
1:D:89:LEU:O	1:D:91:VAL:HG13	1.99	0.63
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.79	0.63
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.81	0.63
1:C:117:CYS:HB3	1:C:122:PRO:HA	1.80	0.63
1:A:282:LEU:CD1	1:C:211:ALA:HA	2.29	0.63
1:D:31:TRP:CE2	1:D:95:ASN:HB2	2.34	0.63
1:A:202:LEU:HD12	1:A:202:LEU:C	2.19	0.62
1:D:58:LEU:HD21	1:D:80:HIS:NE2	2.14	0.62
1:D:225:THR:HG22	1:D:266:ALA:HB2	1.81	0.62
1:A:129:ALA:HB2	1:C:290:GLU:HG3	1.82	0.62
1:B:108:PRO:HB3	1:B:132:PRO:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HB3	1:A:137:LYS:NZ	2.13	0.62
1:A:222:ARG:O	1:A:223:PHE:HB2	1.99	0.62
1:B:69:GLN:HE22	1:B:71:GLY:C	2.02	0.62
1:D:249:ILE:C	1:D:249:ILE:HD12	2.20	0.62
1:B:49:MET:SD	1:B:49:MET:N	2.72	0.62
1:C:28:ASN:HB2	1:C:146:GLY:HA3	1.82	0.62
1:B:83:GLN:O	1:B:84:ASN:CB	2.47	0.62
1:A:270:GLU:HA	1:A:273:GLN:N	2.08	0.62
1:D:294:PHE:C	1:D:294:PHE:CD2	2.69	0.62
1:A:73:VAL:CG2	1:A:73:VAL:O	2.48	0.62
1:A:122:PRO:HB3	1:B:9:PRO:HG2	1.81	0.62
1:D:168:PRO:HA	2:E:1:02J:O	1.99	0.62
1:C:50:LEU:H	1:C:50:LEU:HD23	1.65	0.62
1:A:201:THR:HG23	1:C:239:TYR:HB3	1.80	0.62
1:C:32:LEU:HD12	1:C:37:TYR:CE2	2.34	0.61
1:C:202:LEU:O	1:C:202:LEU:HG	2.01	0.61
1:C:54:TYR:O	1:C:56:ASP:N	2.29	0.61
1:B:37:TYR:N	1:B:37:TYR:CD2	2.67	0.61
1:B:40:ARG:HH11	1:B:82:MET:CE	2.13	0.61
1:B:45:THR:O	1:B:46:ALA:HB3	2.00	0.61
1:D:57:LEU:C	1:D:61:LYS:HZ2	2.03	0.61
1:D:161:TYR:CE1	1:D:163:HIS:HB2	2.26	0.61
1:A:292:THR:HA	1:C:203:ASN:OD1	2.01	0.61
1:B:52:PRO:HD2	1:B:188:ARG:CZ	2.30	0.61
1:D:86:LEU:CD2	1:D:179:GLY:HA2	2.30	0.61
1:A:264:MET:O	1:A:267:ALA:HB3	2.01	0.61
1:C:186:VAL:HG22	1:C:188:ARG:HH11	1.65	0.61
1:D:55:GLU:CD	1:D:55:GLU:H	2.03	0.61
1:A:230:PHE:HZ	1:A:268:LEU:HD23	1.66	0.61
1:C:63:ASN:HD21	1:C:79:GLY:H	1.44	0.61
1:B:4:ARG:HH11	1:B:4:ARG:HB3	1.66	0.60
1:B:40:ARG:HH11	1:B:82:MET:HE3	1.66	0.60
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.01	0.60
1:B:188:ARG:O	1:B:190:THR:N	2.34	0.60
1:A:20:VAL:HG12	1:A:42:VAL:HG21	1.83	0.60
1:C:33:ASP:O	1:C:94:SER:HA	2.01	0.60
1:C:253:LEU:HD12	1:C:253:LEU:N	2.16	0.60
1:D:58:LEU:CB	1:D:61:LYS:HD3	2.30	0.60
1:A:50:LEU:HD13	1:A:51:ASN:H	1.66	0.60
1:C:132:PRO:HD2	1:C:197:ASP:OD1	2.02	0.60
1:D:286:ILE:HD12	1:D:286:ILE:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HG2	1:A:280:THR:N	2.14	0.60
1:B:201:THR:HG23	1:B:202:LEU:N	2.16	0.60
1:D:58:LEU:HB3	1:D:61:LYS:NZ	2.17	0.60
1:A:50:LEU:HD22	1:A:51:ASN:HB2	1.83	0.60
1:A:63:ASN:HD21	1:A:78:ILE:C	2.05	0.60
1:B:53:ASN:O	1:B:57:LEU:HB2	2.02	0.60
1:B:221:ASN:HB2	1:D:223:PHE:CD1	2.35	0.60
1:D:242:LEU:HB2	1:D:246:HIS:ND1	2.17	0.59
1:B:133:ASN:HD22	1:B:197:ASP:HB2	1.66	0.59
1:D:279:ARG:HH11	1:D:279:ARG:CB	2.15	0.59
1:A:45:THR:O	1:A:47:GLU:N	2.32	0.59
1:A:223:PHE:CZ	1:C:270:GLU:HB2	2.36	0.59
1:B:140:PHE:HD1	1:B:172:HIS:CD2	2.20	0.59
1:B:293:PRO:O	1:B:297:VAL:HG23	2.03	0.59
1:A:102:LYS:NZ	1:A:103:PHE:H	1.99	0.59
1:C:294:PHE:C	1:C:296:VAL:N	2.55	0.59
1:B:221:ASN:H	1:B:221:ASN:ND2	1.98	0.59
1:D:233:VAL:HG11	1:D:269:LYS:HG3	1.85	0.59
1:A:122:PRO:O	1:A:123:SER:CB	2.44	0.58
1:B:217:ARG:O	1:B:220:LEU:HB2	2.02	0.58
1:D:218:TRP:CD1	1:D:218:TRP:C	2.76	0.58
1:A:145:CYS:SG	2:H:5:PJE:CA	2.91	0.58
1:A:145:CYS:SG	2:H:5:PJE:C20	2.92	0.58
1:A:102:LYS:HA	1:A:102:LYS:HE2	1.85	0.58
1:D:6:MET:HG3	1:D:6:MET:O	2.04	0.58
1:A:95:ASN:OD1	1:A:97:LYS:HG3	2.03	0.58
1:A:201:THR:CG2	1:C:239:TYR:HD2	2.15	0.58
1:A:270:GLU:CB	1:A:273:GLN:HB2	2.33	0.58
1:B:104:VAL:CG1	1:B:105:ARG:N	2.66	0.58
1:C:41:HIS:O	1:C:44:CYS:HB2	2.04	0.58
1:C:54:TYR:HD1	1:C:54:TYR:H	1.52	0.58
1:C:78:ILE:O	1:C:90:LYS:HB2	2.04	0.58
1:C:200:ILE:HG21	1:C:203:ASN:ND2	2.19	0.58
1:D:10:SER:O	1:D:14:GLU:HG3	2.04	0.57
1:A:230:PHE:CZ	1:A:268:LEU:HD23	2.38	0.57
1:A:293:PRO:O	1:A:297:VAL:HG23	2.03	0.57
1:D:102:LYS:NZ	1:D:158:SER:HB2	2.20	0.57
1:D:138:GLY:H	1:D:172:HIS:CE1	2.22	0.57
1:D:148:VAL:HA	1:D:161:TYR:O	2.04	0.57
1:A:270:GLU:HA	1:A:273:GLN:HG3	1.86	0.57
1:A:290:GLU:HG3	1:C:129:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:C	1:B:61:LYS:H	2.06	0.57
1:D:80:HIS:O	1:D:80:HIS:CD2	2.57	0.57
1:D:152:ILE:HG22	1:D:153:ASP:N	2.19	0.57
1:A:45:THR:C	1:A:47:GLU:H	2.07	0.57
1:A:248:ASP:O	1:A:251:GLY:N	2.36	0.57
1:A:261:VAL:HG23	1:A:262:LEU:H	1.69	0.57
1:B:201:THR:CG2	1:B:202:LEU:N	2.67	0.57
1:C:223:PHE:N	1:C:223:PHE:CD1	2.73	0.57
1:D:88:ARG:O	1:D:89:LEU:HD23	2.04	0.57
1:C:63:ASN:ND2	1:C:77:VAL:O	2.38	0.57
1:D:19:GLN:NE2	1:D:26:THR:HG21	2.19	0.57
1:D:58:LEU:HD12	1:D:58:LEU:C	2.23	0.57
1:B:73:VAL:HG12	1:B:74:GLN:O	2.05	0.57
1:B:203:ASN:CB	1:D:291:PHE:O	2.50	0.57
1:D:63:ASN:O	1:D:65:SER:N	2.35	0.57
1:B:30:LEU:HD13	1:B:32:LEU:HD11	1.86	0.57
1:D:18:VAL:CG1	1:D:70:ALA:HB2	2.33	0.57
1:D:148:VAL:HG21	1:D:159:PHE:CD1	2.40	0.57
1:D:286:ILE:HD12	1:D:286:ILE:N	2.20	0.57
1:A:24:THR:HG22	1:A:25:THR:HG23	1.87	0.57
1:A:138:GLY:O	1:A:172:HIS:HE1	1.88	0.57
1:B:59:ILE:O	1:B:60:ARG:CB	2.53	0.57
1:A:133:ASN:O	1:A:134:HIS:HB2	2.05	0.56
1:A:279:ARG:HD2	1:C:218:TRP:CD2	2.40	0.56
1:A:291:PHE:CE1	1:C:3:PHE:CE2	2.92	0.56
1:A:70:ALA:O	1:A:73:VAL:HG13	2.05	0.56
1:A:198:THR:HG22	1:C:238:ASN:OD1	2.05	0.56
1:B:100:LYS:NZ	1:B:156:CYS:HB2	2.19	0.56
1:A:104:VAL:HG13	1:A:158:SER:HB2	1.87	0.56
1:B:141:LEU:HD11	1:C:300:CYS:HA	1.88	0.56
1:B:268:LEU:HD21	1:B:272:LEU:HG	1.86	0.56
1:D:217:ARG:O	1:D:217:ARG:CG	2.53	0.56
1:D:154:TYR:C	1:D:156:CYS:H	2.08	0.56
1:B:75:LEU:HD13	1:B:91:VAL:HG11	1.87	0.56
1:B:145:CYS:SG	2:F:5:PJE:C25	2.93	0.56
1:A:140:PHE:CE2	1:A:163:HIS:HD2	2.24	0.56
1:D:249:ILE:CD1	1:D:293:PRO:HG3	2.35	0.56
1:C:114:VAL:O	1:C:125:VAL:HG23	2.06	0.56
1:D:58:LEU:HD13	1:D:62:SER:CA	2.36	0.56
1:B:233:VAL:HG11	1:B:269:LYS:HG3	1.87	0.56
1:C:186:VAL:CG2	1:C:188:ARG:NH1	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:02J:O	2:F:3:VAL:HG23	2.06	0.56
1:A:50:LEU:HD22	1:A:51:ASN:CB	2.36	0.56
1:B:39:PRO:C	1:B:40:ARG:O	2.40	0.56
1:D:168:PRO:HA	2:E:1:02J:C	2.36	0.56
1:C:145:CYS:SG	2:G:5:PJE:C21	2.93	0.56
1:C:161:TYR:HE2	1:C:163:HIS:HB2	1.70	0.56
1:D:52:PRO:HD2	1:D:188:ARG:NH2	2.21	0.56
1:D:79:GLY:O	1:D:80:HIS:HB3	2.06	0.56
1:C:252:PRO:HB2	1:C:253:LEU:HD12	1.88	0.55
1:D:131:ARG:HB3	1:D:197:ASP:OD2	2.06	0.55
1:B:104:VAL:HG12	1:B:105:ARG:N	2.21	0.55
1:D:164:HIS:CD2	1:D:175:THR:HG23	2.41	0.55
1:A:140:PHE:CD2	1:A:163:HIS:CD2	2.95	0.55
1:B:282:LEU:HG	1:D:211:ALA:HB2	1.87	0.55
1:D:169:THR:O	1:D:171:VAL:N	2.38	0.55
1:A:72:ASN:O	1:A:73:VAL:C	2.44	0.55
1:A:83:GLN:HG3	1:A:88:ARG:NH2	2.22	0.55
1:A:280:THR:HG22	1:A:285:THR:HG22	1.89	0.55
1:C:157:VAL:HG11	1:C:159:PHE:CZ	2.41	0.55
1:D:19:GLN:HE21	1:D:26:THR:HG21	1.71	0.55
1:A:5:LYS:NZ	1:B:4:ARG:HH22	2.05	0.55
1:C:233:VAL:HG22	1:C:233:VAL:O	2.06	0.55
1:C:40:ARG:HG2	1:C:85:CYS:O	2.07	0.55
1:C:145:CYS:SG	2:G:5:PJE:CA	2.95	0.55
1:D:234:ALA:O	1:D:236:LYS:N	2.40	0.55
1:D:239:TYR:O	1:D:240:GLU:O	2.25	0.55
1:B:291:PHE:CZ	1:D:5:LYS:HG3	2.41	0.55
1:D:233:VAL:HG13	1:D:273:GLN:HE21	1.71	0.54
1:A:197:ASP:O	1:A:198:THR:HG23	2.07	0.54
1:C:276:MET:HE1	1:C:281:ILE:HG13	1.87	0.54
1:D:88:ARG:C	1:D:89:LEU:HD23	2.27	0.54
1:A:33:ASP:O	1:A:94:SER:HA	2.08	0.54
1:B:281:ILE:HD11	1:D:219:PHE:CE2	2.42	0.54
1:A:102:LYS:HA	1:A:102:LYS:HZ3	1.71	0.54
1:B:187:ASP:N	1:B:187:ASP:OD1	2.32	0.54
1:C:83:GLN:HG3	1:C:83:GLN:O	2.06	0.54
1:B:58:LEU:HD21	1:B:82:MET:HB2	1.89	0.54
1:B:198:THR:HG22	1:D:238:ASN:OD1	2.08	0.54
1:C:58:LEU:HD11	1:C:80:HIS:HD2	1.73	0.54
1:A:41:HIS:CG	2:H:4:LEU:HD23	2.43	0.54
1:B:281:ILE:O	1:B:282:LEU:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:O	1:A:106:ILE:O	2.26	0.53
1:A:184:PRO:HD2	1:A:185:PHE:CE2	2.42	0.53
1:C:10:SER:HB2	1:C:115:LEU:CD1	2.38	0.53
1:C:293:PRO:O	1:C:294:PHE:HB2	2.08	0.53
1:B:105:ARG:NH1	1:B:176:ASP:OD2	2.41	0.53
1:D:27:LEU:HD11	1:D:39:PRO:HD2	1.91	0.53
1:D:74:GLN:O	1:D:75:LEU:HD23	2.08	0.53
1:A:254:SER:HA	1:C:209:TYR:CE2	2.43	0.53
1:D:115:LEU:HD11	1:D:122:PRO:HB3	1.91	0.53
2:H:3:VAL:O	2:H:3:VAL:CG1	2.55	0.53
1:A:113:SER:O	1:A:149:GLY:HA2	2.09	0.53
1:A:282:LEU:HD13	1:C:211:ALA:HA	1.90	0.53
1:B:223:PHE:O	1:B:224:THR:CB	2.55	0.53
1:A:62:SER:OG	1:A:63:ASN:N	2.41	0.53
1:B:253:LEU:HD12	1:B:253:LEU:H	1.73	0.53
1:D:58:LEU:HA	1:D:60:ARG:HB2	1.91	0.53
1:A:222:ARG:HD3	1:C:267:ALA:CB	2.39	0.53
1:C:225:THR:HG22	1:C:266:ALA:HB2	1.90	0.53
1:D:18:VAL:HG12	1:D:70:ALA:CB	2.37	0.53
1:D:20:VAL:CG1	1:D:42:VAL:HG21	2.37	0.53
1:B:133:ASN:ND2	1:B:197:ASP:HB2	2.24	0.53
1:D:24:THR:HG21	1:D:45:THR:HG23	1.89	0.53
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.44	0.53
1:A:222:ARG:HD3	1:C:267:ALA:HA	1.90	0.53
1:A:230:PHE:C	1:A:230:PHE:CD2	2.82	0.53
1:A:247:VAL:HG12	1:A:261:VAL:HG21	1.88	0.53
1:D:58:LEU:HB3	1:D:61:LYS:CE	2.39	0.53
1:A:23:GLY:O	1:A:24:THR:CB	2.55	0.52
1:A:101:TYR:HA	1:A:157:VAL:O	2.09	0.52
1:B:206:ALA:HB1	1:D:293:PRO:HA	1.90	0.52
1:B:221:ASN:CB	1:D:223:PHE:CG	2.92	0.52
1:D:34:ASP:O	1:D:90:LYS:HA	2.08	0.52
1:A:73:VAL:O	1:A:73:VAL:HG22	2.09	0.52
1:A:135:THR:HG21	1:A:171:VAL:HG21	1.91	0.52
1:A:140:PHE:CG	1:A:163:HIS:CD2	2.97	0.52
1:B:200:ILE:O	1:B:204:VAL:HG23	2.08	0.52
1:B:282:LEU:HD12	1:D:207:TRP:NE1	2.24	0.52
1:C:40:ARG:HA	1:C:87:LEU:HG	1.92	0.52
1:D:194:ALA:O	1:D:195:GLY:O	2.26	0.52
1:D:279:ARG:HH11	1:D:279:ARG:HB2	1.72	0.52
1:A:30:LEU:HD22	1:A:32:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:HB3	1:B:4:ARG:NH1	2.24	0.52
1:B:40:ARG:C	1:B:42:VAL:H	2.13	0.52
1:D:36:VAL:HG12	1:D:36:VAL:O	2.09	0.52
1:D:227:LEU:HD11	1:D:231:ASN:ND2	2.24	0.52
1:A:261:VAL:HG23	1:A:262:LEU:N	2.25	0.52
1:B:249:ILE:O	1:B:252:PRO:HD2	2.10	0.52
1:D:19:GLN:HE21	1:D:26:THR:CG2	2.23	0.52
1:D:193:ALA:O	1:D:194:ALA:CB	2.56	0.52
1:A:262:LEU:HA	1:A:265:CYS:HB2	1.90	0.52
1:A:223:PHE:HE2	1:C:270:GLU:CB	2.23	0.52
1:D:58:LEU:HB3	1:D:61:LYS:CD	2.40	0.52
1:D:233:VAL:CG1	1:D:273:GLN:HE21	2.23	0.52
1:D:234:ALA:C	1:D:236:LYS:H	2.13	0.52
1:B:103:PHE:CE1	1:B:177:LEU:HB3	2.45	0.52
1:A:51:ASN:HD22	1:A:188:ARG:HH21	1.58	0.52
1:A:279:ARG:HD2	1:C:218:TRP:CG	2.45	0.52
1:C:243:THR:O	1:C:247:VAL:HG22	2.11	0.51
1:D:89:LEU:O	1:D:90:LYS:C	2.48	0.51
1:C:59:ILE:HA	1:C:61:LYS:O	2.09	0.51
1:A:49:MET:CG	1:A:50:LEU:N	2.74	0.51
1:A:114:VAL:HG11	1:A:126:TYR:CZ	2.45	0.51
1:A:220:LEU:O	1:A:222:ARG:HG3	2.10	0.51
1:B:33:ASP:H	1:B:98:THR:HG21	1.76	0.51
1:B:186:VAL:O	1:B:192:GLN:NE2	2.43	0.51
1:B:287:LEU:HA	1:D:207:TRP:CZ3	2.45	0.51
1:C:8:PHE:HB3	1:C:152:ILE:HD12	1.92	0.51
1:C:63:ASN:ND2	1:C:79:GLY:N	2.54	0.51
1:B:40:ARG:HD2	1:B:82:MET:SD	2.50	0.51
1:B:107:GLN:HB2	1:B:110:GLN:HE21	1.76	0.51
1:B:161:TYR:CE2	1:B:163:HIS:HB2	2.46	0.51
1:B:288:GLU:HB2	1:D:207:TRP:CD2	2.46	0.51
1:D:106:ILE:CD1	1:D:110:GLN:HB2	2.22	0.51
1:C:55:GLU:HA	1:C:58:LEU:HB3	1.91	0.51
1:C:101:TYR:HE1	1:C:103:PHE:CE2	2.28	0.51
1:C:171:VAL:HG12	1:C:172:HIS:H	1.75	0.51
1:C:105:ARG:HG3	1:C:182:TYR:HE2	1.74	0.51
1:C:225:THR:OG1	1:C:226:THR:N	2.43	0.51
1:D:17:MET:CE	1:D:148:VAL:HG12	2.41	0.51
1:A:140:PHE:CE2	1:A:163:HIS:CD2	2.99	0.51
1:B:238:ASN:O	1:B:238:ASN:ND2	2.44	0.51
1:B:288:GLU:O	1:D:204:VAL:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:C	1:B:154:TYR:CD2	2.84	0.51
1:B:208:LEU:O	1:B:211:ALA:HB3	2.11	0.51
1:D:52:PRO:HD2	1:D:188:ARG:CZ	2.41	0.51
1:D:133:ASN:HB3	1:D:197:ASP:HB2	1.93	0.51
1:A:230:PHE:O	1:A:233:VAL:HG23	2.11	0.51
1:A:254:SER:HA	1:C:209:TYR:HE2	1.75	0.51
1:A:111:THR:HG23	1:C:292:THR:HG22	1.92	0.50
1:A:270:GLU:HB2	1:A:273:GLN:HB2	1.94	0.50
1:C:31:TRP:HB2	1:C:36:VAL:CG2	2.36	0.50
1:C:242:LEU:HD13	1:C:243:THR:N	2.25	0.50
1:D:61:LYS:O	1:D:62:SER:C	2.49	0.50
1:A:8:PHE:CD1	1:A:152:ILE:HB	2.46	0.50
1:B:226:THR:C	1:B:228:ASN:N	2.65	0.50
1:D:223:PHE:O	1:D:224:THR:C	2.50	0.50
1:A:227:LEU:HD23	1:A:231:ASN:ND2	2.27	0.50
1:C:153:ASP:O	1:C:154:TYR:HB2	2.11	0.50
1:B:52:PRO:HD2	1:B:188:ARG:NE	2.27	0.50
1:B:268:LEU:O	1:B:269:LYS:C	2.49	0.50
1:C:73:VAL:HG12	1:C:75:LEU:HD23	1.93	0.50
1:C:102:LYS:HD3	1:C:156:CYS:SG	2.51	0.50
1:A:28:ASN:ND2	1:A:28:ASN:N	2.56	0.50
1:B:103:PHE:CD1	1:B:177:LEU:HB3	2.47	0.50
1:C:48:ASP:O	1:C:50:LEU:N	2.44	0.50
1:A:28:ASN:ND2	1:A:145:CYS:O	2.43	0.50
1:A:126:TYR:HB3	1:B:6:MET:HB3	1.94	0.50
1:A:224:THR:HB	1:A:263:ASP:OD2	2.12	0.50
1:C:161:TYR:CE2	1:C:163:HIS:HB2	2.47	0.50
1:A:1:SER:HB3	1:B:166:GLU:OE1	2.11	0.50
1:B:200:ILE:HD12	1:D:289:ASP:CG	2.32	0.50
1:C:111:THR:HG22	1:C:129:ALA:HA	1.94	0.50
1:D:58:LEU:HD13	1:D:62:SER:HA	1.94	0.50
1:A:208:LEU:HD22	1:A:219:PHE:CE1	2.47	0.50
1:C:105:ARG:HG3	1:C:182:TYR:CE2	2.46	0.50
1:A:250:LEU:O	1:A:251:GLY:C	2.50	0.49
1:B:233:VAL:HG23	1:B:237:TYR:HE1	1.77	0.49
1:D:276:MET:HG2	1:D:279:ARG:H	1.77	0.49
1:D:294:PHE:HD2	1:D:294:PHE:O	1.95	0.49
1:B:45:THR:O	1:B:46:ALA:CB	2.59	0.49
1:B:62:SER:OG	1:B:63:ASN:N	2.45	0.49
1:D:105:ARG:HD2	1:D:176:ASP:OD2	2.11	0.49
1:B:295:ASP:OD1	1:B:295:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HG21	1:B:264:MET:HE1	1.95	0.49
1:C:54:TYR:N	1:C:54:TYR:CD1	2.79	0.49
1:A:64:HIS:C	1:A:66:PHE:H	2.16	0.49
1:C:244:GLN:HA	1:C:247:VAL:CG2	2.42	0.49
1:A:72:ASN:O	1:A:74:GLN:N	2.45	0.49
1:A:28:ASN:H	1:A:28:ASN:HD22	1.60	0.49
1:B:108:PRO:CB	1:B:132:PRO:HA	2.43	0.49
1:B:161:TYR:HE2	1:B:163:HIS:HB2	1.78	0.49
1:C:67:LEU:HD12	1:C:69:GLN:HG3	1.95	0.49
1:C:130:MET:HA	1:C:136:ILE:HG22	1.94	0.49
1:D:225:THR:O	1:D:262:LEU:HD22	2.12	0.49
1:A:296:VAL:HG11	1:C:210:ALA:HB2	1.95	0.49
1:B:58:LEU:HA	1:B:61:LYS:HG3	1.95	0.49
1:B:239:TYR:CE1	1:D:199:THR:HB	2.47	0.49
1:D:77:VAL:HA	1:D:91:VAL:HG12	1.93	0.49
1:D:242:LEU:HD23	1:D:242:LEU:O	2.13	0.49
1:A:282:LEU:HD11	1:C:211:ALA:HA	1.95	0.49
1:B:36:VAL:HG22	1:B:89:LEU:HB2	1.94	0.49
1:B:200:ILE:HD13	1:D:289:ASP:O	2.13	0.49
1:C:31:TRP:CB	1:C:36:VAL:HG22	2.40	0.49
1:C:49:MET:CE	2:G:6:010:H1	2.43	0.49
1:C:62:SER:O	1:C:64:HIS:N	2.46	0.49
1:C:207:TRP:O	1:C:210:ALA:HB3	2.12	0.49
1:B:49:MET:O	1:B:52:PRO:HG3	2.13	0.48
1:B:201:THR:CG2	1:B:202:LEU:H	2.26	0.48
1:B:300:CYS:O	1:B:301:SER:C	2.51	0.48
1:C:227:LEU:O	1:C:230:PHE:N	2.37	0.48
1:D:61:LYS:HB2	1:D:65:SER:OG	2.13	0.48
2:F:3:VAL:O	2:F:4:LEU:C	2.51	0.48
1:A:167:LEU:N	1:A:167:LEU:HD23	2.28	0.48
1:A:279:ARG:HD2	1:C:218:TRP:CE2	2.48	0.48
1:A:281:ILE:HG23	1:C:211:ALA:HB1	1.94	0.48
1:C:101:TYR:CE1	1:C:103:PHE:CE2	3.01	0.48
1:C:285:THR:O	1:C:286:ILE:C	2.49	0.48
1:D:59:ILE:HD12	1:D:62:SER:OG	2.13	0.48
1:A:131:ARG:HE	1:A:131:ARG:HA	1.78	0.48
1:B:49:MET:CE	1:B:50:LEU:HB2	2.44	0.48
1:C:48:ASP:C	1:C:50:LEU:HD23	2.33	0.48
1:C:55:GLU:O	1:C:58:LEU:O	2.31	0.48
1:D:40:ARG:HA	1:D:87:LEU:CD2	2.43	0.48
1:D:220:LEU:O	1:D:222:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:CG2	1:A:25:THR:N	2.76	0.48
1:A:243:THR:O	1:A:247:VAL:HG23	2.13	0.48
1:B:209:TYR:OH	1:D:261:VAL:HA	2.13	0.48
1:D:186:VAL:C	1:D:188:ARG:H	2.17	0.48
1:B:52:PRO:HD2	1:B:188:ARG:NH2	2.28	0.48
1:B:233:VAL:O	1:B:237:TYR:HD1	1.97	0.48
1:B:246:HIS:CD2	1:B:246:HIS:H	2.32	0.48
1:D:40:ARG:HD2	1:D:82:MET:SD	2.54	0.48
1:D:133:ASN:C	1:D:133:ASN:OD1	2.52	0.48
1:D:31:TRP:CD1	1:D:31:TRP:C	2.87	0.48
1:D:106:ILE:HD13	1:D:107:GLN:N	2.29	0.48
1:D:230:PHE:O	1:D:234:ALA:N	2.47	0.48
1:B:101:TYR:O	1:B:102:LYS:HB3	2.14	0.47
1:B:223:PHE:CZ	1:B:269:LYS:CE	2.97	0.47
1:C:78:ILE:HD11	1:C:92:ASP:CA	2.44	0.47
1:A:217:ARG:HB2	1:A:220:LEU:HD12	1.95	0.47
1:D:153:ASP:CG	1:D:153:ASP:O	2.51	0.47
1:A:85:CYS:HB2	1:A:179:GLY:O	2.14	0.47
1:C:118:TYR:CZ	1:C:141:LEU:HB2	2.49	0.47
1:C:292:THR:HG23	1:C:295:ASP:OD2	2.14	0.47
1:A:66:PHE:HB2	1:A:77:VAL:HG21	1.96	0.47
1:A:231:ASN:HA	1:A:234:ALA:HB3	1.96	0.47
1:C:54:TYR:C	1:C:55:GLU:HG3	2.35	0.47
1:C:188:ARG:HH11	1:C:188:ARG:HB3	1.79	0.47
1:D:105:ARG:NH1	1:D:180:LYS:O	2.43	0.47
1:D:207:TRP:O	1:D:210:ALA:HB3	2.15	0.47
1:B:218:TRP:CE3	1:B:219:PHE:HA	2.49	0.47
1:B:237:TYR:O	1:B:239:TYR:N	2.48	0.47
1:C:190:THR:C	1:C:192:GLN:H	2.17	0.47
1:D:279:ARG:NH1	1:D:279:ARG:CB	2.75	0.47
1:A:188:ARG:HB2	1:A:190:THR:HG22	1.97	0.47
1:A:261:VAL:O	1:A:265:CYS:N	2.44	0.47
1:C:218:TRP:CG	1:C:219:PHE:N	2.83	0.47
1:A:92:ASP:OD1	1:A:93:THR:HG23	2.14	0.47
1:A:133:ASN:O	1:A:134:HIS:CB	2.61	0.47
1:A:201:THR:CG2	1:C:239:TYR:CD2	2.93	0.47
1:A:299:GLN:HG2	1:A:299:GLN:O	2.14	0.47
1:B:37:TYR:H	1:B:37:TYR:HD2	1.63	0.47
1:C:145:CYS:SG	2:G:5:PJE:C25	3.03	0.47
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.15	0.47
1:C:181:PHE:CE1	1:C:187:ASP:HB3	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:MET:CE	1:C:281:ILE:HG13	2.44	0.47
1:D:18:VAL:HG22	1:D:29:GLY:O	2.15	0.47
1:D:161:TYR:HE1	1:D:163:HIS:CB	2.18	0.47
1:D:232:LEU:HD12	1:D:233:VAL:N	2.30	0.47
1:D:237:TYR:N	1:D:237:TYR:CD1	2.82	0.47
1:C:43:ILE:O	1:C:43:ILE:HG13	2.14	0.47
1:D:101:TYR:O	1:D:101:TYR:CD1	2.67	0.47
1:A:141:LEU:HD11	1:D:300:CYS:HA	1.96	0.47
1:A:224:THR:HB	1:A:263:ASP:CG	2.35	0.47
1:C:48:ASP:C	1:C:50:LEU:H	2.18	0.47
1:D:58:LEU:HA	1:D:60:ARG:N	2.26	0.47
1:D:249:ILE:HD11	1:D:293:PRO:HG3	1.96	0.47
1:A:201:THR:O	1:A:202:LEU:C	2.54	0.46
1:B:133:ASN:O	1:B:134:HIS:HB2	2.14	0.46
1:B:237:TYR:O	1:B:238:ASN:C	2.53	0.46
1:B:238:ASN:CB	1:D:198:THR:HG22	2.42	0.46
1:D:32:LEU:HD13	1:D:101:TYR:CE2	2.50	0.46
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.77	0.46
1:D:101:TYR:CD1	1:D:101:TYR:C	2.89	0.46
1:A:31:TRP:CZ2	1:A:75:LEU:HD21	2.51	0.46
1:C:86:LEU:HG	1:C:179:GLY:CA	2.46	0.46
1:D:43:ILE:HD12	1:D:57:LEU:HD23	1.97	0.46
1:B:133:ASN:HB2	1:B:195:GLY:O	2.15	0.46
1:B:165:MET:HA	2:F:4:LEU:HA	1.96	0.46
1:C:39:PRO:O	1:C:40:ARG:O	2.34	0.46
1:D:102:LYS:HG3	1:D:156:CYS:SG	2.55	0.46
1:A:5:LYS:HZ3	1:B:4:ARG:HH22	1.64	0.46
1:A:140:PHE:CD1	1:A:163:HIS:CD2	3.04	0.46
1:C:286:ILE:HD12	1:C:287:LEU:N	2.31	0.46
1:D:63:ASN:C	1:D:65:SER:H	2.18	0.46
1:A:50:LEU:O	1:A:51:ASN:HB2	2.16	0.46
1:A:114:VAL:HG11	1:A:126:TYR:CE1	2.51	0.46
1:A:166:GLU:OE1	1:B:1:SER:OG	2.33	0.46
1:B:58:LEU:O	1:B:59:ILE:HG22	2.15	0.46
1:B:118:TYR:CZ	1:B:141:LEU:HB2	2.49	0.46
1:D:28:ASN:ND2	1:D:117:CYS:O	2.48	0.46
1:A:131:ARG:NH2	1:C:289:ASP:OD2	2.49	0.46
1:D:237:TYR:CE2	1:D:272:LEU:O	2.69	0.46
1:A:40:ARG:O	1:A:43:ILE:HG12	2.16	0.46
1:A:138:GLY:O	1:A:172:HIS:CE1	2.68	0.46
1:A:140:PHE:CG	1:A:163:HIS:NE2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:C	1:B:220:LEU:H	2.19	0.46
1:C:86:LEU:HG	1:C:179:GLY:HA2	1.97	0.46
1:C:103:PHE:CD1	1:C:177:LEU:HB3	2.51	0.46
1:C:235:MET:SD	1:C:235:MET:N	2.83	0.46
1:D:27:LEU:HD13	1:D:39:PRO:HD2	1.97	0.46
1:A:103:PHE:CD1	1:A:177:LEU:HB3	2.51	0.46
1:A:133:ASN:C	1:A:134:HIS:CD2	2.89	0.46
1:A:192:GLN:H	1:A:192:GLN:HG2	1.49	0.46
1:B:60:ARG:CB	1:B:60:ARG:HH11	2.29	0.46
1:B:276:MET:HE2	1:B:281:ILE:HG12	1.98	0.46
1:C:30:LEU:CD1	1:C:32:LEU:HD11	2.46	0.46
1:C:218:TRP:CD2	1:C:219:PHE:N	2.84	0.46
1:D:56:ASP:OD2	1:D:56:ASP:N	2.48	0.46
1:B:223:PHE:HZ	1:B:269:LYS:CE	2.28	0.46
1:A:141:LEU:CD1	1:D:300:CYS:HA	2.46	0.45
1:B:239:TYR:HB3	1:D:201:THR:OG1	2.15	0.45
1:A:25:THR:HG21	1:A:44:CYS:O	2.16	0.45
1:A:104:VAL:CG1	1:A:158:SER:HB2	2.46	0.45
1:A:111:THR:HA	1:A:128:CYS:O	2.16	0.45
1:A:277:ASN:O	1:A:279:ARG:N	2.48	0.45
1:B:31:TRP:HE1	1:B:91:VAL:HG21	1.80	0.45
1:C:67:LEU:HD12	1:C:69:GLN:CG	2.46	0.45
1:D:67:LEU:HG	1:D:68:VAL:N	2.31	0.45
1:A:121:SER:HA	1:A:122:PRO:HD2	1.59	0.45
1:A:205:LEU:HB2	1:C:250:LEU:HD21	1.97	0.45
1:A:266:ALA:O	1:A:269:LYS:HB3	2.17	0.45
1:B:39:PRO:O	1:B:40:ARG:O	2.34	0.45
1:B:103:PHE:N	1:B:103:PHE:CD2	2.84	0.45
1:C:209:TYR:O	1:C:213:ILE:HG12	2.16	0.45
1:D:43:ILE:CD1	1:D:57:LEU:HD23	2.47	0.45
1:B:33:ASP:O	1:B:94:SER:CA	2.57	0.45
1:B:150:PHE:N	1:B:150:PHE:CD2	2.84	0.45
1:A:141:LEU:HD23	1:A:142:ASN:H	1.81	0.45
1:A:226:THR:OG1	1:A:229:ASP:HB2	2.16	0.45
1:C:83:GLN:O	1:C:83:GLN:CG	2.64	0.45
1:A:201:THR:O	1:A:204:VAL:N	2.47	0.45
1:A:279:ARG:HD2	1:C:218:TRP:CD1	2.52	0.45
1:C:165:MET:HB2	2:G:3:VAL:O	2.17	0.45
1:C:243:THR:O	1:C:246:HIS:HB2	2.15	0.45
1:A:218:TRP:CD2	1:A:219:PHE:N	2.85	0.45
1:A:268:LEU:HG	1:A:272:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:CZ	1:B:269:LYS:HE2	2.52	0.45
1:C:234:ALA:O	1:C:236:LYS:N	2.50	0.45
2:E:4:LEU:HB2	2:E:5:PJE:CA	2.45	0.45
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.46	0.45
1:A:270:GLU:HG2	1:C:223:PHE:CE2	2.52	0.45
1:A:281:ILE:CG2	1:C:211:ALA:CB	2.95	0.45
1:B:69:GLN:OE1	1:B:72:ASN:HA	2.17	0.45
1:B:244:GLN:O	1:B:244:GLN:HG3	2.16	0.45
1:C:58:LEU:HD12	1:C:58:LEU:HA	1.80	0.45
1:A:133:ASN:C	1:A:133:ASN:OD1	2.54	0.45
1:A:199:THR:HG22	1:A:200:ILE:N	2.31	0.45
1:D:63:ASN:H	1:D:80:HIS:HE1	1.61	0.45
1:D:239:TYR:O	1:D:240:GLU:C	2.54	0.45
2:F:3:VAL:O	2:F:3:VAL:HG12	2.17	0.45
1:B:103:PHE:CE1	1:B:177:LEU:O	2.70	0.45
1:C:31:TRP:CD2	1:C:95:ASN:HB2	2.51	0.45
1:C:54:TYR:O	1:C:55:GLU:HG3	2.17	0.45
1:C:270:GLU:HG3	1:C:271:LEU:N	2.31	0.45
1:A:59:ILE:HG23	1:A:59:ILE:O	2.16	0.44
1:C:25:THR:HG22	1:C:42:VAL:HG23	1.99	0.44
1:C:261:VAL:HG23	1:C:262:LEU:N	2.33	0.44
1:A:238:ASN:HD21	1:C:198:THR:HG22	1.82	0.44
1:A:268:LEU:HD22	1:C:205:LEU:HD23	1.98	0.44
1:C:58:LEU:HD12	1:C:59:ILE:H	1.82	0.44
1:D:70:ALA:O	1:D:72:ASN:N	2.49	0.44
1:D:102:LYS:O	1:D:103:PHE:HD2	2.00	0.44
1:D:106:ILE:HG22	1:D:182:TYR:OH	2.17	0.44
1:A:106:ILE:HG13	1:A:110:GLN:HB2	1.99	0.44
1:A:202:LEU:HD21	1:C:249:ILE:HG21	1.99	0.44
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.53	0.44
1:C:49:MET:HE1	2:G:6:010:H1	1.99	0.44
1:D:84:ASN:HB2	1:D:179:GLY:HA3	1.99	0.44
1:B:50:LEU:C	1:B:52:PRO:HD3	2.38	0.44
1:D:148:VAL:HG21	1:D:159:PHE:HD1	1.81	0.44
1:D:200:ILE:HG21	1:D:203:ASN:ND2	2.33	0.44
1:B:22:CYS:CB	1:B:65:SER:O	2.66	0.44
1:B:130:MET:HG3	1:B:130:MET:O	2.17	0.44
1:B:250:LEU:O	1:B:251:GLY:C	2.56	0.44
1:B:270:GLU:HG3	1:D:220:LEU:HD11	2.00	0.44
1:C:73:VAL:HG12	1:C:74:GLN:O	2.17	0.44
1:D:74:GLN:HG2	1:D:75:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:THR:OG1	1:D:295:ASP:OD1	2.32	0.44
1:B:30:LEU:HD12	1:B:177:LEU:CD1	2.47	0.44
1:B:101:TYR:HA	1:B:157:VAL:O	2.17	0.44
1:D:99:PRO:O	1:D:100:LYS:C	2.55	0.44
1:C:167:LEU:HB3	1:C:168:PRO:HD2	2.00	0.44
1:A:141:LEU:C	2:H:5:PJE:H11	2.37	0.44
1:A:237:TYR:CB	1:A:272:LEU:HD12	2.48	0.44
1:B:18:VAL:HG12	1:B:70:ALA:CB	2.48	0.44
1:B:27:LEU:C	1:B:27:LEU:HD12	2.38	0.44
1:D:232:LEU:C	1:D:234:ALA:N	2.69	0.44
2:H:1:02J:C	2:H:3:VAL:HG23	2.47	0.44
1:A:125:VAL:HG13	1:A:125:VAL:O	2.18	0.43
1:A:143:GLY:H	2:H:5:PJE:C21	2.31	0.43
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.76	0.43
1:A:268:LEU:C	1:A:270:GLU:H	2.20	0.43
1:B:37:TYR:N	1:B:37:TYR:HD2	2.14	0.43
1:B:238:ASN:O	1:B:238:ASN:CG	2.56	0.43
1:D:236:LYS:HE3	1:D:236:LYS:HB3	1.88	0.43
1:A:223:PHE:O	1:A:224:THR:CG2	2.66	0.43
1:B:221:ASN:ND2	1:B:221:ASN:N	2.65	0.43
1:B:300:CYS:O	1:B:301:SER:O	2.36	0.43
1:C:20:VAL:HG12	1:C:20:VAL:O	2.17	0.43
1:C:90:LYS:HB3	1:C:90:LYS:HZ3	1.83	0.43
1:A:265:CYS:O	1:A:269:LYS:HB2	2.19	0.43
1:B:165:MET:HE1	1:B:167:LEU:HD23	2.00	0.43
1:C:78:ILE:H	1:C:78:ILE:HG13	1.35	0.43
1:D:31:TRP:NE1	1:D:95:ASN:HB2	2.34	0.43
1:D:131:ARG:HE	1:D:131:ARG:HA	1.84	0.43
1:A:6:MET:HG2	1:B:126:TYR:HD2	1.84	0.43
1:A:230:PHE:O	1:A:233:VAL:N	2.51	0.43
1:B:56:ASP:OD2	1:B:56:ASP:C	2.57	0.43
1:B:88:ARG:HB2	1:B:88:ARG:CZ	2.47	0.43
1:D:88:ARG:HB2	1:D:88:ARG:HH11	1.83	0.43
1:D:251:GLY:O	1:D:254:SER:HB3	2.17	0.43
1:A:64:HIS:C	1:A:66:PHE:N	2.72	0.43
1:B:204:VAL:HG22	1:D:289:ASP:HB3	2.00	0.43
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.75	0.43
1:C:40:ARG:O	1:C:42:VAL:HG12	2.18	0.43
1:C:95:ASN:HA	1:C:96:PRO:HD2	1.73	0.43
1:D:37:TYR:N	1:D:37:TYR:CD2	2.86	0.43
1:D:58:LEU:HD13	1:D:62:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:CE3	1:B:219:PHE:N	2.86	0.43
1:C:78:ILE:HD11	1:C:92:ASP:HA	2.01	0.43
1:A:2:GLY:HA3	1:B:139:SER:HA	2.01	0.43
1:A:117:CYS:HA	1:A:122:PRO:O	2.18	0.43
1:A:223:PHE:HE2	1:C:270:GLU:HB3	1.83	0.43
1:C:53:ASN:ND2	1:C:56:ASP:HB2	2.33	0.43
1:D:22:CYS:HB3	1:D:42:VAL:O	2.18	0.43
1:D:220:LEU:HB3	1:D:221:ASN:H	1.50	0.43
1:D:292:THR:HB	1:D:293:PRO:HD2	2.00	0.43
1:B:60:ARG:NH1	1:B:60:ARG:HB2	2.34	0.43
1:B:133:ASN:C	1:B:133:ASN:OD1	2.57	0.43
1:B:223:PHE:CZ	1:B:269:LYS:CD	3.02	0.43
1:C:118:TYR:CE1	1:C:144:SER:HB3	2.54	0.43
1:C:227:LEU:HD11	1:C:242:LEU:HD12	2.00	0.43
1:C:243:THR:H	1:C:246:HIS:HB2	1.84	0.43
1:A:240:GLU:O	1:A:241:PRO:C	2.57	0.43
1:A:270:GLU:C	1:A:272:LEU:N	2.66	0.43
1:A:270:GLU:HB3	1:A:273:GLN:CG	2.49	0.43
1:B:50:LEU:O	1:B:52:PRO:HD3	2.18	0.43
1:C:118:TYR:OH	1:C:141:LEU:HB2	2.19	0.43
1:A:11:GLY:N	1:B:14:GLU:OE2	2.46	0.43
1:B:20:VAL:HG12	1:B:42:VAL:HG21	2.01	0.43
1:B:101:TYR:HB2	1:B:159:PHE:HE2	1.84	0.43
1:B:140:PHE:HB2	1:B:172:HIS:CD2	2.53	0.43
1:B:282:LEU:O	1:B:283:GLY:C	2.55	0.43
1:D:117:CYS:SG	1:D:122:PRO:HA	2.59	0.43
1:A:253:LEU:HD12	1:A:253:LEU:H	1.84	0.42
1:B:100:LYS:HZ3	1:B:156:CYS:HB2	1.82	0.42
1:D:213:ILE:O	1:D:213:ILE:HG22	2.18	0.42
1:A:64:HIS:O	1:A:64:HIS:CG	2.71	0.42
1:B:13:VAL:HG21	1:B:150:PHE:CG	2.54	0.42
1:D:22:CYS:CB	1:D:42:VAL:HG22	2.48	0.42
1:A:140:PHE:CE1	1:A:163:HIS:CD2	3.08	0.42
1:A:175:THR:HG22	1:A:181:PHE:CD1	2.54	0.42
1:B:226:THR:C	1:B:228:ASN:H	2.23	0.42
1:C:101:TYR:CE1	1:C:103:PHE:HE2	2.37	0.42
1:D:243:THR:O	1:D:246:HIS:HB2	2.20	0.42
1:D:249:ILE:HD13	1:D:293:PRO:HG3	2.01	0.42
1:A:2:GLY:N	1:A:214:ASN:OD1	2.52	0.42
1:A:230:PHE:CE2	1:A:234:ALA:HB2	2.54	0.42
1:A:277:ASN:C	1:A:279:ARG:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PHE:CG	1:B:163:HIS:CD2	3.08	0.42
1:C:236:LYS:HE3	1:C:236:LYS:HA	2.00	0.42
1:D:57:LEU:HB3	1:D:61:LYS:NZ	2.35	0.42
1:D:100:LYS:NZ	1:D:155:ASP:OD1	2.53	0.42
1:A:140:PHE:CD1	1:A:163:HIS:NE2	2.87	0.42
1:C:59:ILE:HD12	1:C:59:ILE:HA	1.89	0.42
1:C:117:CYS:H	1:C:147:SER:HB3	1.84	0.42
1:C:236:LYS:HA	1:C:236:LYS:CE	2.49	0.42
1:D:38:CYS:O	1:D:86:LEU:HB2	2.20	0.42
1:A:28:ASN:HB3	1:A:120:GLY:H	1.85	0.42
1:A:41:HIS:CG	2:H:4:LEU:CD2	3.03	0.42
1:A:95:ASN:HA	1:A:96:PRO:HD2	1.91	0.42
1:A:276:MET:HE3	1:A:285:THR:O	2.20	0.42
1:B:281:ILE:O	1:B:284:SER:N	2.53	0.42
1:C:33:ASP:C	1:C:94:SER:HA	2.40	0.42
1:D:46:ALA:O	1:D:49:MET:N	2.45	0.42
1:A:184:PRO:HD2	1:A:185:PHE:CD2	2.54	0.42
1:B:103:PHE:N	1:B:103:PHE:HD2	2.16	0.42
1:D:102:LYS:HZ1	1:D:158:SER:HB2	1.85	0.42
1:A:49:MET:CG	1:A:50:LEU:H	2.31	0.42
1:A:140:PHE:CE1	1:A:163:HIS:HD2	2.37	0.42
1:B:63:ASN:OD1	1:B:80:HIS:CD2	2.53	0.42
1:B:94:SER:O	1:B:96:PRO:HD3	2.20	0.42
1:B:218:TRP:CE3	1:B:219:PHE:CA	3.03	0.42
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.74	0.42
1:D:135:THR:HG21	1:D:171:VAL:HG21	2.00	0.42
1:D:247:VAL:HG13	1:D:261:VAL:HG21	2.02	0.42
1:A:133:ASN:OD1	1:A:135:THR:HG23	2.20	0.42
1:B:22:CYS:HB2	1:B:65:SER:O	2.20	0.42
1:B:30:LEU:O	1:B:36:VAL:HA	2.20	0.42
1:B:188:ARG:O	1:B:189:GLN:C	2.58	0.42
1:D:95:ASN:HA	1:D:96:PRO:HD2	1.87	0.42
1:D:187:ASP:OD1	1:D:187:ASP:N	2.44	0.42
1:A:6:MET:HE3	1:A:6:MET:HB3	1.85	0.42
1:A:166:GLU:O	1:A:166:GLU:HG2	2.19	0.42
1:A:227:LEU:CD2	1:A:231:ASN:ND2	2.83	0.42
1:B:201:THR:HB	1:D:239:TYR:O	2.19	0.42
1:C:103:PHE:CD1	1:C:177:LEU:CB	3.03	0.42
1:C:293:PRO:O	1:C:294:PHE:CB	2.68	0.42
1:D:54:TYR:O	1:D:56:ASP:N	2.53	0.42
1:D:213:ILE:O	1:D:213:ILE:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ASN:HD22	1:D:214:ASN:HA	1.72	0.42
1:A:240:GLU:HA	1:A:241:PRO:HD2	1.94	0.41
1:A:279:ARG:CG	1:A:280:THR:H	2.17	0.41
1:D:68:VAL:HG23	1:D:75:LEU:HB2	2.01	0.41
1:D:227:LEU:HD13	1:D:227:LEU:C	2.40	0.41
1:A:6:MET:HG2	1:B:126:TYR:CD2	2.55	0.41
1:A:24:THR:HG22	1:A:25:THR:N	2.35	0.41
1:B:32:LEU:O	1:B:34:ASP:N	2.53	0.41
1:B:58:LEU:CD2	1:B:82:MET:HB2	2.50	0.41
1:B:133:ASN:O	1:B:134:HIS:CB	2.68	0.41
1:B:141:LEU:O	1:B:144:SER:HB3	2.21	0.41
1:B:168:PRO:HB3	2:F:1:02J:C4	2.50	0.41
1:B:245:ASP:O	1:B:248:ASP:N	2.53	0.41
1:B:269:LYS:O	1:B:272:LEU:HB2	2.20	0.41
1:D:45:THR:O	1:D:45:THR:HG22	2.20	0.41
1:A:34:ASP:HB3	1:A:94:SER:OG	2.19	0.41
1:A:130:MET:HE1	1:A:182:TYR:CD1	2.55	0.41
1:C:98:THR:HA	1:C:99:PRO:HD3	1.87	0.41
1:D:17:MET:HG2	1:D:117:CYS:SG	2.60	0.41
1:D:112:PHE:O	1:D:112:PHE:CD1	2.73	0.41
1:B:59:ILE:C	1:B:61:LYS:N	2.72	0.41
1:B:227:LEU:HD13	1:B:227:LEU:C	2.40	0.41
1:C:294:PHE:C	1:C:296:VAL:H	2.23	0.41
1:D:68:VAL:HG23	1:D:68:VAL:O	2.19	0.41
1:D:196:THR:O	1:D:197:ASP:HB3	2.20	0.41
1:A:86:LEU:HG	1:A:179:GLY:HA2	2.03	0.41
1:B:30:LEU:HD12	1:B:177:LEU:HD13	2.02	0.41
1:B:100:LYS:HZ2	1:B:156:CYS:HB2	1.84	0.41
1:C:107:GLN:HB2	1:C:110:GLN:OE1	2.20	0.41
1:C:136:ILE:HG13	1:C:136:ILE:O	2.18	0.41
1:D:57:LEU:HB3	1:D:61:LYS:HZ2	1.85	0.41
1:D:175:THR:HA	1:D:181:PHE:HA	2.03	0.41
1:D:190:THR:O	1:D:192:GLN:HG2	2.21	0.41
1:A:137:LYS:HB3	1:A:137:LYS:HZ3	1.84	0.41
1:A:269:LYS:C	1:A:270:GLU:HG3	2.40	0.41
1:C:140:PHE:CG	1:C:163:HIS:CD2	3.08	0.41
1:D:22:CYS:HB2	1:D:42:VAL:HG22	2.02	0.41
1:C:157:VAL:CG1	1:C:159:PHE:CZ	3.03	0.41
1:D:234:ALA:C	1:D:236:LYS:N	2.74	0.41
1:A:199:THR:CG2	1:A:200:ILE:N	2.84	0.41
1:C:19:GLN:NE2	1:C:21:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG12	1:C:159:PHE:CE2	2.55	0.41
1:A:132:PRO:HG2	1:A:198:THR:O	2.20	0.41
1:A:222:ARG:HB3	1:A:223:PHE:CD2	2.56	0.41
1:A:223:PHE:CE2	1:C:270:GLU:HB3	2.52	0.41
1:B:21:THR:OG1	1:B:26:THR:HG23	2.21	0.41
1:B:212:VAL:C	1:B:214:ASN:N	2.75	0.41
1:B:237:TYR:CD1	1:B:237:TYR:N	2.88	0.41
1:B:292:THR:HA	1:D:203:ASN:OD1	2.20	0.41
1:C:31:TRP:CH2	1:C:75:LEU:HD11	2.56	0.41
1:C:54:TYR:C	1:C:56:ASP:N	2.74	0.41
1:C:247:VAL:HG12	1:C:261:VAL:CG2	2.45	0.41
1:D:125:VAL:CG2	1:D:126:TYR:N	2.83	0.41
1:B:221:ASN:CB	1:D:223:PHE:CD1	3.03	0.41
1:C:78:ILE:O	1:C:79:GLY:O	2.39	0.41
1:D:145:CYS:SG	1:D:164:HIS:O	2.78	0.41
1:D:222:ARG:HG3	1:D:222:ARG:O	2.21	0.41
1:A:10:SER:O	1:A:11:GLY:C	2.60	0.40
1:A:270:GLU:C	1:A:270:GLU:CD	2.79	0.40
1:A:296:VAL:CG1	1:C:210:ALA:HB2	2.51	0.40
1:B:245:ASP:O	1:B:248:ASP:HB2	2.21	0.40
1:D:68:VAL:O	1:D:68:VAL:CG2	2.68	0.40
1:A:197:ASP:O	1:A:198:THR:CB	2.69	0.40
1:C:130:MET:HE1	1:C:134:HIS:O	2.22	0.40
1:C:171:VAL:HG12	1:C:172:HIS:N	2.36	0.40
1:D:58:LEU:HB2	1:D:61:LYS:HD3	2.03	0.40
1:D:167:LEU:HD12	1:D:171:VAL:HG23	2.03	0.40
1:A:5:LYS:NZ	1:B:4:ARG:NH2	2.68	0.40
1:A:20:VAL:HG22	1:A:68:VAL:HG22	2.03	0.40
1:A:222:ARG:HD3	1:C:267:ALA:CA	2.51	0.40
1:A:222:ARG:HD3	1:C:267:ALA:HB2	2.03	0.40
1:A:268:LEU:HD22	1:C:205:LEU:CD2	2.51	0.40
1:B:268:LEU:CD2	1:B:268:LEU:C	2.90	0.40
1:C:104:VAL:HG22	1:C:160:CYS:HB3	2.04	0.40
1:D:97:LYS:H	1:D:97:LYS:HG2	1.79	0.40
1:D:167:LEU:HB3	1:D:168:PRO:CD	2.39	0.40
1:A:171:VAL:HG23	1:A:172:HIS:N	2.36	0.40
1:B:199:THR:CG2	1:B:200:ILE:N	2.84	0.40
1:B:212:VAL:O	1:B:214:ASN:N	2.55	0.40
1:B:223:PHE:CE1	1:B:269:LYS:HD3	2.56	0.40
1:C:131:ARG:HD3	1:C:137:LYS:HE2	2.02	0.40
1:D:40:ARG:HB3	1:D:85:CYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLN:HG2	1:D:75:LEU:H	1.87	0.40
1:D:87:LEU:HB2	1:D:89:LEU:HD21	2.02	0.40
1:A:218:TRP:CE3	1:A:219:PHE:HA	2.56	0.40
1:C:26:THR:C	1:C:27:LEU:HD23	2.42	0.40
1:C:58:LEU:HD22	1:C:87:LEU:HD21	2.03	0.40
1:C:243:THR:OG1	1:C:244:GLN:N	2.55	0.40
1:D:112:PHE:CD1	1:D:149:GLY:HA3	2.57	0.40
1:D:251:GLY:N	1:D:252:PRO:HD2	2.35	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	299/306 (98%)	238 (80%)	32 (11%)	29 (10%)	0 3
1	B	299/306 (98%)	230 (77%)	43 (14%)	26 (9%)	1 4
1	C	298/306 (97%)	230 (77%)	43 (14%)	25 (8%)	1 5
1	D	298/306 (97%)	223 (75%)	47 (16%)	28 (9%)	0 3
2	E	3/6 (50%)	3 (100%)	0	0	100 100
2	F	3/6 (50%)	2 (67%)	1 (33%)	0	100 100
2	G	3/6 (50%)	3 (100%)	0	0	100 100
2	H	3/6 (50%)	1 (33%)	1 (33%)	1 (33%)	0 0
All	All	1206/1248 (97%)	930 (77%)	167 (14%)	109 (9%)	1 4

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	51	ASN

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Mol	Chain	Res	Type
1	A	106	ILE
1	A	122	PRO
1	A	123	SER
1	A	191	ALA
1	A	221	ASN
1	A	223	PHE
1	A	224	THR
1	A	261	VAL
1	A	270	GLU
1	B	40	ARG
1	B	41	HIS
1	B	84	ASN
1	B	106	ILE
1	B	189	GLN
1	B	223	PHE
1	B	224	THR
1	B	238	ASN
1	B	251	GLY
1	C	40	ARG
1	C	41	HIS
1	C	50	LEU
1	C	55	GLU
1	C	79	GLY
1	C	272	LEU
1	C	273	GLN
1	C	294	PHE
1	D	36	VAL
1	D	49	MET
1	D	55	GLU
1	D	63	ASN
1	D	64	HIS
1	D	155	ASP
1	D	193	ALA
1	D	194	ALA
1	D	195	GLY
1	D	222	ARG
1	A	46	ALA
1	A	89	LEU
1	A	195	GLY
1	A	251	GLY
1	B	33	ASP
1	B	59	ILE

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Mol	Chain	Res	Type
1	B	213	ILE
1	C	63	ASN
1	C	72	ASN
1	C	155	ASP
1	C	191	ALA
1	C	217	ARG
1	C	227	LEU
1	C	236	LYS
1	D	68	VAL
1	D	71	GLY
1	D	80	HIS
1	D	170	GLY
1	D	221	ASN
1	D	224	THR
1	D	235	MET
2	H	4	LEU
1	A	50	LEU
1	A	73	VAL
1	A	134	HIS
1	A	277	ASN
1	A	278	GLY
1	B	52	PRO
1	B	60	ARG
1	B	261	VAL
1	B	274	ASN
1	C	235	MET
1	D	90	LYS
1	D	234	ALA
1	A	197	ASP
1	A	198	THR
1	B	23	GLY
1	B	46	ALA
1	B	56	ASP
1	B	134	HIS
1	C	43	ILE
1	C	49	MET
1	C	276	MET
1	D	84	ASN
1	D	187	ASP
1	A	84	ASN
1	A	241	PRO
1	B	256	GLN

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Mol	Chain	Res	Type
1	B	282	LEU
1	C	286	ILE
1	D	62	SER
1	D	73	VAL
1	D	240	GLU
1	A	23	GLY
1	B	11	GLY
1	B	167	LEU
1	B	269	LYS
1	C	48	ASP
1	C	59	ILE
1	C	251	GLY
1	D	119	ASN
1	D	278	GLY
1	C	184	PRO
1	C	252	PRO
1	A	15	GLY
1	A	171	VAL
1	B	9	PRO
1	D	167	LEU
1	A	249	ILE
1	D	200	ILE
1	A	43	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	259/263 (98%)	211 (82%)	48 (18%)	1 8
1	B	259/263 (98%)	210 (81%)	49 (19%)	1 8
1	C	258/263 (98%)	204 (79%)	54 (21%)	1 6
1	D	258/263 (98%)	199 (77%)	59 (23%)	1 4
2	E	2/2 (100%)	0	2 (100%)	0 0
2	F	2/2 (100%)	1 (50%)	1 (50%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	2/2 (100%)	0	2 (100%)	0 0
2	H	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	1042/1060 (98%)	826 (79%)	216 (21%)	1 6

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	22	CYS
1	A	24	THR
1	A	28	ASN
1	A	30	LEU
1	A	44	CYS
1	A	47	GLU
1	A	48	ASP
1	A	49	MET
1	A	50	LEU
1	A	51	ASN
1	A	58	LEU
1	A	59	ILE
1	A	62	SER
1	A	64	HIS
1	A	73	VAL
1	A	76	ARG
1	A	78	ILE
1	A	102	LYS
1	A	106	ILE
1	A	114	VAL
1	A	115	LEU
1	A	119	ASN
1	A	122	PRO
1	A	131	ARG
1	A	136	ILE
1	A	137	LYS
1	A	141	LEU
1	A	181	PHE
1	A	185	PHE
1	A	186	VAL
1	A	188	ARG
1	A	189	GLN
1	A	190	THR

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Mol	Chain	Res	Type
1	A	196	THR
1	A	200	ILE
1	A	232	LEU
1	A	233	VAL
1	A	236	LYS
1	A	244	GLN
1	A	256	GLN
1	A	263	ASP
1	A	270	GLU
1	A	271	LEU
1	A	272	LEU
1	A	282	LEU
1	A	286	ILE
1	A	301	SER
1	B	12	LYS
1	B	21	THR
1	B	27	LEU
1	B	30	LEU
1	B	37	TYR
1	B	41	HIS
1	B	43	ILE
1	B	47	GLU
1	B	49	MET
1	B	56	ASP
1	B	57	LEU
1	B	58	LEU
1	B	59	ILE
1	B	69	GLN
1	B	75	LEU
1	B	78	ILE
1	B	83	GLN
1	B	94	SER
1	B	123	SER
1	B	125	VAL
1	B	131	ARG
1	B	142	ASN
1	B	153	ASP
1	B	155	ASP
1	B	169	THR
1	B	178	GLU
1	B	180	LYS
1	B	181	PHE

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Mol	Chain	Res	Type
1	B	186	VAL
1	B	189	GLN
1	B	192	GLN
1	B	196	THR
1	B	200	ILE
1	B	201	THR
1	B	202	LEU
1	B	221	ASN
1	B	222	ARG
1	B	223	PHE
1	B	227	LEU
1	B	233	VAL
1	B	236	LYS
1	B	238	ASN
1	B	250	LEU
1	B	268	LEU
1	B	271	LEU
1	B	273	GLN
1	B	286	ILE
1	B	295	ASP
1	B	297	VAL
1	C	1	SER
1	C	19	GLN
1	C	24	THR
1	C	25	THR
1	C	30	LEU
1	C	32	LEU
1	C	40	ARG
1	C	50	LEU
1	C	53	ASN
1	C	54	TYR
1	C	55	GLU
1	C	57	LEU
1	C	67	LEU
1	C	76	ARG
1	C	78	ILE
1	C	83	GLN
1	C	90	LYS
1	C	104	VAL
1	C	121	SER
1	C	128	CYS
1	C	133	ASN

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Mol	Chain	Res	Type
1	C	136	ILE
1	C	147	SER
1	C	158	SER
1	C	169	THR
1	C	181	PHE
1	C	190	THR
1	C	202	LEU
1	C	213	ILE
1	C	216	ASP
1	C	222	ARG
1	C	223	PHE
1	C	224	THR
1	C	225	THR
1	C	228	ASN
1	C	232	LEU
1	C	235	MET
1	C	236	LYS
1	C	243	THR
1	C	245	ASP
1	C	247	VAL
1	C	248	ASP
1	C	249	ILE
1	C	263	ASP
1	C	268	LEU
1	C	269	LYS
1	C	270	GLU
1	C	274	ASN
1	C	280	THR
1	C	286	ILE
1	C	289	ASP
1	C	290	GLU
1	C	292	THR
1	C	298	ARG
1	D	17	MET
1	D	19	GLN
1	D	24	THR
1	D	30	LEU
1	D	35	THR
1	D	38	CYS
1	D	51	ASN
1	D	53	ASN
1	D	56	ASP

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Mol	Chain	Res	Type
1	D	57	LEU
1	D	58	LEU
1	D	61	LYS
1	D	67	LEU
1	D	68	VAL
1	D	72	ASN
1	D	77	VAL
1	D	81	SER
1	D	86	LEU
1	D	87	LEU
1	D	103	PHE
1	D	106	ILE
1	D	125	VAL
1	D	127	GLN
1	D	128	CYS
1	D	131	ARG
1	D	133	ASN
1	D	141	LEU
1	D	148	VAL
1	D	153	ASP
1	D	156	CYS
1	D	158	SER
1	D	165	MET
1	D	172	HIS
1	D	178	GLU
1	D	180	LYS
1	D	181	PHE
1	D	187	ASP
1	D	190	THR
1	D	192	GLN
1	D	208	LEU
1	D	216	ASP
1	D	218	TRP
1	D	219	PHE
1	D	220	LEU
1	D	221	ASN
1	D	226	THR
1	D	228	ASN
1	D	232	LEU
1	D	242	LEU
1	D	245	ASP
1	D	248	ASP

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Mol	Chain	Res	Type
1	D	261	VAL
1	D	262	LEU
1	D	264	MET
1	D	279	ARG
1	D	285	THR
1	D	286	ILE
1	D	294	PHE
1	D	295	ASP
2	H	4	LEU
2	F	4	LEU
2	G	3	VAL
2	G	4	LEU
2	E	3	VAL
2	E	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	28	ASN
1	A	41	HIS
1	A	51	ASN
1	A	63	ASN
1	A	107	GLN
1	A	134	HIS
1	A	151	ASN
1	A	163	HIS
1	A	228	ASN
1	A	238	ASN
1	A	246	HIS
1	B	64	HIS
1	B	69	GLN
1	B	72	ASN
1	B	80	HIS
1	B	119	ASN
1	B	134	HIS
1	B	164	HIS
1	B	274	ASN
1	C	19	GLN
1	C	53	ASN
1	C	63	ASN
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	151	ASN
1	C	172	HIS
1	D	19	GLN
1	D	51	ASN
1	D	53	ASN
1	D	69	GLN
1	D	107	GLN
1	D	119	ASN
1	D	134	HIS
1	D	172	HIS
1	D	214	ASN
1	D	228	ASN
1	D	273	GLN
1	D	274	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	02J	F	1	2	6,8,9	2.78	4 (66%)	4,10,12	4.27	1 (25%)
2	02J	E	1	2	6,8,9	3.55	4 (66%)	4,10,12	3.03	1 (25%)
2	PJE	H	5	2	12,13,14	6.23	6 (50%)	12,16,18	2.41	4 (33%)
2	02J	H	1	2	6,8,9	3.38	4 (66%)	4,10,12	4.79	2 (50%)
2	PJE	F	5	2	12,13,14	7.43	7 (58%)	12,16,18	4.27	7 (58%)
2	PJE	G	5	2	12,13,14	6.62	6 (50%)	12,16,18	4.34	6 (50%)
2	PJE	E	5	2	12,13,14	6.69	6 (50%)	12,16,18	3.08	10 (83%)
2	02J	G	1	2	6,8,9	2.98	3 (50%)	4,10,12	3.52	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	02J	F	1	2	-	0/0/2/4	0/1/1/1
2	PJE	H	5	2	1/1/3/7	5/7/18/19	0/1/1/1
2	02J	E	1	2	-	0/0/2/4	0/1/1/1
2	02J	H	1	2	-	0/0/2/4	0/1/1/1
2	PJE	G	5	2	1/1/3/7	4/7/18/19	0/1/1/1
2	PJE	E	5	2	1/1/3/7	4/7/18/19	0/1/1/1
2	PJE	F	5	2	-	3/7/18/19	0/1/1/1
2	02J	G	1	2	-	0/0/2/4	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	PJE	C29-N6	22.03	1.57	1.33
2	H	5	PJE	C29-N6	19.61	1.54	1.33
2	E	5	PJE	C29-N6	19.60	1.54	1.33
2	G	5	PJE	C29-N6	19.56	1.54	1.33
2	F	5	PJE	O8-C29	8.46	1.40	1.23
2	E	5	PJE	O8-C29	8.21	1.39	1.23
2	G	5	PJE	O8-C29	8.08	1.39	1.23
2	E	1	02J	CA-C	6.63	1.55	1.48
2	F	5	PJE	C26-C29	6.46	1.60	1.52
2	E	5	PJE	C26-C29	6.17	1.59	1.52
2	H	1	02J	CA-C	5.84	1.54	1.48
2	G	5	PJE	C26-C29	5.66	1.59	1.52
2	H	5	PJE	C26-C29	5.29	1.58	1.52
2	F	5	PJE	C21-C20	5.26	1.54	1.33
2	H	5	PJE	C21-C20	5.14	1.53	1.33
2	G	5	PJE	C21-C20	5.02	1.53	1.33
2	E	5	PJE	C21-C20	5.00	1.53	1.33
2	H	1	02J	C6-C5	4.58	1.54	1.48
2	G	1	02J	C6-C5	4.48	1.53	1.48
2	G	1	02J	CA-C	4.45	1.53	1.48
2	F	1	02J	C6-C5	4.33	1.53	1.48
2	E	1	02J	C6-C5	4.29	1.53	1.48
2	F	5	PJE	C27-C28	-4.24	1.46	1.53
2	F	1	02J	CA-C	3.85	1.52	1.48
2	G	5	PJE	C27-C28	-3.33	1.47	1.53
2	E	5	PJE	C27-C28	-3.13	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	5	PJE	C21-C	3.04	1.53	1.44
2	E	5	PJE	C21-C	2.91	1.53	1.44
2	G	1	02J	C4-C5	-2.87	1.35	1.39
2	H	5	PJE	CA-C20	2.85	1.53	1.50
2	H	5	PJE	O8-C29	2.69	1.28	1.23
2	F	5	PJE	C21-C	2.68	1.52	1.44
2	G	5	PJE	C21-C	2.62	1.52	1.44
2	F	5	PJE	CA-C20	2.58	1.53	1.50
2	F	1	02J	C4-C5	-2.58	1.36	1.39
2	H	1	02J	C4-C5	-2.44	1.36	1.39
2	E	1	02J	C4-CA	2.31	1.44	1.39
2	H	1	02J	C4-CA	2.26	1.43	1.39
2	E	1	02J	C4-C5	-2.24	1.36	1.39
2	F	1	02J	C4-CA	2.01	1.43	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5	PJE	O8-C29-N6	-10.55	110.90	125.54
2	G	5	PJE	CA-C20-C21	-9.49	110.85	124.41
2	H	1	02J	O-C-CA	-9.12	115.58	124.22
2	F	1	02J	O-C-CA	-8.39	116.27	124.22
2	G	5	PJE	O8-C29-C26	-7.89	116.95	126.23
2	G	1	02J	O-C-CA	-6.64	117.93	124.22
2	F	5	PJE	O8-C29-C26	-5.94	119.25	126.23
2	G	5	PJE	O8-C29-N6	-5.71	117.62	125.54
2	E	5	PJE	O8-C29-C26	-5.60	119.65	126.23
2	E	1	02J	O-C-CA	-5.42	119.09	124.22
2	F	5	PJE	C25-C26-C29	5.08	124.05	112.89
2	H	5	PJE	C25-C26-C27	4.99	135.68	117.31
2	E	5	PJE	O8-C29-N6	-4.31	119.57	125.54
2	G	5	PJE	C25-C26-C29	4.13	121.97	112.89
2	F	5	PJE	CA-C20-C21	-4.02	118.67	124.41
2	H	5	PJE	O8-C29-N6	-3.87	120.17	125.54
2	E	5	PJE	C28-N6-C29	-3.47	107.03	113.84
2	F	5	PJE	C27-C28-N6	3.46	108.50	103.43
2	G	5	PJE	C27-C28-N6	3.34	108.32	103.43
2	E	5	PJE	C28-C27-C26	2.92	110.48	105.75
2	E	5	PJE	CA-C20-C21	-2.86	120.32	124.41
2	E	5	PJE	C25-C26-C29	2.85	119.16	112.89
2	E	5	PJE	C27-C28-N6	2.69	107.37	103.43
2	E	5	PJE	C20-CA-N	-2.55	105.06	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	5	PJE	O-C-C21	-2.51	117.09	125.67
2	H	5	PJE	C25-C26-C29	2.49	118.37	112.89
2	E	5	PJE	O-C-C21	-2.43	117.38	125.67
2	H	1	02J	CA-C4-C5	2.34	109.06	106.06
2	F	5	PJE	C25-CA-N	2.31	115.47	110.32
2	F	5	PJE	C28-N6-C29	-2.21	109.51	113.84
2	E	5	PJE	C25-CA-N	2.18	115.18	110.32
2	G	5	PJE	O-C-C21	-2.01	118.81	125.67

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	5	PJE	C26
2	G	5	PJE	CA
2	E	5	PJE	CA

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	5	PJE	C26-C25-CA-C20
2	H	5	PJE	C26-C25-CA-N
2	H	5	PJE	O-C-C21-C20
2	H	5	PJE	CA-C25-C26-C29
2	F	5	PJE	O-C-C21-C20
2	F	5	PJE	CA-C25-C26-C27
2	G	5	PJE	C26-C25-CA-C20
2	G	5	PJE	C26-C25-CA-N
2	G	5	PJE	O-C-C21-C20
2	E	5	PJE	C21-C20-CA-C25
2	E	5	PJE	C26-C25-CA-C20
2	E	5	PJE	C26-C25-CA-N
2	E	5	PJE	O-C-C21-C20
2	F	5	PJE	CA-C20-C21-C
2	H	5	PJE	C21-C20-CA-C25
2	G	5	PJE	C21-C20-CA-C25

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	02J	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	02J	2	0
2	H	5	PJE	5	0
2	H	1	02J	2	0
2	F	5	PJE	4	0
2	G	5	PJE	4	0
2	E	5	PJE	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/306 (98%)	0.17	5 (1%) 70 57	58, 78, 102, 127	0
1	B	301/306 (98%)	0.19	5 (1%) 70 57	55, 84, 112, 134	0
1	C	300/306 (98%)	0.15	2 (0%) 87 81	57, 75, 102, 122	0
1	D	300/306 (98%)	0.60	33 (11%) 5 3	67, 96, 147, 159	0
2	E	3/6 (50%)	2.20	1 (33%) 0 0	127, 127, 130, 140	0
2	F	3/6 (50%)	0.22	0 100 100	104, 104, 106, 112	0
2	G	3/6 (50%)	0.93	0 100 100	81, 81, 87, 95	0
2	H	3/6 (50%)	0.97	0 100 100	101, 101, 103, 114	0
All	All	1214/1248 (97%)	0.28	46 (3%) 40 26	55, 83, 123, 159	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	LEU	7.7
1	B	301	SER	4.4
1	D	56	ASP	4.2
1	A	72	ASN	3.8
2	E	2	ALA	3.7
1	D	47	GLU	3.7
1	A	50	LEU	3.6
1	D	53	ASN	3.3
1	D	229	ASP	3.3
1	D	300	CYS	3.2
1	C	300	CYS	3.0
1	C	222	ARG	2.9
1	A	48	ASP	2.9
1	D	94	SER	2.8
1	D	25	THR	2.8
1	D	51	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	191	ALA	2.7
1	B	242	LEU	2.6
1	D	45	THR	2.6
1	D	89	LEU	2.6
1	D	75	LEU	2.6
1	D	167	LEU	2.5
1	D	67	LEU	2.5
1	D	232	LEU	2.5
1	D	49	MET	2.5
1	D	81	SER	2.4
1	D	72	ASN	2.4
1	D	165	MET	2.4
1	D	227	LEU	2.3
1	D	76	ARG	2.3
1	D	35	THR	2.3
1	D	87	LEU	2.3
1	D	54	TYR	2.3
1	D	60	ARG	2.3
1	A	53	ASN	2.2
1	D	44	CYS	2.2
1	B	34	ASP	2.2
1	D	192	GLN	2.2
1	D	241	PRO	2.2
1	B	221	ASN	2.2
1	D	230	PHE	2.2
1	D	231	ASN	2.1
1	D	80	HIS	2.1
1	B	300	CYS	2.0
1	D	190	THR	2.0
1	A	49	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	02J	E	1	8/9	0.22	0.98	148,151,152,152	0
2	02J	H	1	8/9	0.73	0.51	119,124,125,126	0
2	02J	F	1	8/9	0.81	0.47	115,119,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	02J	G	1	8/9	0.83	0.50	103,106,108,108	0
2	PJE	F	5	13/14	0.85	0.35	103,104,109,110	0
2	PJE	H	5	13/14	0.90	0.33	102,103,115,116	0
2	PJE	E	5	13/14	0.93	0.25	123,125,129,129	0
2	PJE	G	5	13/14	0.94	0.26	77,79,83,85	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.