Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 12:48 PM JST

PDB ID	:	4TRZ
Title	:	Structure of BACE1 complex with 2-thiophenyl HEA-type inhibitor
Authors	:	Akaji, K.; Teruya, K.; Akiyama, T.; Sanjho, A.; Yamashita, E.; Nakagawa, A.
Deposited on	:	2014-06-18
Resolution	:	3.25 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 (i)) were used in the production of this report:

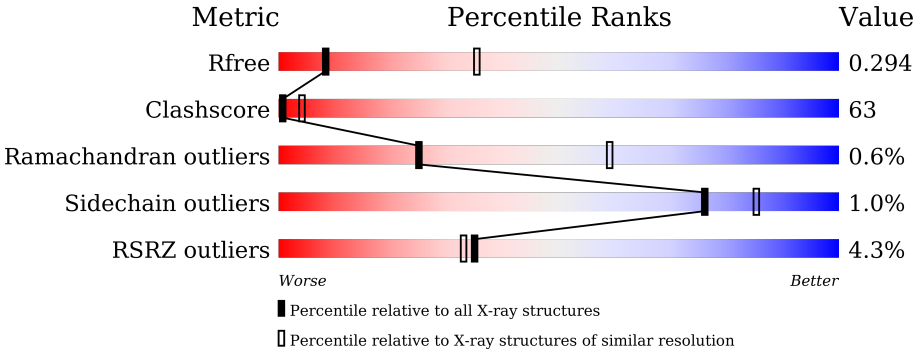
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	388	4% 43% 56% ·
1	B	388	4% 38% 60% ·
1	C	388	5% 38% 61% ·
2	D	4	50% 25% 25%
2	E	4	25% 50% 25%
2	F	4	50% 25% 25%

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	TIH	D	3	-	-	X	-
2	TVA	D	4	-	-	X	-
2	TVA	E	4	-	-	X	-
2	TIH	F	3	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9299 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3050	1954	506	576	14	0	0	0
1	B	388	3050	1954	506	576	14	0	0	0
1	C	388	3050	1954	506	576	14	0	0	0

- Molecule 2 is a protein called 2-thiophenyl HEA-type inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	4	46	31	5	8	2	0	0	0
2	E	4	46	31	5	8	2	0	0	0
2	F	4	46	31	5	8	2	0	0	0

- Molecule 3 is water.

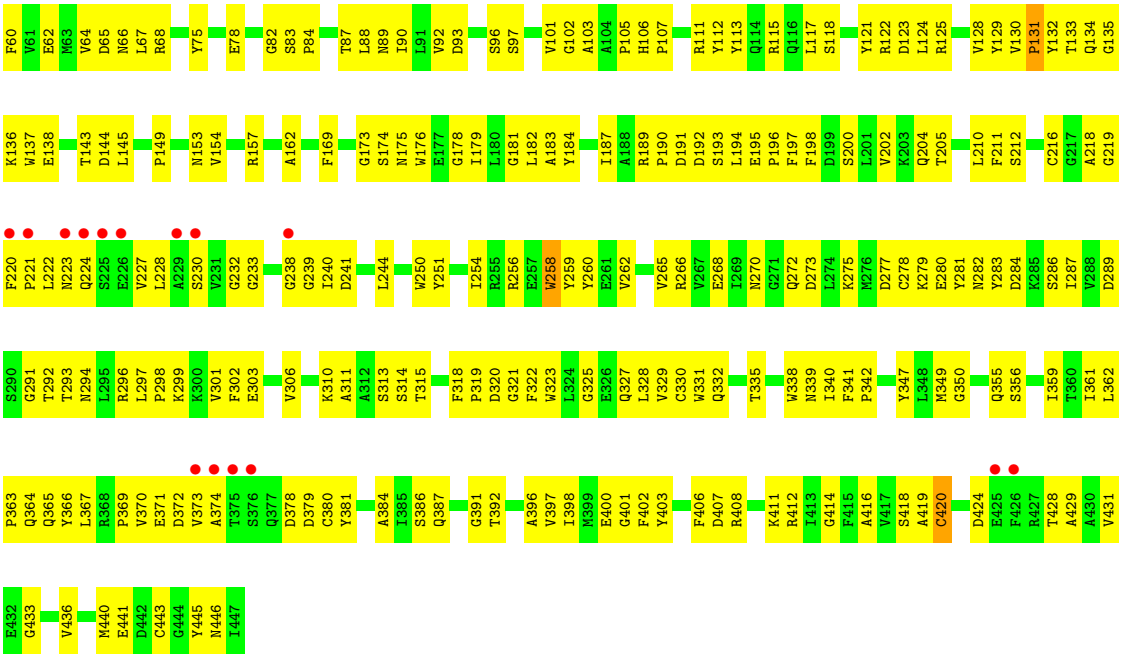
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
3	B	6	6	6	0	0
3	C	2	2	2	0	0
3	F	1	1	1	0	0

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.

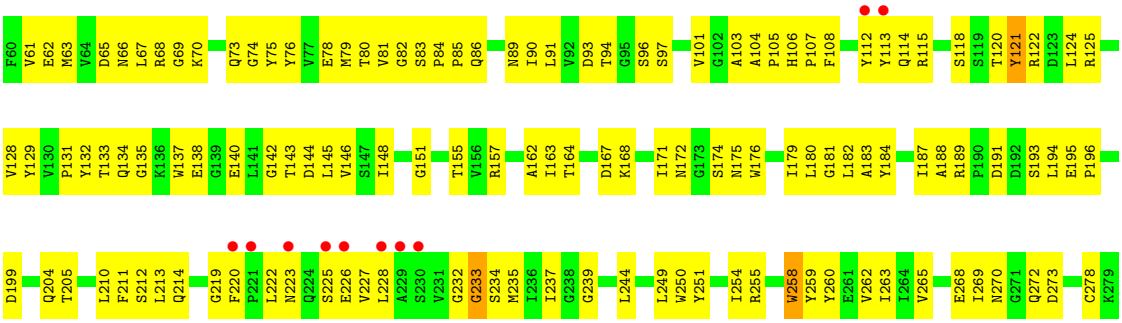
• Molecule 1: Beta-secretase 1

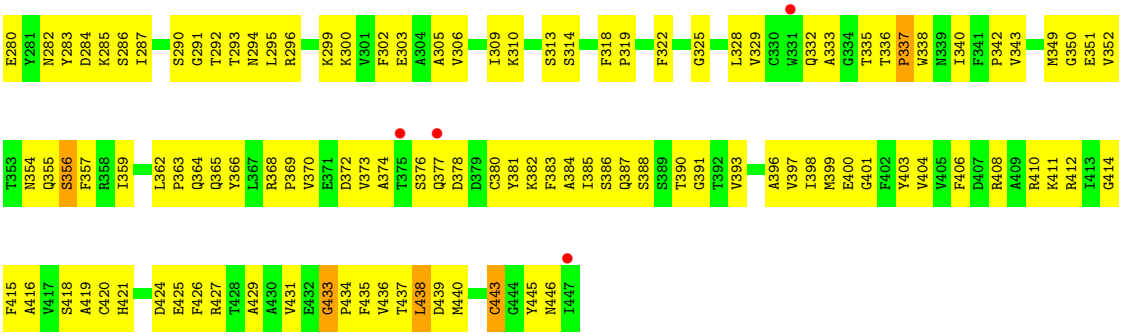
Chain A:



• Molecule 1: Beta-secretase 1

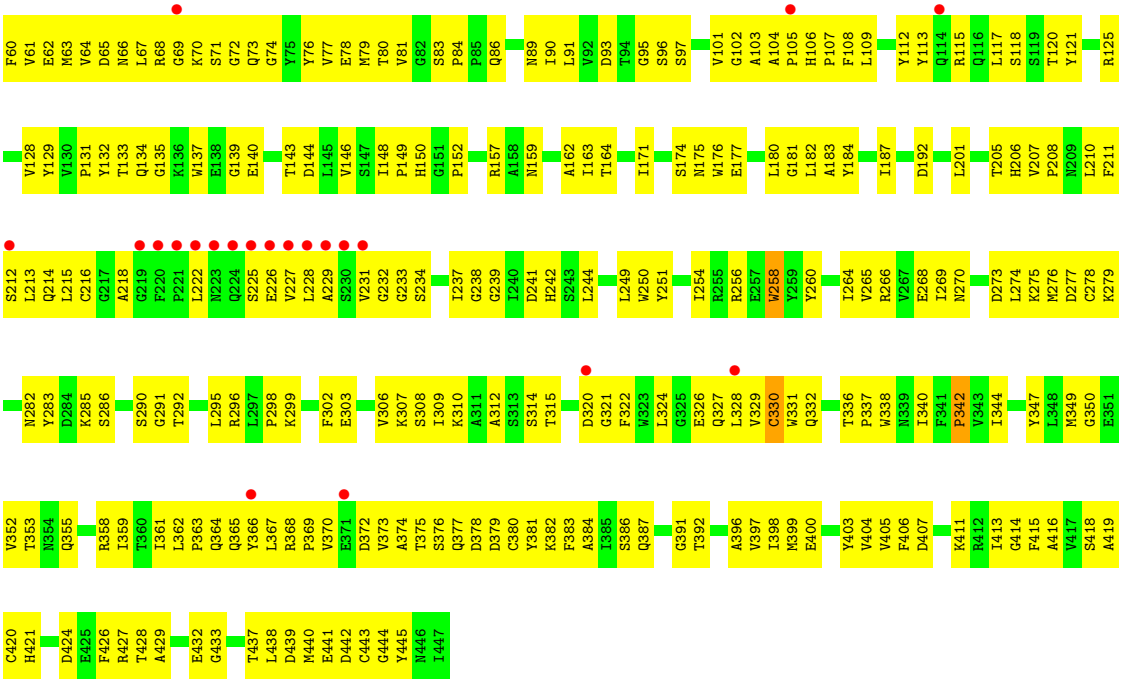
Chain B:





- Molecule 1: Beta-secretase 1

Chain C:



- Molecule 2: 2-thiophenyl HEA-type inhibitor

Chain D:

- Molecule 2: 2-thiophenyl HEA-type inhibitor

Chain E:

- Molecule 2: 2-thiophenyl HEA-type inhibitor

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.87Å 102.42Å 101.59Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	49.10 – 3.25 49.09 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.10-3.25) 99.3 (49.09-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.263 , 0.295 0.263 , 0.294	Depositor DCC
R_{free} test set	1315 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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 (i)

5.1 Standard geometry (i)

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

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	0.93	0/3128	0.73	0/4254
1	B	0.89	0/3128	0.77	2/4254 (0.0%)
1	C	0.88	0/3128	0.73	0/4254
2	D	0.30	0/16	0.69	0/20
2	E	2.04	1/16 (6.2%)	1.83	1/20 (5.0%)
2	F	0.36	0/16	0.69	0/20
All	All	0.90	1/9432 (0.0%)	0.75	3/12822 (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
2	D	0	1
2	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	GLU	CD-OE1	-5.10	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	B	121	TYR	N-CA-C	-5.49	96.17	111.00
1	B	433	GLY	C-N-CD	-5.02	109.55	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	TIH	Mainchain
2	F	3	TIH	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	3050	0	2962	340	0
1	B	3050	0	2962	374	0
1	C	3050	0	2964	432	0
2	D	46	0	38	26	0
2	E	46	0	39	21	0
2	F	46	0	38	19	0
3	A	2	0	0	0	0
3	B	6	0	0	3	0
3	C	2	0	0	0	0
3	F	1	0	0	0	0
All	All	9299	0	9003	1143	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 63.

All (1143) 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:C:225:SER:HA	1:C:226:GLU:CG	1.34	1.57
1:B:287:ILE:CD1	2:E:4:TVA:H48	1.33	1.56
1:B:259:TYR:CD1	2:E:4:TVA:H47	1.50	1.43
1:C:216:CYS:HB3	1:C:420:CYS:SG	1.60	1.42
1:C:376:SER:CB	1:C:377:GLN:HA	1.43	1.39
1:B:106:HIS:ND1	1:B:107:PRO:HD2	1.08	1.36
1:B:182:LEU:HD13	1:B:211:PHE:CZ	1.59	1.35
1:C:366:TYR:CZ	1:C:383:PHE:HE1	1.44	1.33
1:C:225:SER:CA	1:C:226:GLU:HG3	1.57	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ILE:HD12	2:E:4:TVA:C30	1.61	1.29
1:C:331:TRP:CZ3	1:C:381:TYR:HD2	1.50	1.28
1:B:350:GLY:HA3	1:B:355:GLN:O	1.31	1.27
1:B:106:HIS:ND1	1:B:107:PRO:CD	1.96	1.26
1:C:314:SER:O	1:C:315:THR:CG2	1.83	1.26
1:B:66:ASN:OD1	1:B:67:LEU:HG	1.35	1.22
1:C:216:CYS:CB	1:C:420:CYS:SG	2.30	1.19
1:C:421:HIS:CE1	1:C:429:ALA:HB2	1.77	1.19
1:C:363:PRO:HA	1:C:366:TYR:CB	1.73	1.18
1:C:328:LEU:HD11	1:C:370:VAL:HG21	1.23	1.18
1:C:106:HIS:ND1	1:C:107:PRO:HD2	1.58	1.18
1:C:331:TRP:HZ3	1:C:381:TYR:CD2	1.62	1.17
1:A:129:TYR:CE2	1:C:61:VAL:HG13	1.78	1.16
1:C:106:HIS:CE1	1:C:107:PRO:HD2	1.80	1.16
1:C:366:TYR:CZ	1:C:383:PHE:CE1	2.33	1.16
1:C:331:TRP:CZ3	1:C:381:TYR:CD2	2.35	1.15
1:B:106:HIS:CE1	1:B:107:PRO:HD2	1.81	1.14
1:C:115:ARG:HG2	1:C:121:TYR:CE2	1.81	1.14
1:A:145:LEU:HD23	1:A:157:ARG:HG2	1.15	1.14
1:A:329:VAL:HG23	1:A:331:TRP:CZ3	1.83	1.14
1:C:225:SER:CA	1:C:226:GLU:CG	2.18	1.12
1:C:175:ASN:HD21	1:C:228:LEU:HD21	1.08	1.12
1:A:340:ILE:HD11	1:A:341:PHE:CZ	1.85	1.12
1:B:363:PRO:CG	1:B:427:ARG:HH22	1.61	1.11
1:C:134:GLN:HB2	2:F:3:TIH:HB3	1.29	1.11
1:C:274:LEU:HB3	1:C:276:MET:HE3	1.33	1.11
1:C:312:ALA:CB	1:C:342:PRO:HG3	1.79	1.11
1:A:122:ARG:HH12	1:A:157:ARG:HD3	1.13	1.11
1:C:115:ARG:HD2	1:C:121:TYR:CZ	1.85	1.10
1:B:283:TYR:CD2	1:B:445:TYR:CE2	2.40	1.10
1:C:314:SER:O	1:C:315:THR:HG22	0.92	1.09
1:B:283:TYR:HD2	1:B:445:TYR:CE2	1.70	1.09
1:C:376:SER:CB	1:C:377:GLN:CA	2.29	1.09
1:B:182:LEU:HD13	1:B:211:PHE:CE2	1.88	1.08
1:B:270:ASN:HD22	1:B:342:PRO:CB	1.64	1.08
1:C:421:HIS:CE1	1:C:429:ALA:CB	2.37	1.08
1:C:363:PRO:HA	1:C:366:TYR:HB3	1.28	1.07
1:B:363:PRO:HG3	1:B:427:ARG:HH22	1.04	1.07
1:A:371:GLU:HG3	1:A:372:ASP:N	1.65	1.06
1:B:108:PHE:HE2	1:B:172:ASN:HB2	1.14	1.06
1:A:145:LEU:CD2	1:A:157:ARG:HG2	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLY:HA2	1:B:144:ASP:OD2	1.54	1.05
1:B:328:LEU:HD21	1:B:370:VAL:HG21	1.32	1.05
1:C:363:PRO:HD2	1:C:364:GLN:OE1	1.54	1.04
1:C:115:ARG:CD	1:C:121:TYR:CZ	2.39	1.04
1:A:340:ILE:HD11	1:A:341:PHE:CE1	1.92	1.03
1:B:214:GLN:OE1	1:B:244:LEU:HG	1.57	1.03
1:C:366:TYR:CE2	1:C:383:PHE:HE1	1.75	1.03
1:C:331:TRP:O	1:C:378:ASP:HB3	1.57	1.02
1:A:129:TYR:HE2	1:C:61:VAL:CG1	1.72	1.02
1:B:94:THR:HG22	1:B:182:LEU:HD12	1.41	1.02
1:C:413:ILE:HG22	1:C:415:PHE:CE1	1.94	1.02
1:A:173:GLY:HA3	1:A:224:GLN:OE1	1.58	1.02
1:B:106:HIS:CG	1:B:107:PRO:CD	2.42	1.02
1:C:309:ILE:HD13	1:C:366:TYR:OH	1.58	1.02
1:A:174:SER:HB2	1:A:176:TRP:CD1	1.95	1.01
1:B:259:TYR:CD1	2:E:4:TVA:C30	2.43	1.01
1:A:129:TYR:HE2	1:C:61:VAL:HG13	0.86	1.00
1:B:259:TYR:CE1	2:E:4:TVA:H47	1.96	1.00
1:C:336:THR:HB	1:C:338:TRP:CZ3	1.95	1.00
1:A:329:VAL:CG2	1:A:331:TRP:CH2	2.43	1.00
1:B:66:ASN:OD1	1:B:67:LEU:CG	2.09	1.00
1:B:328:LEU:HD21	1:B:370:VAL:CG2	1.90	1.00
1:A:174:SER:HB2	1:A:176:TRP:NE1	1.77	1.00
1:B:322:PHE:CD2	1:B:329:VAL:HG13	1.97	1.00
1:C:376:SER:HB2	1:C:377:GLN:CA	1.91	1.00
1:B:106:HIS:CG	1:B:107:PRO:HD2	1.97	0.99
1:B:328:LEU:CD2	1:B:370:VAL:HG21	1.92	0.99
1:C:65:ASP:H	1:C:234:SER:HB3	1.22	0.99
1:C:364:GLN:OE1	1:C:364:GLN:N	1.96	0.99
1:B:328:LEU:CD2	1:B:370:VAL:CG2	2.40	0.99
1:B:129:TYR:HD2	1:B:138:GLU:HG2	1.23	0.98
1:C:295:LEU:HD13	1:C:398:ILE:CG1	1.92	0.98
1:B:299:LYS:HG3	1:B:387:GLN:OE1	1.63	0.98
1:B:284:ASP:OD1	1:B:285:LYS:HG2	1.65	0.97
1:C:350:GLY:HA3	1:C:355:GLN:OE1	1.63	0.97
1:C:331:TRP:C	1:C:378:ASP:HB3	1.86	0.96
1:B:438:LEU:HD12	1:B:439:ASP:H	1.28	0.96
1:C:216:CYS:SG	1:C:420:CYS:CB	2.53	0.96
1:C:328:LEU:HD11	1:C:370:VAL:CG2	1.93	0.96
1:A:130:VAL:HG21	1:A:137:TRP:CZ2	2.00	0.96
1:C:376:SER:HB3	1:C:377:GLN:HA	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:THR:HB	1:C:338:TRP:CH2	2.02	0.95
1:C:363:PRO:CA	1:C:366:TYR:HB3	1.96	0.94
1:B:270:ASN:HD22	1:B:342:PRO:HB3	1.29	0.94
1:B:269:ILE:O	1:B:270:ASN:OD1	1.85	0.94
1:C:302:PHE:O	1:C:306:VAL:HG23	1.68	0.94
1:B:259:TYR:HD1	2:E:4:TVA:H47	1.26	0.94
1:C:350:GLY:HA3	1:C:355:GLN:O	1.66	0.94
1:B:113:TYR:HH	1:B:121:TYR:HD1	1.02	0.94
1:B:363:PRO:CG	1:B:427:ARG:NH2	2.28	0.94
1:C:106:HIS:CG	1:C:107:PRO:CD	2.51	0.94
1:B:222:LEU:HD21	1:B:227:VAL:H	1.29	0.93
1:C:177:GLU:OE2	1:C:177:GLU:N	2.01	0.93
1:C:363:PRO:CD	1:C:364:GLN:OE1	2.15	0.93
1:C:363:PRO:HA	1:C:366:TYR:HB2	1.50	0.93
1:A:329:VAL:HG21	1:A:331:TRP:CH2	2.04	0.93
1:B:287:ILE:CD1	2:E:4:TVA:C30	2.29	0.93
1:C:70:LYS:HG2	1:C:72:GLY:H	1.31	0.93
1:C:376:SER:HB2	1:C:377:GLN:HA	0.95	0.93
1:A:329:VAL:HG23	1:A:331:TRP:CH2	2.03	0.92
1:B:108:PHE:CE2	1:B:172:ASN:HB2	2.03	0.92
1:B:113:TYR:OH	1:B:121:TYR:CD1	2.20	0.92
1:B:322:PHE:HD2	1:B:329:VAL:HG13	1.31	0.92
1:B:287:ILE:HD13	2:E:4:TVA:H48	1.47	0.92
1:C:205:THR:HG22	1:C:206:HIS:N	1.84	0.92
1:C:366:TYR:OH	1:C:383:PHE:CE1	2.20	0.92
1:A:340:ILE:HD11	1:A:341:PHE:CE2	2.05	0.92
1:C:216:CYS:SG	1:C:420:CYS:HB3	2.10	0.91
1:B:244:LEU:HD23	1:B:403:TYR:CE1	2.06	0.91
1:C:332:GLN:HA	1:C:378:ASP:CG	1.90	0.91
1:A:299:LYS:O	1:A:303:GLU:HG3	1.71	0.91
1:A:315:THR:HG21	1:B:340:ILE:HD11	1.49	0.91
1:A:338:TRP:CH2	1:A:364:GLN:HA	2.05	0.91
1:B:322:PHE:CD2	1:B:329:VAL:CG1	2.54	0.91
1:B:283:TYR:HD2	1:B:445:TYR:CD2	1.89	0.90
1:C:175:ASN:HD21	1:C:228:LEU:CD2	1.84	0.90
1:C:366:TYR:CE2	1:C:383:PHE:CE1	2.58	0.90
1:C:115:ARG:CG	1:C:121:TYR:CE2	2.53	0.90
1:B:124:LEU:HD11	1:B:143:THR:HG23	1.53	0.90
1:B:219:GLY:O	1:B:220:PHE:CD1	2.24	0.89
1:C:295:LEU:HD13	1:C:398:ILE:HG13	1.54	0.89
1:A:363:PRO:HA	1:A:366:TYR:CE1	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:CD2	1:A:157:ARG:CG	2.49	0.89
1:A:145:LEU:HD23	1:A:157:ARG:CG	2.02	0.89
1:B:103:ALA:CB	1:B:162:ALA:HB1	2.03	0.89
1:B:183:ALA:HB1	1:B:187:ILE:HD11	1.54	0.89
1:B:108:PHE:HE2	1:B:172:ASN:CB	1.85	0.89
1:B:363:PRO:HG3	1:B:427:ARG:NH2	1.87	0.89
1:A:244:LEU:O	1:A:419:ALA:HB2	1.72	0.89
1:A:306:VAL:CG1	1:A:310:LYS:HE3	2.02	0.88
1:A:420:CYS:SG	1:A:420:CYS:O	2.30	0.88
1:C:182:LEU:HD13	1:C:211:PHE:CE2	2.07	0.88
1:A:122:ARG:NH1	1:A:157:ARG:HD3	1.88	0.88
1:C:365:GLN:N	1:C:365:GLN:OE1	2.04	0.88
1:B:270:ASN:HD22	1:B:342:PRO:HB2	1.35	0.88
1:C:314:SER:C	1:C:315:THR:HG22	1.92	0.88
1:B:140:GLU:OE2	1:B:164:THR:HG21	1.74	0.88
1:C:328:LEU:CD1	1:C:370:VAL:HG21	2.04	0.88
1:C:274:LEU:HD13	1:C:276:MET:HE1	1.56	0.87
1:B:349:MET:HE1	1:B:440:MET:HA	1.55	0.87
1:B:120:THR:O	1:B:122:ARG:HG3	1.74	0.87
1:C:68:ARG:HG2	1:C:231:VAL:HG12	1.55	0.87
1:A:277:ASP:O	1:A:280:GLU:HB2	1.74	0.87
1:A:306:VAL:HG12	1:A:310:LYS:HE3	1.55	0.87
1:A:371:GLU:HG3	1:A:372:ASP:H	1.35	0.87
1:C:372:ASP:HB3	1:C:374:ALA:O	1.74	0.87
1:A:297:LEU:HD23	1:A:392:THR:HG23	1.54	0.87
1:A:87:THR:HG22	1:A:111:ARG:HH12	1.40	0.86
1:C:265:VAL:O	1:C:266:ARG:HG2	1.74	0.86
1:B:305:ALA:O	1:B:309:ILE:HG13	1.75	0.86
1:C:291:GLY:O	2:F:2:ILE:HG13	1.73	0.86
1:C:312:ALA:HB2	1:C:342:PRO:HG3	1.57	0.86
1:C:376:SER:HB3	1:C:377:GLN:CA	2.02	0.86
1:A:173:GLY:CA	1:A:224:GLN:OE1	2.23	0.86
1:B:113:TYR:OH	1:B:121:TYR:HD1	1.54	0.86
1:A:134:GLN:HB2	2:D:3:TIH:HB3	1.56	0.85
1:C:396:ALA:O	1:C:400:GLU:HG3	1.74	0.85
1:B:368:ARG:HG3	1:B:369:PRO:HD2	1.59	0.85
1:C:115:ARG:HG2	1:C:121:TYR:CD2	2.10	0.85
1:C:367:LEU:CD2	1:C:383:PHE:HA	2.06	0.85
1:A:216:CYS:HB2	1:A:232:GLY:O	1.75	0.85
1:C:225:SER:HA	1:C:226:GLU:HG2	1.55	0.85
1:C:106:HIS:ND1	1:C:107:PRO:CD	2.38	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:MET:CE	1:B:440:MET:HA	2.05	0.85
1:B:106:HIS:CG	1:B:107:PRO:HD3	2.12	0.85
1:B:108:PHE:HD2	1:B:172:ASN:HA	1.39	0.85
1:B:182:LEU:CD1	1:B:211:PHE:CE2	2.60	0.85
1:B:182:LEU:CD1	1:B:211:PHE:CZ	2.54	0.85
1:C:312:ALA:CB	1:C:342:PRO:CG	2.54	0.85
1:B:129:TYR:HD2	1:B:138:GLU:CG	1.90	0.84
1:C:241:ASP:HB3	1:C:244:LEU:HD13	1.59	0.84
1:C:225:SER:H	1:C:226:GLU:HG2	1.40	0.84
1:B:291:GLY:O	2:E:2:ILE:HG13	1.77	0.84
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.12	0.84
1:B:332:GLN:HA	1:B:378:ASP:HA	1.60	0.84
1:C:115:ARG:CD	1:C:121:TYR:CE2	2.61	0.84
1:A:223:ASN:O	1:A:227:VAL:HG23	1.77	0.84
1:C:362:LEU:HB3	1:C:363:PRO:HD2	1.59	0.84
1:B:108:PHE:CD2	1:B:172:ASN:HA	2.13	0.83
1:A:371:GLU:CG	1:A:372:ASP:N	2.40	0.83
1:B:82:GLY:CA	1:B:144:ASP:OD2	2.25	0.83
1:C:413:ILE:CG2	1:C:415:PHE:CE1	2.61	0.83
1:A:259:TYR:OH	2:D:4:TVA:H42	1.78	0.83
1:A:259:TYR:HE1	2:D:4:TVA:H43	1.43	0.83
1:B:115:ARG:HG2	1:B:121:TYR:CZ	2.14	0.83
1:A:82:GLY:HA2	1:A:144:ASP:OD2	1.79	0.83
1:A:291:GLY:O	2:D:2:ILE:HG13	1.79	0.83
1:C:143:THR:HG22	1:C:159:ASN:HA	1.58	0.82
1:B:129:TYR:CD2	1:B:138:GLU:HG2	2.11	0.82
1:B:106:HIS:CE1	1:B:107:PRO:CD	2.55	0.82
1:C:171:ILE:HD11	2:F:2:ILE:HG22	1.62	0.82
1:C:249:LEU:HD23	1:C:416:ALA:HB2	1.59	0.82
1:C:134:GLN:HB2	2:F:3:TIH:CB	2.10	0.81
1:B:94:THR:CG2	1:B:182:LEU:HD12	2.10	0.81
1:B:222:LEU:HD21	1:B:227:VAL:N	1.93	0.81
1:C:175:ASN:ND2	1:C:228:LEU:HD21	1.93	0.81
1:C:421:HIS:HE1	1:C:429:ALA:HB2	1.36	0.81
1:A:340:ILE:CD1	1:A:341:PHE:CE1	2.63	0.81
1:B:349:MET:CE	1:B:440:MET:CA	2.59	0.81
1:A:371:GLU:CG	1:A:372:ASP:H	1.92	0.80
1:A:428:THR:HG22	1:A:429:ALA:O	1.81	0.80
1:B:306:VAL:O	1:B:310:LYS:HG3	1.81	0.80
1:C:134:GLN:CB	2:F:3:TIH:HB3	2.11	0.80
1:C:312:ALA:HB3	1:C:342:PRO:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:CD	1:C:121:TYR:OH	2.28	0.80
1:C:225:SER:N	1:C:226:GLU:HG2	1.96	0.80
1:C:322:PHE:CD1	1:C:329:VAL:HG13	2.17	0.80
1:B:383:PHE:CZ	1:B:385:ILE:HD12	2.17	0.80
1:B:250:TRP:CH2	1:B:433:GLY:HA3	2.17	0.80
1:C:214:GLN:OE1	1:C:216:CYS:SG	2.40	0.79
1:C:215:LEU:HD11	1:C:399:MET:CE	2.12	0.79
1:B:294:ASN:HB2	1:B:384:ALA:O	1.82	0.79
1:A:366:TYR:O	1:A:384:ALA:HB3	1.83	0.79
1:A:361:ILE:HG23	1:A:365:GLN:CB	2.13	0.79
1:B:287:ILE:HD12	2:E:4:TVA:H48	0.79	0.79
1:C:283:TYR:HD2	1:C:445:TYR:CE1	2.01	0.79
1:C:205:THR:HG22	1:C:206:HIS:H	1.45	0.79
1:B:356:SER:O	1:B:435:PHE:HB2	1.83	0.78
1:C:225:SER:N	1:C:226:GLU:HA	1.98	0.78
1:B:270:ASN:ND2	1:B:342:PRO:CB	2.46	0.78
1:B:113:TYR:HE2	1:B:121:TYR:HE1	1.26	0.78
1:A:87:THR:HG22	1:A:111:ARG:NH1	1.99	0.78
1:A:340:ILE:HD11	1:A:341:PHE:CD1	2.18	0.78
1:A:294:ASN:HB3	1:A:384:ALA:O	1.83	0.78
1:A:340:ILE:CD1	1:A:341:PHE:CD1	2.66	0.78
1:B:283:TYR:CE2	1:B:445:TYR:CE2	2.71	0.78
1:B:350:GLY:CA	1:B:355:GLN:O	2.26	0.78
1:B:299:LYS:O	1:B:303:GLU:HG3	1.84	0.77
1:B:103:ALA:HB2	1:B:162:ALA:HB1	1.65	0.77
1:B:436:VAL:O	1:B:436:VAL:HG13	1.85	0.77
1:B:332:GLN:HA	1:B:378:ASP:OD1	1.85	0.77
1:B:328:LEU:HD23	1:B:370:VAL:CG2	2.14	0.77
1:B:438:LEU:HD12	1:B:439:ASP:N	1.99	0.77
1:A:365:GLN:O	1:A:397:VAL:HB	1.85	0.77
1:B:263:ILE:HD13	1:B:440:MET:HG3	1.66	0.77
1:B:115:ARG:HD2	1:B:121:TYR:CE2	2.20	0.77
1:C:320:ASP:OD1	1:C:321:GLY:N	2.18	0.77
2:F:1:GLU:OE1	2:F:3:TIH:HE1	1.84	0.77
1:A:361:ILE:HG23	1:A:365:GLN:HG3	1.67	0.76
1:C:225:SER:CA	1:C:226:GLU:HG2	2.11	0.76
1:C:366:TYR:OH	1:C:383:PHE:CZ	2.36	0.76
1:C:132:TYR:HB2	1:C:135:GLY:O	1.84	0.76
1:A:329:VAL:HG21	1:A:331:TRP:HH2	1.50	0.76
1:A:68:ARG:NH1	1:A:228:LEU:HA	2.01	0.76
1:A:293:THR:OG1	2:D:2:ILE:HG12	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ARG:HA	1:B:386:SER:O	1.86	0.76
1:B:349:MET:HE1	1:B:440:MET:CA	2.15	0.76
1:C:265:VAL:HA	1:C:278:CYS:SG	2.26	0.76
1:B:105:PRO:HG3	1:B:112:TYR:CE2	2.21	0.75
1:B:222:LEU:HD23	1:B:223:ASN:O	1.86	0.75
1:C:328:LEU:HD21	1:C:380:CYS:HB3	1.66	0.75
1:C:367:LEU:HD22	1:C:383:PHE:HA	1.68	0.75
1:B:283:TYR:CD2	1:B:445:TYR:HE2	1.98	0.75
1:C:322:PHE:CA	1:C:327:GLN:HB2	2.15	0.75
1:A:134:GLN:CB	2:D:3:TIH:HB3	2.17	0.75
1:C:65:ASP:HB3	1:C:231:VAL:HG21	1.69	0.75
1:C:115:ARG:HD2	1:C:121:TYR:OH	1.87	0.75
1:A:244:LEU:HD22	1:A:403:TYR:CE1	2.21	0.75
1:B:270:ASN:ND2	1:B:342:PRO:HB3	2.02	0.75
1:C:363:PRO:O	1:C:366:TYR:N	2.20	0.75
1:C:331:TRP:HZ3	1:C:381:TYR:HD2	0.81	0.74
1:A:361:ILE:CG2	1:A:365:GLN:HB2	2.18	0.74
1:B:328:LEU:CD2	1:B:370:VAL:HG23	2.18	0.74
1:C:283:TYR:CD2	1:C:445:TYR:CE1	2.76	0.74
1:C:205:THR:HG21	1:C:207:VAL:HG23	1.70	0.74
1:A:361:ILE:HG23	1:A:365:GLN:CG	2.17	0.74
1:C:358:ARG:NH2	1:C:432:GLU:OE1	2.21	0.74
1:C:322:PHE:CE1	1:C:329:VAL:HG13	2.22	0.74
1:A:219:GLY:O	1:A:220:PHE:CD1	2.40	0.73
1:B:113:TYR:HE2	1:B:121:TYR:CE1	2.06	0.73
1:C:309:ILE:HD13	1:C:366:TYR:CZ	2.23	0.73
1:A:329:VAL:CG2	1:A:331:TRP:CZ3	2.64	0.73
1:C:115:ARG:HD3	1:C:121:TYR:OH	1.88	0.73
1:C:421:HIS:CE1	1:C:429:ALA:HB3	2.22	0.73
1:A:103:ALA:CB	1:A:162:ALA:HB1	2.19	0.73
1:A:349:MET:HA	1:A:440:MET:CE	2.19	0.73
1:B:66:ASN:ND2	1:B:235:MET:H	1.86	0.73
1:B:372:ASP:OD1	1:B:373:VAL:N	2.20	0.73
1:B:222:LEU:HD11	1:B:227:VAL:HA	1.70	0.72
1:C:367:LEU:CD2	1:C:383:PHE:HD1	2.01	0.72
1:B:66:ASN:HD21	1:B:235:MET:H	1.36	0.72
1:C:254:ILE:O	1:C:411:LYS:HE2	1.89	0.72
1:A:273:ASP:OD1	1:A:275:LYS:N	2.21	0.72
1:B:404:VAL:HG22	1:B:415:PHE:CD1	2.24	0.72
1:C:250:TRP:CH2	1:C:433:GLY:HA3	2.23	0.72
1:C:76:TYR:OH	1:C:175:ASN:ND2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:VAL:HG22	1:C:78:GLU:N	2.04	0.72
1:C:312:ALA:HB1	1:C:342:PRO:HD3	1.70	0.72
1:C:65:ASP:N	1:C:234:SER:HB3	2.02	0.72
1:B:332:GLN:HB3	1:B:378:ASP:OD1	1.90	0.72
1:C:322:PHE:N	1:C:327:GLN:HB2	2.05	0.72
1:B:244:LEU:CD2	1:B:403:TYR:CE1	2.73	0.71
1:C:367:LEU:HD21	1:C:383:PHE:HD1	1.54	0.71
1:B:294:ASN:OD1	1:B:296:ARG:HG2	1.90	0.71
1:C:205:THR:CG2	1:C:206:HIS:N	2.53	0.71
1:B:332:GLN:CB	1:B:378:ASP:OD1	2.38	0.71
1:C:78:GLU:O	1:C:149:PRO:HD3	1.90	0.71
1:C:106:HIS:CG	1:C:107:PRO:HD3	2.25	0.71
1:C:336:THR:CB	1:C:338:TRP:CH2	2.74	0.71
1:A:138:GLU:CD	1:C:61:VAL:HG22	2.10	0.71
1:C:350:GLY:CA	1:C:355:GLN:OE1	2.38	0.71
1:A:283:TYR:HD1	1:A:445:TYR:CE2	2.09	0.70
1:B:222:LEU:HD11	1:B:227:VAL:CA	2.21	0.70
1:B:349:MET:HE2	1:B:440:MET:CA	2.21	0.70
1:C:322:PHE:CE1	1:C:329:VAL:HG22	2.25	0.70
1:B:113:TYR:CE2	1:B:121:TYR:CE1	2.79	0.70
1:C:78:GLU:O	1:C:149:PRO:CD	2.39	0.70
1:B:270:ASN:ND2	1:B:342:PRO:HB2	2.06	0.70
1:B:404:VAL:HG22	1:B:415:PHE:HD1	1.56	0.70
1:C:70:LYS:HG2	1:C:72:GLY:N	2.06	0.70
1:C:368:ARG:HG3	1:C:369:PRO:HD2	1.73	0.70
1:C:279:LYS:HA	1:C:443:CYS:O	1.92	0.70
1:C:265:VAL:HG12	1:C:443:CYS:SG	2.32	0.70
1:B:108:PHE:CE2	1:B:172:ASN:CB	2.68	0.70
1:A:349:MET:HA	1:A:440:MET:HE1	1.73	0.70
1:C:350:GLY:CA	1:C:355:GLN:O	2.37	0.69
1:B:349:MET:HE2	1:B:440:MET:N	2.06	0.69
1:B:397:VAL:HG23	1:B:398:ILE:HD13	1.74	0.69
1:B:336:THR:HB	1:B:338:TRP:CH2	2.28	0.69
1:A:218:ALA:HB2	1:A:222:LEU:HD11	1.74	0.69
1:A:402:PHE:HB3	1:A:416:ALA:O	1.93	0.69
1:B:332:GLN:CA	1:B:378:ASP:OD1	2.41	0.69
1:B:183:ALA:CB	1:B:187:ILE:HD11	2.22	0.69
1:C:205:THR:CG2	1:C:207:VAL:HG23	2.23	0.69
1:C:328:LEU:HD23	1:C:329:VAL:N	2.08	0.69
1:A:223:ASN:OD1	1:A:224:GLN:N	2.25	0.69
1:C:133:THR:HB	2:F:3:TIH:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TYR:HD2	1:A:138:GLU:HB3	1.59	0.68
1:B:365:GLN:NE2	1:B:401:GLY:HA3	2.07	0.68
1:C:322:PHE:CZ	1:C:329:VAL:HG22	2.28	0.68
1:A:339:ASN:OD1	1:A:340:ILE:N	2.25	0.68
1:B:115:ARG:CD	1:B:121:TYR:OH	2.40	0.68
1:B:349:MET:CE	1:B:440:MET:HB2	2.22	0.68
1:A:96:SER:O	1:A:181:GLY:CA	2.42	0.68
1:A:216:CYS:N	1:A:232:GLY:O	2.22	0.68
1:B:143:THR:C	1:B:157:ARG:HH12	1.94	0.68
1:B:66:ASN:OD1	1:B:67:LEU:N	2.27	0.68
1:B:383:PHE:HZ	1:B:385:ILE:HD12	1.58	0.68
1:A:244:LEU:HD22	1:A:403:TYR:HE1	1.56	0.68
1:B:65:ASP:H	1:B:234:SER:HB3	1.59	0.68
1:C:214:GLN:NE2	1:C:244:LEU:HG	2.09	0.68
1:A:258:TRP:HD1	1:A:258:TRP:H	1.42	0.68
1:A:66:ASN:OD1	1:A:67:LEU:N	2.27	0.68
1:A:338:TRP:CZ2	1:A:364:GLN:HG3	2.29	0.68
1:B:349:MET:HE1	1:B:440:MET:CB	2.25	0.67
1:C:283:TYR:HD2	1:C:445:TYR:CD1	2.11	0.67
1:A:192:ASP:OD1	1:A:193:SER:N	2.27	0.67
1:B:94:THR:HG22	1:B:182:LEU:CD1	2.21	0.67
1:C:299:LYS:HG3	1:C:387:GLN:OE1	1.94	0.67
1:A:103:ALA:HB2	1:A:162:ALA:HB1	1.76	0.67
1:A:259:TYR:HE1	2:D:4:TVA:C28	2.07	0.67
1:B:222:LEU:CD2	1:B:227:VAL:HB	2.23	0.67
1:C:274:LEU:HD13	1:C:276:MET:CE	2.25	0.67
1:C:70:LYS:O	1:C:74:GLY:N	2.28	0.67
1:A:299:LYS:O	1:A:303:GLU:CG	2.42	0.67
1:A:313:SER:CB	1:A:340:ILE:HD13	2.25	0.67
1:C:205:THR:CG2	1:C:206:HIS:H	2.08	0.67
1:C:329:VAL:HG23	1:C:331:TRP:CH2	2.30	0.67
1:C:413:ILE:CG2	1:C:415:PHE:CZ	2.78	0.67
1:A:123:ASP:OD1	1:A:125:ARG:N	2.20	0.67
1:B:96:SER:O	1:B:181:GLY:HA3	1.95	0.67
1:C:103:ALA:HB2	1:C:162:ALA:HB1	1.76	0.67
1:A:130:VAL:CG2	1:A:137:TRP:CZ2	2.78	0.66
1:A:216:CYS:CB	1:A:232:GLY:O	2.43	0.66
1:A:83:SER:HA	1:A:84:PRO:C	2.13	0.66
1:C:115:ARG:HD3	1:C:121:TYR:CZ	2.28	0.66
1:A:90:ILE:HD12	1:A:178:GLY:HA3	1.75	0.66
1:C:149:PRO:CD	1:C:150:HIS:H	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:HA3	1:A:355:GLN:OE1	1.95	0.66
1:C:413:ILE:HG21	1:C:415:PHE:CZ	2.30	0.66
1:B:404:VAL:HG13	1:B:415:PHE:CE1	2.31	0.66
1:A:68:ARG:NH1	1:A:228:LEU:O	2.29	0.66
1:C:363:PRO:C	1:C:366:TYR:H	1.99	0.66
1:A:340:ILE:HD11	1:A:341:PHE:CD2	2.31	0.66
1:B:106:HIS:HE1	1:B:108:PHE:HD1	1.43	0.66
1:B:115:ARG:CG	1:B:121:TYR:CZ	2.79	0.66
1:A:289:ASP:OD1	1:A:291:GLY:N	2.27	0.66
1:A:244:LEU:O	1:A:419:ALA:CB	2.44	0.65
1:B:212:SER:HB3	1:B:403:TYR:CZ	2.31	0.65
1:B:268:GLU:HG2	1:B:273:ASP:HA	1.77	0.65
1:B:445:TYR:CD1	1:B:446:ASN:N	2.64	0.65
1:A:338:TRP:CZ3	1:A:364:GLN:HA	2.32	0.65
1:B:319:PRO:O	1:B:322:PHE:HB3	1.96	0.65
1:C:337:PRO:O	1:C:340:ILE:HG12	1.96	0.65
1:A:102:GLY:O	1:A:113:TYR:N	2.24	0.65
1:B:96:SER:O	1:B:181:GLY:CA	2.45	0.65
1:B:302:PHE:O	1:B:306:VAL:HG23	1.96	0.65
1:A:68:ARG:HH12	1:A:228:LEU:HG	1.60	0.65
1:A:338:TRP:CH2	1:A:364:GLN:HG3	2.32	0.65
1:A:130:VAL:HG21	1:A:137:TRP:CH2	2.32	0.65
1:A:371:GLU:HG3	1:A:372:ASP:OD1	1.96	0.65
1:A:340:ILE:HD12	1:A:341:PHE:CD1	2.31	0.65
1:B:322:PHE:CD2	1:B:329:VAL:HG11	2.31	0.65
1:C:118:SER:HB3	1:C:121:TYR:HB2	1.79	0.65
1:C:282:ASN:ND2	1:C:286:SER:OG	2.30	0.65
1:A:179:ILE:CD1	2:D:4:TVA:S2	2.85	0.65
1:B:259:TYR:HD1	2:E:4:TVA:C30	1.96	0.65
1:B:411:LYS:O	1:B:411:LYS:HG2	1.97	0.65
1:C:295:LEU:HD22	1:C:398:ILE:HD11	1.79	0.65
1:B:363:PRO:HA	1:B:366:TYR:CE2	2.33	0.64
1:B:377:GLN:OE1	1:B:377:GLN:N	2.20	0.64
1:A:169:PHE:HE1	2:D:4:TVA:S2	2.20	0.64
1:B:65:ASP:HA	1:B:233:GLY:O	1.97	0.64
1:C:225:SER:N	1:C:226:GLU:CG	2.55	0.64
1:C:226:GLU:HB2	1:C:229:ALA:H	1.62	0.64
1:B:90:ILE:HG21	1:B:180:LEU:HB2	1.79	0.64
1:C:215:LEU:HD11	1:C:399:MET:HE2	1.80	0.64
1:A:322:PHE:O	1:A:325:GLY:N	2.30	0.64
1:B:140:GLU:OE2	1:B:164:THR:CG2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLY:HA2	1:B:227:VAL:HG21	1.80	0.64
1:A:244:LEU:CD2	1:A:403:TYR:CE1	2.80	0.64
1:A:283:TYR:OH	1:C:225:SER:CB	2.45	0.64
1:B:184:TYR:OH	1:B:254:ILE:HD13	1.98	0.64
1:A:210:LEU:O	1:A:238:GLY:N	2.30	0.64
1:B:262:VAL:O	1:B:286:SER:HB2	1.98	0.64
1:B:425:GLU:HB2	1:B:426:PHE:CE1	2.33	0.64
1:A:115:ARG:CD	1:A:121:TYR:CZ	2.81	0.64
1:A:145:LEU:HD21	1:A:157:ARG:HE	1.63	0.64
1:B:255:ARG:NH2	1:B:445:TYR:O	2.31	0.64
2:F:3:TIH:O	2:F:4:TVA:H37	1.98	0.64
1:B:292:THR:HA	2:E:2:ILE:O	1.98	0.63
1:A:283:TYR:CD1	1:A:445:TYR:CE2	2.86	0.63
1:C:283:TYR:O	1:C:391:GLY:HA2	1.98	0.63
1:C:295:LEU:HD13	1:C:398:ILE:CD1	2.28	0.63
1:C:336:THR:HG21	1:C:338:TRP:CE2	2.33	0.63
1:A:350:GLY:H	1:A:440:MET:HE1	1.63	0.63
1:A:361:ILE:CG2	1:A:365:GLN:CB	2.76	0.63
1:B:294:ASN:OD1	1:B:296:ARG:CG	2.46	0.63
1:A:82:GLY:CA	1:A:144:ASP:OD2	2.45	0.63
1:B:97:SER:N	1:B:183:ALA:HB3	2.14	0.63
1:B:265:VAL:HG21	1:B:437:THR:CB	2.28	0.63
1:B:343:VAL:HG12	1:B:362:LEU:HD23	1.80	0.63
1:A:366:TYR:O	1:A:384:ALA:CB	2.46	0.63
1:B:115:ARG:HG3	3:B:505:HOH:O	1.98	0.63
1:B:283:TYR:CD2	1:B:445:TYR:CD2	2.78	0.63
1:C:314:SER:O	1:C:315:THR:CB	2.47	0.63
1:A:227:VAL:HA	1:A:230:SER:HB2	1.81	0.63
1:C:309:ILE:HD13	1:C:366:TYR:CE1	2.33	0.63
2:E:1:GLU:OE1	2:E:3:TIH:HE1	1.98	0.63
1:C:256:ARG:HD3	1:C:258:TRP:CD1	2.34	0.62
1:C:364:GLN:NE2	1:C:424:ASP:OD2	2.32	0.62
1:A:259:TYR:CE1	2:D:4:TVA:C28	2.81	0.62
1:C:250:TRP:CZ2	1:C:433:GLY:HA3	2.34	0.62
1:B:349:MET:HE1	1:B:440:MET:HB2	1.80	0.62
1:A:179:ILE:HD12	2:D:4:TVA:S2	2.39	0.62
1:C:120:THR:HB	1:C:157:ARG:HH12	1.63	0.62
1:B:418:SER:O	1:B:421:HIS:ND1	2.32	0.62
1:C:309:ILE:HG21	1:C:366:TYR:OH	1.99	0.62
1:C:149:PRO:HD2	1:C:150:HIS:H	1.64	0.62
1:A:328:LEU:HD22	1:A:370:VAL:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PHE:HA	1:C:327:GLN:HB2	1.81	0.62
1:A:174:SER:CB	1:A:176:TRP:CD1	2.78	0.62
1:A:328:LEU:C	1:A:328:LEU:HD12	2.19	0.62
1:A:223:ASN:O	1:A:227:VAL:N	2.31	0.62
1:A:322:PHE:CD1	1:A:329:VAL:HG13	2.34	0.62
1:B:115:ARG:CD	1:B:121:TYR:CZ	2.82	0.62
1:C:182:LEU:HD13	1:C:211:PHE:CZ	2.34	0.62
1:C:336:THR:HG21	1:C:338:TRP:CZ2	2.35	0.62
1:A:189:ARG:O	1:A:194:LEU:HD23	1.99	0.61
1:B:258:TRP:HD1	1:B:258:TRP:H	1.47	0.61
1:B:269:ILE:O	1:B:270:ASN:CG	2.38	0.61
1:C:363:PRO:CG	1:C:364:GLN:OE1	2.48	0.61
1:A:87:THR:CG2	1:A:111:ARG:HH12	2.11	0.61
1:C:336:THR:HB	1:C:338:TRP:CE3	2.34	0.61
1:C:366:TYR:HD2	1:C:367:LEU:HG	1.64	0.61
1:C:215:LEU:CD1	1:C:399:MET:HE2	2.31	0.61
1:A:364:GLN:HE22	1:A:424:ASP:HB2	1.64	0.61
1:B:89:ASN:HB2	1:B:176:TRP:HA	1.83	0.61
1:B:283:TYR:CE2	1:B:445:TYR:HE2	2.14	0.61
1:A:411:LYS:O	1:A:411:LYS:HG2	2.01	0.61
1:B:332:GLN:HA	1:B:378:ASP:CA	2.30	0.61
1:C:134:GLN:HB2	2:F:3:TIH:N	2.15	0.61
1:A:122:ARG:HH22	1:A:157:ARG:HB3	1.66	0.61
1:B:79:MET:SD	1:B:90:ILE:HG13	2.41	0.61
1:A:122:ARG:HH12	1:A:157:ARG:CD	2.01	0.61
1:B:436:VAL:O	1:B:436:VAL:CG1	2.49	0.61
1:C:215:LEU:CD1	1:C:399:MET:CE	2.79	0.61
2:D:1:GLU:OE1	2:D:3:TIH:HE1	2.01	0.61
1:C:411:LYS:O	1:C:411:LYS:HG2	1.99	0.61
1:B:73:GLN:HG2	1:B:171:ILE:HG21	1.83	0.61
1:C:296:ARG:NH1	1:C:387:GLN:O	2.34	0.61
1:B:337:PRO:HB2	1:B:340:ILE:HG12	1.83	0.60
1:B:115:ARG:HD2	1:B:121:TYR:CZ	2.36	0.60
1:B:179:ILE:HD12	2:E:4:TVA:S2	2.41	0.60
1:C:101:VAL:O	1:C:163:ILE:HG13	2.00	0.60
2:D:4:TVA:N	2:D:4:TVA:H30	2.16	0.60
1:A:130:VAL:HG12	1:A:132:TYR:CE2	2.37	0.60
1:C:67:LEU:HB2	1:C:233:GLY:O	2.00	0.60
1:C:201:LEU:O	1:C:205:THR:HB	2.01	0.60
1:A:210:LEU:HD11	1:A:239:GLY:N	2.16	0.60
1:C:312:ALA:CB	1:C:342:PRO:HD3	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:O	1:A:181:GLY:HA3	2.02	0.60
1:C:106:HIS:CE1	1:C:107:PRO:CD	2.73	0.60
1:C:212:SER:OG	1:C:405:VAL:HG22	2.01	0.60
1:C:329:VAL:O	1:C:380:CYS:HA	2.01	0.60
1:B:335:THR:HG22	1:B:335:THR:O	2.01	0.60
1:C:174:SER:O	1:C:175:ASN:HB3	2.02	0.60
1:B:81:VAL:HG12	1:B:146:VAL:HG22	1.84	0.60
1:B:83:SER:O	1:B:118:SER:HA	2.02	0.60
1:B:263:ILE:CD1	1:B:440:MET:HG3	2.32	0.60
1:C:77:VAL:HG22	1:C:78:GLU:H	1.65	0.60
1:C:258:TRP:HD1	1:C:258:TRP:H	1.50	0.60
1:C:376:SER:HB3	1:C:378:ASP:N	2.17	0.60
1:A:212:SER:HB3	1:A:403:TYR:CZ	2.37	0.59
1:B:374:ALA:C	1:B:376:SER:H	2.05	0.59
1:C:274:LEU:HB3	1:C:276:MET:CE	2.20	0.59
1:A:362:LEU:O	1:A:365:GLN:HB2	2.01	0.59
1:A:128:VAL:HG22	1:A:129:TYR:N	2.17	0.59
1:B:80:THR:HA	1:B:86:GLN:O	2.02	0.59
1:C:225:SER:HA	1:C:226:GLU:HG3	0.63	0.59
1:A:130:VAL:CG1	1:A:132:TYR:CE2	2.86	0.59
1:B:107:PRO:HD2	1:B:108:PHE:H	1.67	0.59
1:C:270:ASN:HB2	1:C:342:PRO:HB2	1.84	0.59
1:C:307:LYS:O	1:C:310:LYS:N	2.34	0.59
1:C:329:VAL:CG2	1:C:331:TRP:CH2	2.85	0.59
1:C:367:LEU:HD23	1:C:383:PHE:HA	1.85	0.59
1:A:219:GLY:O	1:A:220:PHE:HD1	1.82	0.59
1:B:145:LEU:HD23	1:B:155:THR:HG21	1.83	0.59
1:C:210:LEU:HD11	1:C:239:GLY:N	2.18	0.59
1:A:198:PHE:O	1:A:202:VAL:HG23	2.03	0.59
1:B:115:ARG:HD3	1:B:121:TYR:OH	2.03	0.59
1:B:250:TRP:CZ2	1:B:433:GLY:HA3	2.38	0.59
1:B:106:HIS:CE1	1:B:108:PHE:HD1	2.20	0.59
1:B:313:SER:HA	1:B:340:ILE:HG22	1.83	0.59
1:C:274:LEU:O	1:C:275:LYS:HB2	2.01	0.59
1:A:294:ASN:CB	1:A:384:ALA:O	2.51	0.58
1:B:293:THR:HG21	2:E:1:GLU:HB3	1.86	0.58
1:B:363:PRO:CD	1:B:427:ARG:NH2	2.66	0.58
1:C:312:ALA:CB	1:C:342:PRO:CD	2.82	0.58
1:A:101:VAL:HG12	1:A:102:GLY:N	2.17	0.58
1:B:283:TYR:O	1:B:391:GLY:HA2	2.03	0.58
1:B:349:MET:CE	1:B:440:MET:CB	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:SER:C	1:B:183:ALA:HB3	2.22	0.58
1:B:295:LEU:HB2	1:B:398:ILE:HD11	1.84	0.58
1:C:362:LEU:HD11	1:C:428:THR:HA	1.84	0.58
1:C:363:PRO:HG2	1:C:364:GLN:OE1	2.03	0.58
1:A:135:GLY:O	1:A:136:LYS:HG3	2.03	0.58
1:A:145:LEU:CD2	1:A:157:ARG:HG3	2.33	0.58
1:B:133:THR:OG1	2:E:3:TIH:HB2	2.03	0.58
1:B:66:ASN:OD1	1:B:67:LEU:CD2	2.52	0.58
1:B:76:TYR:CD2	1:B:89:ASN:HB3	2.39	0.58
1:B:113:TYR:CE2	1:B:121:TYR:HE1	2.12	0.58
1:B:174:SER:O	1:B:175:ASN:HB3	2.04	0.58
1:B:284:ASP:OD1	1:B:285:LYS:N	2.37	0.58
1:C:273:ASP:O	1:C:275:LYS:HG3	2.04	0.58
1:A:292:THR:HG21	1:A:296:ARG:HD2	1.86	0.57
1:A:340:ILE:HD11	1:A:341:PHE:CG	2.38	0.57
1:B:94:THR:HB	1:B:260:TYR:CE2	2.39	0.57
1:C:68:ARG:CG	1:C:231:VAL:HG12	2.31	0.57
1:C:93:ASP:HA	1:C:290:SER:OG	2.04	0.57
1:A:306:VAL:O	1:A:310:LYS:HG3	2.03	0.57
1:B:143:THR:HB	1:B:157:ARG:HH11	1.68	0.57
1:A:88:LEU:CD1	1:A:101:VAL:HG11	2.35	0.57
1:A:259:TYR:CZ	2:D:4:TVA:H42	2.39	0.57
1:B:86:GLN:NE2	1:B:114:GLN:O	2.37	0.57
1:B:124:LEU:CD1	1:B:143:THR:HG23	2.30	0.57
1:C:216:CYS:HB2	1:C:232:GLY:O	2.05	0.57
1:A:183:ALA:CB	1:A:187:ILE:HD11	2.34	0.57
1:A:340:ILE:CD1	1:A:341:PHE:CG	2.87	0.57
1:B:368:ARG:CG	1:B:369:PRO:HD2	2.33	0.57
1:C:83:SER:HA	1:C:84:PRO:C	2.23	0.57
1:B:204:GLN:C	1:B:205:THR:HG23	2.25	0.57
1:B:268:GLU:HA	1:B:272:GLN:O	2.04	0.57
1:C:182:LEU:CD1	1:C:211:PHE:CE2	2.86	0.57
1:A:287:ILE:CD1	1:A:289:ASP:HB2	2.34	0.57
1:B:374:ALA:HB3	1:B:376:SER:HB2	1.86	0.57
1:B:171:ILE:HB	1:B:174:SER:HB3	1.87	0.57
1:B:210:LEU:HD11	1:B:239:GLY:CA	2.35	0.57
1:B:306:VAL:HG12	1:B:310:LYS:HE3	1.86	0.57
1:B:406:PHE:N	1:B:406:PHE:CD1	2.73	0.57
1:C:73:GLN:OE1	1:C:174:SER:HA	2.05	0.57
1:C:406:PHE:N	1:C:406:PHE:CD1	2.73	0.57
1:C:171:ILE:HD11	2:F:2:ILE:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:SER:HB3	1:A:184:TYR:O	2.05	0.56
1:A:355:GLN:HG2	1:A:356:SER:N	2.19	0.56
1:B:420:CYS:O	1:B:420:CYS:SG	2.63	0.56
1:C:103:ALA:CB	1:C:162:ALA:HB1	2.35	0.56
1:C:225:SER:N	1:C:226:GLU:CA	2.66	0.56
1:C:336:THR:CG2	1:C:338:TRP:CE2	2.88	0.56
1:A:174:SER:CB	1:A:176:TRP:NE1	2.59	0.56
1:A:320:ASP:HA	1:A:323:TRP:HD1	1.70	0.56
1:A:397:VAL:HG23	1:A:398:ILE:N	2.20	0.56
1:B:97:SER:OG	1:B:188:ALA:HA	2.06	0.56
1:B:115:ARG:HG2	1:B:121:TYR:CE1	2.39	0.56
1:B:199:ASP:OD1	1:B:408:ARG:NH2	2.38	0.56
1:B:349:MET:SD	1:B:440:MET:HB2	2.45	0.56
1:C:171:ILE:HB	1:C:174:SER:HB3	1.86	0.56
1:C:254:ILE:HB	1:C:411:LYS:HG2	1.87	0.56
1:C:426:PHE:CD1	1:C:426:PHE:N	2.73	0.56
1:B:108:PHE:CD2	1:B:172:ASN:CA	2.88	0.56
1:A:240:ILE:HA	1:A:403:TYR:OH	2.06	0.56
1:B:265:VAL:HG12	1:B:443:CYS:SG	2.46	0.56
1:C:352:VAL:HG12	1:C:353:THR:N	2.20	0.56
1:A:210:LEU:O	1:A:238:GLY:HA2	2.06	0.56
1:C:175:ASN:ND2	1:C:228:LEU:CD2	2.61	0.56
1:C:438:LEU:O	1:C:439:ASP:HB2	2.04	0.56
1:B:336:THR:HG21	1:B:338:TRP:CZ2	2.40	0.56
1:C:270:ASN:HB2	1:C:342:PRO:CB	2.36	0.56
1:C:349:MET:HE2	1:C:440:MET:HB3	1.86	0.56
1:A:78:GLU:O	1:A:149:PRO:HD2	2.06	0.56
1:A:183:ALA:HB1	1:A:187:ILE:HD11	1.88	0.56
1:B:269:ILE:N	1:B:272:GLN:O	2.37	0.56
1:C:60:PHE:O	1:C:62:GLU:N	2.38	0.56
1:A:117:LEU:HD23	1:A:117:LEU:N	2.21	0.56
1:A:319:PRO:HB2	1:A:327:GLN:NE2	2.21	0.56
1:B:284:ASP:OD1	1:B:390:THR:O	2.24	0.56
1:C:106:HIS:HE1	1:C:108:PHE:CD2	2.23	0.56
1:A:129:TYR:OH	1:A:136:LYS:HD3	2.06	0.56
1:A:258:TRP:CG	1:A:259:TYR:N	2.69	0.56
1:B:106:HIS:HE1	1:B:108:PHE:CD1	2.24	0.56
1:B:184:TYR:OH	1:B:254:ILE:CD1	2.54	0.56
1:B:222:LEU:HD22	1:B:227:VAL:HB	1.88	0.56
1:B:424:ASP:OD1	1:B:427:ARG:O	2.24	0.56
1:C:295:LEU:HD13	1:C:398:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HA	1:A:386:SER:O	2.06	0.55
1:A:363:PRO:C	1:A:365:GLN:N	2.57	0.55
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.69	0.55
1:A:299:LYS:HB2	1:A:387:GLN:OE1	2.07	0.55
1:B:363:PRO:HG2	1:B:427:ARG:NH2	2.19	0.55
1:C:216:CYS:N	1:C:232:GLY:O	2.37	0.55
1:A:244:LEU:CD2	1:A:403:TYR:HE1	2.17	0.55
1:C:241:ASP:CB	1:C:244:LEU:HD13	2.33	0.55
1:C:376:SER:HB3	1:C:377:GLN:C	2.27	0.55
1:A:174:SER:O	1:A:175:ASN:HB3	2.07	0.55
1:A:218:ALA:HB2	1:A:222:LEU:CD1	2.37	0.55
1:B:204:GLN:C	1:B:205:THR:CG2	2.75	0.55
1:B:212:SER:HB3	1:B:403:TYR:OH	2.07	0.55
1:C:68:ARG:O	1:C:76:TYR:CE2	2.59	0.55
1:A:130:VAL:CG2	1:A:137:TRP:CH2	2.90	0.55
1:A:258:TRP:N	1:A:258:TRP:CD1	2.72	0.55
1:C:117:LEU:HD12	1:C:117:LEU:N	2.21	0.55
1:C:384:ALA:HB1	1:C:397:VAL:HG11	1.87	0.55
1:A:293:THR:OG1	2:D:2:ILE:N	2.38	0.55
1:A:328:LEU:HD13	1:A:380:CYS:HB3	1.87	0.55
1:A:359:ILE:HG22	1:A:431:VAL:HG13	1.88	0.55
1:B:68:ARG:HA	1:B:232:GLY:H	1.72	0.55
1:B:268:GLU:HG2	1:B:273:ASP:CA	2.36	0.55
1:C:113:TYR:OH	1:C:144:ASP:OD2	2.23	0.55
1:C:132:TYR:HE2	1:C:137:TRP:HE1	1.53	0.55
1:C:277:ASP:OD1	1:C:278:CYS:N	2.40	0.55
1:A:221:PRO:HG2	1:A:371:GLU:HA	1.88	0.55
1:A:283:TYR:O	1:A:391:GLY:HA2	2.07	0.55
1:B:352:VAL:O	1:B:355:GLN:O	2.25	0.55
1:B:354:ASN:O	1:B:435:PHE:O	2.25	0.55
1:B:377:GLN:H	1:B:377:GLN:CD	2.06	0.55
1:C:115:ARG:HD3	1:C:121:TYR:CE2	2.38	0.55
2:D:3:TIH:O	2:D:4:TVA:H38	2.07	0.55
1:A:66:ASN:OD1	1:A:67:LEU:HG	2.07	0.55
1:A:362:LEU:HB3	1:A:364:GLN:OE1	2.06	0.55
1:C:295:LEU:CD2	1:C:398:ILE:HD11	2.37	0.55
1:C:312:ALA:HB1	1:C:342:PRO:CD	2.36	0.55
1:B:76:TYR:HD2	1:B:89:ASN:HB3	1.71	0.55
1:C:109:LEU:HD22	1:C:177:GLU:HG3	1.88	0.55
1:A:174:SER:HB2	1:A:176:TRP:HE1	1.64	0.54
1:A:259:TYR:CE1	2:D:4:TVA:H42	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:CG	1:B:259:TYR:N	2.75	0.54
1:C:106:HIS:CD2	1:C:107:PRO:HD3	2.41	0.54
1:C:128:VAL:HG22	1:C:129:TYR:N	2.22	0.54
1:C:363:PRO:CA	1:C:366:TYR:CB	2.62	0.54
1:A:190:PRO:O	1:A:191:ASP:OD1	2.25	0.54
1:B:63:MET:HG2	1:B:151:GLY:HA2	1.89	0.54
1:B:313:SER:HA	1:B:340:ILE:CG2	2.37	0.54
1:B:328:LEU:HD23	1:B:370:VAL:HG23	1.81	0.54
1:B:357:PHE:N	1:B:357:PHE:CD1	2.76	0.54
1:C:77:VAL:CG2	1:C:78:GLU:N	2.70	0.54
1:A:66:ASN:OD1	1:A:67:LEU:HD23	2.08	0.54
1:C:362:LEU:O	1:C:365:GLN:OE1	2.25	0.54
1:C:441:GLU:OE1	1:C:441:GLU:HA	2.07	0.54
1:B:66:ASN:HD21	1:B:235:MET:HB3	1.72	0.54
1:B:362:LEU:HB3	1:B:364:GLN:OE1	2.08	0.54
1:C:347:TYR:CD2	1:C:358:ARG:HB3	2.42	0.54
1:A:129:TYR:CE2	1:C:61:VAL:CG1	2.62	0.54
1:B:66:ASN:HD21	1:B:235:MET:N	2.04	0.54
1:B:129:TYR:CD2	1:B:138:GLU:CG	2.81	0.54
1:C:137:TRP:HB2	1:C:163:ILE:HG23	1.89	0.54
1:C:226:GLU:OE1	1:C:228:LEU:HB2	2.07	0.54
1:A:115:ARG:HD3	1:A:121:TYR:CZ	2.43	0.54
2:D:4:TVA:N	2:D:4:TVA:C21	2.70	0.54
1:B:97:SER:OG	1:B:188:ALA:CA	2.55	0.53
1:A:294:ASN:ND2	2:D:1:GLU:OE2	2.42	0.53
1:B:212:SER:CB	1:B:403:TYR:OH	2.56	0.53
1:C:218:ALA:HB2	1:C:222:LEU:CD1	2.38	0.53
1:A:129:TYR:HA	1:A:138:GLU:HA	1.91	0.53
1:A:292:THR:HA	2:D:2:ILE:O	2.08	0.53
1:B:265:VAL:HG21	1:B:437:THR:HB	1.90	0.53
1:B:280:GLU:OE2	1:B:300:LYS:HD2	2.08	0.53
1:B:282:ASN:OD1	1:B:286:SER:OG	2.21	0.53
1:C:362:LEU:CD2	1:C:427:ARG:HB2	2.39	0.53
1:C:362:LEU:C	1:C:364:GLN:N	2.58	0.53
1:B:121:TYR:N	1:B:144:ASP:OD1	2.42	0.53
1:C:60:PHE:C	1:C:62:GLU:N	2.58	0.53
1:B:204:GLN:O	1:B:205:THR:HG22	2.08	0.53
1:B:265:VAL:HA	1:B:443:CYS:SG	2.49	0.53
1:A:200:SER:O	1:A:204:GLN:HG3	2.09	0.53
1:A:250:TRP:CH2	1:A:433:GLY:HA3	2.44	0.53
1:B:259:TYR:CE1	2:E:4:TVA:C30	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASN:O	1:B:284:ASP:O	2.27	0.52
1:A:259:TYR:CE1	2:D:4:TVA:H43	2.32	0.52
1:B:118:SER:OG	1:B:144:ASP:OD2	2.22	0.52
1:B:251:TYR:CD1	1:B:414:GLY:HA3	2.45	0.52
1:C:106:HIS:CD2	1:C:107:PRO:CD	2.92	0.52
1:C:212:SER:OG	1:C:405:VAL:HG13	2.09	0.52
1:A:101:VAL:CG1	1:A:102:GLY:N	2.72	0.52
1:B:157:ARG:HG3	1:B:157:ARG:NH1	2.24	0.52
1:B:374:ALA:C	1:B:376:SER:N	2.63	0.52
1:B:425:GLU:CB	1:B:426:PHE:CE1	2.93	0.52
1:C:80:THR:HA	1:C:86:GLN:O	2.10	0.52
1:C:330:CYS:HA	1:C:379:ASP:O	2.09	0.52
1:C:336:THR:HB	1:C:338:TRP:CZ2	2.44	0.52
1:A:328:LEU:HD22	1:A:370:VAL:HG23	1.91	0.52
1:B:310:LYS:O	1:B:314:SER:N	2.43	0.52
1:B:396:ALA:O	1:B:400:GLU:HG3	2.10	0.52
1:A:210:LEU:O	1:A:238:GLY:CA	2.57	0.52
1:B:133:THR:OG1	2:E:3:TIH:CB	2.58	0.52
1:B:383:PHE:CE2	1:B:385:ILE:HB	2.44	0.52
1:C:244:LEU:HD22	1:C:403:TYR:CE1	2.44	0.52
1:C:296:ARG:HA	1:C:386:SER:O	2.10	0.52
1:C:322:PHE:CD1	1:C:327:GLN:O	2.62	0.52
1:A:129:TYR:CD2	1:A:138:GLU:HB3	2.41	0.52
1:C:362:LEU:HD21	1:C:427:ARG:CB	2.40	0.52
2:F:3:TIH:O	2:F:4:TVA:C26	2.58	0.52
1:A:283:TYR:OH	1:C:225:SER:OG	2.26	0.52
1:A:293:THR:O	1:A:397:VAL:HG13	2.11	0.52
1:B:94:THR:HG22	1:B:182:LEU:HB2	1.92	0.52
1:A:212:SER:CB	1:A:403:TYR:OH	2.58	0.51
1:B:204:GLN:O	1:B:205:THR:CG2	2.58	0.51
1:C:67:LEU:CD2	1:C:77:VAL:HB	2.39	0.51
1:C:352:VAL:CG1	1:C:353:THR:N	2.74	0.51
1:C:258:TRP:CD1	1:C:258:TRP:N	2.78	0.51
1:C:373:VAL:HG23	1:C:374:ALA:N	2.25	0.51
1:C:256:ARG:HD3	1:C:258:TRP:NE1	2.25	0.51
1:C:265:VAL:C	1:C:266:ARG:HG2	2.30	0.51
1:C:295:LEU:CD1	1:C:398:ILE:HG13	2.35	0.51
1:A:64:VAL:O	1:A:65:ASP:HB2	2.09	0.51
1:B:328:LEU:HD21	1:B:370:VAL:HG23	1.81	0.51
1:B:362:LEU:HG	1:B:429:ALA:HB2	1.91	0.51
1:A:115:ARG:HD2	1:A:121:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HG2	1:C:61:VAL:HG21	1.93	0.51
1:A:211:PHE:CE1	1:A:406:PHE:CD2	2.99	0.51
1:B:410:ARG:HD3	1:B:412:ARG:HH21	1.75	0.51
1:C:78:GLU:HG2	1:C:149:PRO:HG3	1.92	0.51
1:C:79:MET:HE2	1:C:146:VAL:CG1	2.41	0.51
1:C:268:GLU:HB3	1:C:273:ASP:HA	1.92	0.51
1:C:365:GLN:NE2	1:C:421:HIS:CE1	2.79	0.51
1:A:67:LEU:HB2	1:A:233:GLY:O	2.10	0.51
1:A:371:GLU:CG	1:A:372:ASP:OD1	2.58	0.51
1:A:396:ALA:O	1:A:400:GLU:HG3	2.11	0.51
1:B:293:THR:O	1:B:397:VAL:HG13	2.10	0.51
1:A:210:LEU:CD1	1:A:239:GLY:N	2.73	0.51
1:B:137:TRP:HB2	1:B:163:ILE:CG2	2.41	0.51
1:B:222:LEU:CD2	1:B:223:ASN:O	2.56	0.51
1:C:367:LEU:HD21	1:C:383:PHE:CD1	2.40	0.51
1:A:138:GLU:HG2	1:C:61:VAL:CG2	2.41	0.51
1:A:319:PRO:O	1:A:322:PHE:N	2.33	0.51
1:A:372:ASP:HB2	1:A:374:ALA:O	2.11	0.51
1:B:295:LEU:HD12	1:B:393:VAL:O	2.10	0.51
1:B:336:THR:HG21	1:B:338:TRP:CE2	2.46	0.51
1:B:349:MET:HG2	1:B:350:GLY:O	2.10	0.51
1:C:362:LEU:HB3	1:C:363:PRO:CD	2.36	0.51
1:A:78:GLU:HG2	1:A:149:PRO:HG3	1.92	0.50
1:A:318:PHE:HD2	1:A:323:TRP:CZ2	2.29	0.50
1:C:174:SER:O	1:C:175:ASN:CB	2.60	0.50
1:A:131:PRO:HD2	1:A:189:ARG:HE	1.76	0.50
1:C:93:ASP:OD2	2:F:4:TVA:O6	2.30	0.50
1:A:145:LEU:HD21	1:A:157:ARG:CG	2.38	0.50
1:A:283:TYR:HH	1:C:225:SER:CB	2.22	0.50
1:B:372:ASP:CG	1:B:380:CYS:SG	2.90	0.50
1:C:132:TYR:HE2	1:C:137:TRP:NE1	2.08	0.50
1:C:249:LEU:CD2	1:C:416:ALA:HB2	2.36	0.50
1:B:93:ASP:O	1:B:181:GLY:HA2	2.12	0.50
1:B:249:LEU:HD23	1:B:416:ALA:HB2	1.94	0.50
1:C:77:VAL:CG2	1:C:78:GLU:H	2.24	0.50
1:A:338:TRP:CE3	1:A:363:PRO:HG2	2.47	0.50
2:D:1:GLU:OE1	2:D:3:TIH:CE1	2.60	0.50
1:A:189:ARG:HA	1:A:190:PRO:C	2.32	0.50
1:A:445:TYR:CD1	1:A:445:TYR:C	2.85	0.50
1:C:152:PRO:HD3	1:C:237:ILE:HD12	1.94	0.50
1:C:336:THR:CB	1:C:338:TRP:CZ2	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:SER:HB3	1:C:378:ASP:H	1.76	0.50
2:D:3:TIH:O	2:D:4:TVA:C25	2.59	0.50
1:C:60:PHE:O	1:C:61:VAL:C	2.47	0.50
1:A:118:SER:HB3	1:A:121:TYR:HB2	1.93	0.50
1:A:244:LEU:HD23	1:A:403:TYR:CD1	2.46	0.50
1:A:262:VAL:O	1:A:286:SER:HB2	2.12	0.50
1:B:222:LEU:HG	1:B:226:GLU:HB3	1.94	0.50
1:B:265:VAL:CG2	1:B:437:THR:HB	2.42	0.50
1:C:149:PRO:CG	1:C:150:HIS:N	2.75	0.50
1:A:254:ILE:O	1:A:411:LYS:HE2	2.12	0.50
1:B:137:TRP:HB2	1:B:163:ILE:HG23	1.92	0.50
1:B:445:TYR:CD1	1:B:445:TYR:C	2.85	0.50
1:C:332:GLN:HA	1:C:378:ASP:CB	2.42	0.50
1:A:68:ARG:NH1	1:A:228:LEU:CA	2.73	0.49
1:C:69:GLY:HA2	1:C:227:VAL:CG2	2.42	0.49
1:B:251:TYR:HA	1:B:414:GLY:HA2	1.93	0.49
1:C:83:SER:O	1:C:118:SER:HA	2.12	0.49
1:B:235:MET:HE2	1:B:237:ILE:HD11	1.95	0.49
1:B:359:ILE:O	1:B:359:ILE:HG13	2.10	0.49
1:A:227:VAL:O	1:A:230:SER:O	2.30	0.49
1:A:369:PRO:HA	1:A:381:TYR:HD1	1.77	0.49
1:B:144:ASP:N	1:B:157:ARG:HH12	2.10	0.49
1:C:324:LEU:HB2	1:C:326:GLU:HG2	1.93	0.49
1:C:344:ILE:HD11	1:C:366:TYR:HD1	1.77	0.49
1:B:258:TRP:CD1	1:B:258:TRP:N	2.80	0.49
1:C:421:HIS:NE2	1:C:429:ALA:HB2	2.22	0.49
1:C:62:GLU:HG3	1:C:63:MET:HG2	1.93	0.49
1:C:350:GLY:N	1:C:355:GLN:O	2.46	0.49
1:C:404:VAL:HG13	1:C:415:PHE:CE2	2.47	0.49
1:A:356:SER:HB3	1:A:440:MET:HE3	1.95	0.49
1:A:371:GLU:CD	1:A:372:ASP:H	2.15	0.49
1:A:197:PHE:O	1:A:200:SER:HB2	2.13	0.49
1:C:307:LYS:CG	1:C:308:SER:N	2.75	0.49
1:A:328:LEU:HD21	1:A:373:VAL:CG1	2.43	0.49
1:C:347:TYR:CE2	1:C:358:ARG:HB3	2.48	0.49
1:A:66:ASN:OD1	1:A:67:LEU:CD2	2.60	0.48
1:A:221:PRO:HG3	1:A:370:VAL:C	2.34	0.48
1:A:241:ASP:HB3	1:A:244:LEU:HD13	1.94	0.48
1:A:282:ASN:OD1	1:A:286:SER:OG	2.22	0.48
1:A:313:SER:HB2	1:A:340:ILE:HD13	1.94	0.48
1:C:208:PRO:HD2	1:C:238:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:HD3	1:A:121:TYR:CE1	2.47	0.48
1:A:328:LEU:CD1	1:A:330:CYS:SG	3.01	0.48
1:B:125:ARG:NE	3:B:506:HOH:O	2.45	0.48
1:C:213:LEU:HD12	1:C:406:PHE:CE1	2.48	0.48
1:C:368:ARG:O	1:C:381:TYR:HA	2.13	0.48
1:A:115:ARG:HG2	1:A:121:TYR:CE1	2.48	0.48
1:A:313:SER:HB3	1:A:340:ILE:CD1	2.43	0.48
1:C:312:ALA:HB1	1:C:342:PRO:CG	2.42	0.48
1:A:315:THR:CG2	1:B:340:ILE:HD11	2.33	0.48
1:B:244:LEU:O	1:B:419:ALA:N	2.43	0.48
1:C:139:GLY:HA2	1:C:164:THR:HG23	1.94	0.48
1:A:105:PRO:HD3	1:A:112:TYR:CE2	2.48	0.48
1:B:258:TRP:CD1	1:B:259:TYR:N	2.81	0.48
1:B:369:PRO:HA	1:B:381:TYR:HD1	1.78	0.48
1:C:362:LEU:O	1:C:365:GLN:N	2.45	0.48
1:B:210:LEU:HD11	1:B:239:GLY:HA2	1.95	0.48
1:C:355:GLN:N	1:C:440:MET:HE1	2.28	0.48
2:F:3:TIH:C	2:F:4:TVA:H30	2.44	0.48
1:B:333:ALA:HB2	1:B:377:GLN:O	2.14	0.48
1:C:67:LEU:O	1:C:231:VAL:HB	2.14	0.48
1:C:312:ALA:HB3	1:C:342:PRO:CG	2.35	0.48
1:C:96:SER:O	1:C:181:GLY:CA	2.62	0.48
1:C:102:GLY:O	1:C:112:TYR:HB2	2.14	0.48
1:C:62:GLU:HG3	1:C:63:MET:CG	2.44	0.48
2:D:3:TIH:O	2:D:4:TVA:C26	2.62	0.48
1:A:129:TYR:CZ	1:C:64:VAL:HB	2.49	0.47
1:A:338:TRP:O	1:A:341:PHE:N	2.41	0.47
1:B:82:GLY:O	1:B:85:PRO:HA	2.14	0.47
1:B:343:VAL:CG1	1:B:362:LEU:HD23	2.42	0.47
1:C:244:LEU:CD2	1:C:403:TYR:CE1	2.97	0.47
1:C:331:TRP:CE3	1:C:381:TYR:CD2	2.97	0.47
1:C:413:ILE:HG22	1:C:415:PHE:CZ	2.42	0.47
1:A:173:GLY:HA2	1:A:224:GLN:OE1	2.11	0.47
1:B:84:PRO:HB2	1:B:85:PRO:HD2	1.95	0.47
2:E:2:ILE:C	2:E:3:TIH:HD	2.35	0.47
1:A:128:VAL:CG2	1:A:129:TYR:N	2.77	0.47
1:A:350:GLY:CA	1:A:355:GLN:OE1	2.61	0.47
1:A:361:ILE:HG22	1:A:362:LEU:O	2.14	0.47
1:B:174:SER:O	1:B:175:ASN:CB	2.62	0.47
1:C:60:PHE:C	1:C:62:GLU:H	2.17	0.47
1:C:251:TYR:HA	1:C:414:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LYS:O	1:B:74:GLY:N	2.47	0.47
1:B:325:GLY:O	1:B:382:LYS:HD3	2.14	0.47
1:A:260:TYR:OH	1:A:408:ARG:NH1	2.48	0.47
1:A:66:ASN:OD1	1:A:67:LEU:CG	2.63	0.47
1:B:189:ARG:O	1:B:194:LEU:CD2	2.63	0.47
1:B:225:SER:O	1:B:228:LEU:HB3	2.14	0.47
1:B:336:THR:CG2	1:B:338:TRP:CE2	2.98	0.47
1:B:365:GLN:HE22	1:B:401:GLY:HA3	1.79	0.47
1:C:93:ASP:O	1:C:181:GLY:HA2	2.14	0.47
1:C:286:SER:HA	1:C:392:THR:HB	1.97	0.47
1:C:328:LEU:HD23	1:C:328:LEU:C	2.35	0.47
1:A:445:TYR:O	1:A:446:ASN:OD1	2.32	0.47
1:C:76:TYR:CD1	1:C:89:ASN:HB3	2.49	0.47
1:C:227:VAL:HG13	1:C:228:LEU:N	2.29	0.47
1:C:295:LEU:CD1	1:C:398:ILE:HD11	2.44	0.47
1:B:425:GLU:HB2	1:B:426:PHE:CD1	2.50	0.47
1:C:324:LEU:CB	1:C:326:GLU:HG2	2.45	0.47
1:A:130:VAL:HG11	1:A:132:TYR:CE2	2.50	0.47
1:B:222:LEU:HD21	1:B:227:VAL:HB	1.93	0.47
1:A:355:GLN:HG2	1:A:356:SER:H	1.79	0.46
1:B:191:ASP:OD1	1:B:193:SER:OG	2.28	0.46
1:B:222:LEU:HD21	1:B:227:VAL:CB	2.45	0.46
1:C:66:ASN:OD1	1:C:67:LEU:HG	2.15	0.46
1:C:134:GLN:N	2:F:3:TIH:HB3	2.29	0.46
1:A:96:SER:HB3	1:A:132:TYR:HE1	1.81	0.46
1:A:115:ARG:CD	1:A:121:TYR:CE1	2.98	0.46
1:A:364:GLN:NE2	1:A:424:ASP:HB2	2.30	0.46
1:B:107:PRO:CD	1:B:108:PHE:H	2.26	0.46
1:B:196:PRO:HG2	1:B:199:ASP:OD2	2.16	0.46
1:B:359:ILE:HG22	1:B:431:VAL:HG13	1.97	0.46
1:C:418:SER:O	1:C:421:HIS:HB2	2.15	0.46
1:A:283:TYR:HA	1:A:284:ASP:HA	1.50	0.46
1:A:319:PRO:C	1:A:321:GLY:N	2.67	0.46
1:B:101:VAL:O	1:B:163:ILE:HG13	2.15	0.46
1:B:338:TRP:HZ2	1:B:381:TYR:HH	1.63	0.46
1:C:70:LYS:HG2	1:C:71:SER:N	2.30	0.46
1:A:265:VAL:HG23	1:A:266:ARG:N	2.30	0.46
1:B:68:ARG:HD2	1:B:227:VAL:O	2.15	0.46
1:B:296:ARG:HB3	1:B:388:SER:HB2	1.97	0.46
1:C:328:LEU:HD12	1:C:382:LYS:HE3	1.96	0.46
1:C:336:THR:CG2	1:C:338:TRP:CZ2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:SER:CB	1:A:184:TYR:O	2.64	0.46
1:A:268:GLU:HA	1:A:272:GLN:O	2.15	0.46
1:B:259:TYR:CE1	2:E:4:TVA:H42	2.50	0.46
1:B:118:SER:HB3	1:B:121:TYR:HB2	1.97	0.46
1:B:244:LEU:HD23	1:B:403:TYR:CD1	2.50	0.46
1:B:322:PHE:CE2	1:B:329:VAL:CG1	2.96	0.46
1:B:404:VAL:CG1	1:B:415:PHE:CE1	2.98	0.46
1:A:311:ALA:HA	1:A:314:SER:OG	2.15	0.46
1:B:62:GLU:HA	1:B:62:GLU:OE1	2.16	0.46
1:B:383:PHE:CZ	1:B:385:ILE:HB	2.51	0.46
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.51	0.46
1:B:125:ARG:CD	3:B:506:HOH:O	2.63	0.46
1:C:344:ILE:HD11	1:C:366:TYR:CD1	2.50	0.46
1:C:149:PRO:CG	1:C:150:HIS:H	2.28	0.46
1:A:93:ASP:O	1:A:181:GLY:HA2	2.16	0.45
1:B:336:THR:CG2	1:B:338:TRP:CZ2	2.99	0.45
1:C:68:ARG:HD3	1:C:228:LEU:HA	1.98	0.45
1:C:171:ILE:CD1	2:F:2:ILE:CG2	2.95	0.45
1:C:205:THR:HG22	1:C:207:VAL:H	1.80	0.45
1:C:307:LYS:O	1:C:310:LYS:HB2	2.17	0.45
1:A:60:PHE:N	1:A:62:GLU:OE1	2.50	0.45
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.73	0.45
1:A:132:TYR:O	1:A:133:THR:C	2.54	0.45
1:A:187:ILE:HD13	1:A:258:TRP:O	2.16	0.45
1:A:216:CYS:CA	1:A:232:GLY:O	2.64	0.45
1:B:176:TRP:CE3	1:B:176:TRP:O	2.70	0.45
1:C:331:TRP:CE3	1:C:381:TYR:CE2	3.04	0.45
1:A:283:TYR:OH	1:C:225:SER:HB2	2.15	0.45
1:B:322:PHE:HE2	1:B:329:VAL:HG22	1.80	0.45
1:C:79:MET:HE2	1:C:146:VAL:HG11	1.98	0.45
1:A:210:LEU:HD11	1:A:239:GLY:CA	2.46	0.45
1:A:251:TYR:CD1	1:A:414:GLY:HA3	2.51	0.45
1:A:293:THR:HG1	2:D:2:ILE:HG12	1.79	0.45
1:A:349:MET:HG2	1:A:350:GLY:O	2.16	0.45
1:C:397:VAL:HG23	1:C:398:ILE:N	2.30	0.45
1:A:338:TRP:CZ3	1:A:364:GLN:CA	2.99	0.45
1:C:182:LEU:O	1:C:260:TYR:OH	2.24	0.45
1:C:279:LYS:HE3	1:C:442:ASP:O	2.17	0.45
1:A:221:PRO:CG	1:A:370:VAL:C	2.84	0.45
1:B:108:PHE:CE2	1:B:172:ASN:CA	2.99	0.45
1:B:124:LEU:HD13	1:B:142:GLY:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ILE:HG13	1:C:361:ILE:O	2.15	0.45
1:C:362:LEU:HD21	1:C:427:ARG:HB2	1.98	0.45
1:C:375:THR:O	1:C:376:SER:HB2	2.17	0.45
1:A:318:PHE:CD2	1:A:323:TRP:CZ2	3.05	0.45
1:A:441:GLU:C	1:A:443:CYS:N	2.67	0.45
1:B:75:TYR:OH	1:B:400:GLU:OE1	2.35	0.45
1:B:184:TYR:HD2	1:B:258:TRP:O	2.00	0.45
1:C:218:ALA:HB2	1:C:222:LEU:HD13	1.98	0.45
1:B:94:THR:HA	1:B:182:LEU:HB2	1.99	0.45
1:C:266:ARG:HB2	1:C:347:TYR:CD1	2.52	0.45
1:A:115:ARG:HB3	1:A:121:TYR:CG	2.52	0.45
1:A:298:PRO:HD2	1:A:301:VAL:HB	1.98	0.45
1:C:70:LYS:NZ	1:C:368:ARG:HD2	2.32	0.45
1:C:117:LEU:N	1:C:117:LEU:CD1	2.80	0.45
1:C:176:TRP:O	1:C:176:TRP:CE3	2.69	0.45
1:A:122:ARG:HB2	1:A:143:THR:OG1	2.16	0.44
1:A:204:GLN:C	1:A:205:THR:HG23	2.37	0.44
1:C:118:SER:HG	1:C:144:ASP:CG	2.20	0.44
1:C:149:PRO:CD	1:C:150:HIS:N	2.72	0.44
1:C:321:GLY:O	1:C:324:LEU:HB2	2.18	0.44
1:C:330:CYS:HB3	1:C:378:ASP:O	2.17	0.44
1:A:92:VAL:HG13	1:A:182:LEU:HD11	1.99	0.44
1:A:313:SER:HB3	1:A:340:ILE:HD13	1.99	0.44
1:A:436:VAL:CG2	1:B:436:VAL:HB	2.47	0.44
1:A:192:ASP:O	1:A:193:SER:C	2.55	0.44
1:B:143:THR:HB	1:B:157:ARG:NH1	2.32	0.44
1:C:96:SER:O	1:C:181:GLY:HA3	2.17	0.44
1:C:421:HIS:NE2	1:C:429:ALA:CB	2.79	0.44
1:A:310:LYS:HE2	1:A:323:TRP:CD1	2.52	0.44
1:C:322:PHE:CE1	1:C:328:LEU:HA	2.53	0.44
2:D:3:TIH:N	2:D:4:TVA:H30	2.33	0.44
1:C:242:HIS:CD2	1:C:242:HIS:N	2.85	0.44
1:A:103:ALA:HB3	1:A:162:ALA:HB1	1.97	0.44
1:A:256:ARG:O	1:A:258:TRP:HD1	2.01	0.44
1:A:341:PHE:HA	1:A:342:PRO:HD3	1.58	0.44
1:B:174:SER:HB2	1:B:176:TRP:NE1	2.33	0.44
1:B:439:ASP:O	1:B:443:CYS:HB2	2.18	0.44
1:B:250:TRP:O	1:B:414:GLY:HA2	2.18	0.44
1:B:263:ILE:CG2	1:B:443:CYS:HB3	2.47	0.44
1:A:328:LEU:HD22	1:A:370:VAL:HG21	2.00	0.43
1:A:363:PRO:HA	1:A:366:TYR:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:SER:CB	1:B:183:ALA:O	2.66	0.43
1:A:60:PHE:CZ	1:A:239:GLY:HA3	2.53	0.43
1:A:401:GLY:O	1:A:418:SER:HB2	2.18	0.43
1:C:299:LYS:O	1:C:303:GLU:HG3	2.19	0.43
1:C:269:ILE:HG22	1:C:342:PRO:HB2	2.00	0.43
1:C:283:TYR:CE2	1:C:445:TYR:CE1	3.06	0.43
1:C:292:THR:HA	2:F:2:ILE:O	2.18	0.43
1:A:153:ASN:C	1:A:154:VAL:HG13	2.37	0.43
1:A:258:TRP:CD1	1:A:259:TYR:N	2.81	0.43
1:A:282:ASN:O	1:A:284:ASP:C	2.56	0.43
1:A:302:PHE:O	1:A:306:VAL:HG23	2.19	0.43
1:A:318:PHE:HD2	1:A:323:TRP:HZ2	1.66	0.43
1:B:351:GLU:OE1	1:B:412:ARG:HD2	2.18	0.43
1:A:112:TYR:CD1	1:A:112:TYR:N	2.87	0.43
1:B:78:GLU:O	1:B:148:ILE:HG23	2.19	0.43
1:B:132:TYR:HB2	1:B:135:GLY:O	2.18	0.43
1:C:71:SER:HB2	1:C:396:ALA:CB	2.48	0.43
1:A:135:GLY:O	1:A:136:LYS:CG	2.66	0.43
1:A:313:SER:HA	1:A:340:ILE:HB	2.01	0.43
1:A:359:ILE:O	1:A:359:ILE:HG13	2.17	0.43
1:C:362:LEU:C	1:C:364:GLN:H	2.21	0.43
1:C:407:ASP:O	1:C:411:LYS:N	2.52	0.43
1:A:278:CYS:HA	1:A:281:TYR:CD2	2.54	0.43
1:A:378:ASP:O	1:A:379:ASP:C	2.57	0.43
1:C:104:ALA:HB1	1:C:105:PRO:HD2	2.00	0.43
1:C:109:LEU:CD2	1:C:177:GLU:HG3	2.49	0.43
1:C:295:LEU:HD13	1:C:398:ILE:HG12	1.90	0.43
1:A:266:ARG:HB3	1:A:347:TYR:CD1	2.54	0.43
1:B:120:THR:O	1:B:157:ARG:NH2	2.51	0.43
1:C:68:ARG:O	1:C:76:TYR:CD2	2.72	0.43
1:C:115:ARG:NH1	1:C:140:GLU:OE1	2.44	0.43
1:C:210:LEU:CD1	1:C:239:GLY:N	2.82	0.43
1:C:363:PRO:O	1:C:364:GLN:C	2.54	0.43
1:A:197:PHE:CD1	1:A:197:PHE:C	2.92	0.43
1:A:244:LEU:HD23	1:A:403:TYR:CE1	2.54	0.43
1:C:81:VAL:HG23	1:C:81:VAL:O	2.18	0.43
1:A:89:ASN:O	1:A:90:ILE:HD13	2.18	0.42
1:A:362:LEU:CB	1:A:364:GLN:OE1	2.67	0.42
1:B:234:SER:OG	1:B:244:LEU:HD21	2.19	0.42
1:C:115:ARG:HD2	1:C:121:TYR:CE1	2.47	0.42
1:B:167:ASP:OD1	1:B:168:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:MET:HA	1:B:356:SER:HB3	2.01	0.42
1:A:102:GLY:O	1:A:112:TYR:HB2	2.18	0.42
1:A:250:TRP:CZ2	1:A:433:GLY:HA3	2.54	0.42
1:B:120:THR:O	1:B:122:ARG:CG	2.56	0.42
1:B:182:LEU:HD13	1:B:211:PHE:HZ	1.57	0.42
1:C:244:LEU:O	1:C:419:ALA:CB	2.67	0.42
1:C:359:ILE:O	1:C:359:ILE:HG13	2.19	0.42
1:C:362:LEU:O	1:C:363:PRO:C	2.58	0.42
1:A:103:ALA:HA	1:A:113:TYR:O	2.19	0.42
1:A:315:THR:HG21	1:B:340:ILE:CD1	2.35	0.42
1:C:171:ILE:O	1:C:174:SER:HB3	2.19	0.42
1:C:322:PHE:CZ	1:C:329:VAL:CG2	3.00	0.42
1:A:328:LEU:CD2	1:A:370:VAL:HG21	2.49	0.42
1:B:299:LYS:O	1:B:303:GLU:CG	2.63	0.42
1:C:212:SER:HB2	1:C:403:TYR:OH	2.19	0.42
1:C:250:TRP:CZ2	1:C:433:GLY:CA	3.01	0.42
1:C:364:GLN:HB2	1:C:365:GLN:OE1	2.20	0.42
1:A:279:LYS:HA	1:A:443:CYS:O	2.19	0.42
1:A:332:GLN:O	1:A:335:THR:OG1	2.30	0.42
1:B:189:ARG:O	1:B:194:LEU:HD23	2.19	0.42
1:B:329:VAL:O	1:B:380:CYS:HA	2.19	0.42
1:B:374:ALA:HB3	1:B:376:SER:CB	2.49	0.42
1:C:97:SER:HB3	1:C:184:TYR:O	2.20	0.42
1:A:68:ARG:O	1:A:75:TYR:HA	2.19	0.42
1:C:362:LEU:HD22	1:C:427:ARG:HB2	2.01	0.42
1:A:90:ILE:CD1	1:A:178:GLY:HA3	2.47	0.42
1:A:204:GLN:C	1:A:205:THR:CG2	2.87	0.42
1:A:210:LEU:C	1:A:210:LEU:HD12	2.41	0.42
1:A:363:PRO:C	1:A:365:GLN:H	2.21	0.42
1:A:397:VAL:CG2	1:A:398:ILE:N	2.82	0.42
1:B:227:VAL:HG13	1:B:228:LEU:N	2.33	0.42
1:C:93:ASP:OD1	1:C:95:GLY:N	2.36	0.42
1:A:281:TYR:O	1:A:392:THR:OG1	2.38	0.42
1:A:338:TRP:CE2	1:A:364:GLN:HG3	2.55	0.42
1:A:340:ILE:CD1	1:A:341:PHE:CD2	3.00	0.41
1:A:407:ASP:HB3	1:A:412:ARG:HG2	2.02	0.41
1:B:93:ASP:OD1	1:B:291:GLY:HA3	2.20	0.41
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.81	0.41
1:C:249:LEU:HD23	1:C:416:ALA:CB	2.40	0.41
1:C:331:TRP:CZ3	1:C:381:TYR:CE2	3.01	0.41
1:A:310:LYS:HG2	1:A:323:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:SER:OG	1:C:244:LEU:HD21	2.20	0.41
1:C:273:ASP:OD1	1:C:274:LEU:N	2.54	0.41
1:A:130:VAL:HG11	1:A:132:TYR:CZ	2.55	0.41
1:A:131:PRO:CG	1:A:189:ARG:HH21	2.33	0.41
1:A:363:PRO:O	1:A:364:GLN:C	2.57	0.41
1:B:134:GLN:HB2	2:E:3:TIH:HB3	2.01	0.41
1:C:192:ASP:OD1	1:C:192:ASP:N	2.51	0.41
1:A:115:ARG:HB3	1:A:121:TYR:CD2	2.55	0.41
1:A:123:ASP:OD1	1:A:124:LEU:N	2.53	0.41
1:A:319:PRO:O	1:A:321:GLY:N	2.53	0.41
1:B:61:VAL:O	1:B:62:GLU:C	2.58	0.41
1:B:210:LEU:HD12	1:B:210:LEU:C	2.40	0.41
1:B:222:LEU:HD11	1:B:227:VAL:N	2.35	0.41
1:C:214:GLN:HE22	1:C:244:LEU:HG	1.82	0.41
1:C:227:VAL:CG1	1:C:228:LEU:N	2.82	0.41
1:C:285:LYS:O	1:C:392:THR:N	2.53	0.41
1:B:294:ASN:ND2	1:B:386:SER:OG	2.53	0.41
1:C:61:VAL:HA	1:C:64:VAL:HG23	2.01	0.41
1:C:225:SER:C	1:C:226:GLU:HG3	2.32	0.41
1:C:362:LEU:O	1:C:364:GLN:N	2.53	0.41
1:C:373:VAL:CG2	1:C:374:ALA:N	2.84	0.41
1:A:361:ILE:HG22	1:A:365:GLN:HB2	2.01	0.41
1:B:91:LEU:HD12	1:B:176:TRP:CE2	2.56	0.41
1:C:125:ARG:O	1:C:125:ARG:HG3	2.19	0.41
1:C:363:PRO:O	1:C:367:LEU:N	2.45	0.41
1:A:132:TYR:C	1:A:134:GLN:N	2.74	0.41
1:B:322:PHE:HE2	1:B:329:VAL:CG2	2.33	0.41
1:C:134:GLN:CA	2:F:3:TIH:HB3	2.50	0.41
1:C:183:ALA:CB	1:C:187:ILE:HD11	2.50	0.41
1:C:279:LYS:HE2	1:C:444:GLY:O	2.20	0.41
1:A:302:PHE:CZ	1:A:306:VAL:HG21	2.55	0.41
1:B:365:GLN:HE21	1:B:401:GLY:HA3	1.81	0.41
1:C:91:LEU:HD11	2:F:2:ILE:CD1	2.51	0.41
1:C:132:TYR:CD1	2:F:4:TVA:O6	2.73	0.41
1:A:195:GLU:HA	1:A:196:PRO:HD3	1.93	0.41
1:A:270:ASN:HA	1:B:270:ASN:O	2.21	0.41
1:B:104:ALA:HA	1:B:105:PRO:HD3	1.85	0.41
1:B:322:PHE:CE2	1:B:329:VAL:CG2	3.04	0.41
1:C:90:ILE:HG21	1:C:180:LEU:HB2	2.02	0.41
1:C:177:GLU:N	1:C:177:GLU:CD	2.73	0.41
1:C:216:CYS:O	1:C:232:GLY:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PRO:O	1:C:299:LYS:C	2.59	0.41
1:C:128:VAL:CG2	1:C:129:TYR:N	2.83	0.41
1:C:397:VAL:CG2	1:C:398:ILE:N	2.84	0.41
1:C:420:CYS:SG	1:C:420:CYS:O	2.79	0.41
1:A:197:PHE:O	1:A:200:SER:N	2.53	0.40
1:A:221:PRO:HD3	1:A:369:PRO:HB2	2.02	0.40
1:C:148:ILE:HG22	1:C:149:PRO:HD2	2.02	0.40
1:C:264:ILE:H	1:C:282:ASN:HD21	1.69	0.40
1:C:329:VAL:HG21	1:C:331:TRP:CH2	2.54	0.40
1:C:404:VAL:HG22	1:C:415:PHE:CD2	2.56	0.40
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.90	0.40
1:B:68:ARG:O	1:B:76:TYR:CD1	2.74	0.40
1:B:90:ILE:CG2	1:B:180:LEU:HB2	2.50	0.40
1:B:195:GLU:HA	1:B:196:PRO:HD2	1.89	0.40
1:B:213:LEU:HD23	1:B:235:MET:HA	2.01	0.40
1:C:210:LEU:HD12	1:C:210:LEU:C	2.42	0.40
1:C:265:VAL:HB	1:C:437:THR:HG21	2.03	0.40
1:C:362:LEU:HB3	1:C:364:GLN:OE1	2.20	0.40
1:B:128:VAL:HG22	1:B:129:TYR:N	2.37	0.40
1:A:97:SER:O	1:A:196:PRO:HB3	2.21	0.40
1:A:331:TRP:O	1:A:378:ASP:HB3	2.21	0.40
1:B:290:SER:HA	1:B:399:MET:CE	2.51	0.40
1:B:318:PHE:HA	1:B:319:PRO:HD2	1.93	0.40
1:A:366:TYR:C	1:A:384:ALA:HB3	2.42	0.40
1:B:251:TYR:CD1	1:B:414:GLY:CA	3.05	0.40
1:C:214:GLN:NE2	1:C:244:LEU:CG	2.83	0.40
1:C:251:TYR:CD1	1:C:414:GLY:CA	3.05	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	386/388 (100%)	382 (99%)	3 (1%)	1 (0%)	41	72
1	B	386/388 (100%)	377 (98%)	5 (1%)	4 (1%)	15	47
1	C	386/388 (100%)	379 (98%)	5 (1%)	2 (0%)	29	62
2	D	1/4 (25%)	1 (100%)	0	0	100	100
2	E	1/4 (25%)	1 (100%)	0	0	100	100
2	F	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1161/1176 (99%)	1141 (98%)	13 (1%)	7 (1%)	25	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	GLY
1	C	131	PRO
1	A	131	PRO
1	B	131	PRO
1	B	337	PRO
1	C	342	PRO
1	B	434	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	329 (99%)	2 (1%)	86	91
1	B	331/331 (100%)	326 (98%)	5 (2%)	65	80
1	C	331/331 (100%)	329 (99%)	2 (1%)	86	91
2	D	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	F	2/2 (100%)	2 (100%)	0	100	100
All	All	999/999 (100%)	989 (99%)	10 (1%)	76	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	TRP
1	A	420	CYS
1	B	258	TRP
1	B	278	CYS
1	B	356	SER
1	B	438	LEU
1	B	443	CYS
1	C	258	TRP
1	C	330	CYS
2	E	1	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	242	HIS
1	A	327	GLN
1	A	365	GLN
1	B	175	ASN
1	B	270	ASN
1	C	134	GLN
1	C	175	ASN
1	C	214	GLN
1	C	242	HIS
1	C	282	ASN
1	C	294	ASN
1	C	421	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)

6 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	TVA	D	4	2	19,19,19	0.85	0	14,24,24	3.85	3 (21%)
2	TIH	D	3	2	9,10,11	1.24	1 (11%)	3,12,14	5.10	1 (33%)
2	TVA	F	4	2	19,19,19	0.83	0	14,24,24	3.25	3 (21%)
2	TVA	E	4	2	19,19,19	0.73	0	14,24,24	2.84	3 (21%)
2	TIH	F	3	2	9,10,11	0.94	0	3,12,14	2.18	1 (33%)
2	TIH	E	3	2	9,10,11	1.98	2 (22%)	3,12,14	5.97	1 (33%)

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	TVA	D	4	2	-	12/19/20/20	0/1/1/1
2	TIH	D	3	2	-	1/4/6/8	0/1/1/1
2	TVA	F	4	2	-	7/19/20/20	0/1/1/1
2	TVA	E	4	2	-	3/19/20/20	0/1/1/1
2	TIH	F	3	2	-	0/4/6/8	0/1/1/1
2	TIH	E	3	2	-	0/4/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	TIH	CB-CG	-4.29	1.49	1.50
2	E	3	TIH	CG-SD	-3.24	1.67	1.73
2	D	3	TIH	CG-SD	-2.74	1.68	1.73

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	TVA	C25-C26-N5	11.81	142.23	112.00
2	E	3	TIH	CE1-CE2-SD	-10.30	104.62	112.98
2	F	4	TVA	C25-C26-N5	8.85	134.64	112.00
2	D	3	TIH	CE1-CE2-SD	-8.77	105.86	112.98
2	F	4	TVA	C22-C24-S2	-7.68	106.75	112.98
2	D	4	TVA	C22-C24-S2	-7.54	106.86	112.98
2	E	4	TVA	C22-C24-S2	-7.53	106.87	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	TVA	C25-C26-N5	6.70	129.15	112.00
2	F	3	TIH	CE1-CE2-SD	-3.67	110.00	112.98
2	E	4	TVA	C20-C19-CA	-2.23	109.39	113.37
2	F	4	TVA	C20-C19-CA	-2.21	109.43	113.37
2	D	4	TVA	C20-C19-CA	-2.18	109.49	113.37

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	TVA	C26-C25-CA-N
2	D	4	TVA	CA-C25-C26-N5
2	D	4	TVA	O6-C25-C26-N5
2	D	4	TVA	C25-C26-N5-C27
2	D	4	TVA	C-C27-N5-C26
2	E	4	TVA	N5-C27-C28-C29
2	F	4	TVA	O6-C25-C26-N5
2	D	4	TVA	C27-C28-C29-C30
2	F	4	TVA	C27-C28-C29-C30
2	E	4	TVA	C-C27-C28-C29
2	F	4	TVA	O-C-C27-N5
2	F	4	TVA	OXT-C-C27-N5
2	E	4	TVA	C27-C28-C29-C30
2	F	4	TVA	CA-C25-C26-N5
2	D	4	TVA	O-C-C27-N5
2	D	4	TVA	OXT-C-C27-N5
2	D	4	TVA	C26-C25-CA-C19
2	D	3	TIH	C-CA-CB-CG
2	D	4	TVA	CA-C19-C20-C21
2	F	4	TVA	N5-C27-C28-C29
2	F	4	TVA	C-C27-C28-C29
2	D	4	TVA	O6-C25-CA-C19
2	D	4	TVA	O6-C25-CA-N

There are no ring outliers.

6 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	TVA	16	0
2	D	3	TIH	8	0
2	F	4	TVA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	TVA	13	0
2	F	3	TIH	11	0
2	E	3	TIH	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	388/388 (100%)	0.06	15 (3%)	39	36	46, 73, 142, 201	0
1	B	388/388 (100%)	0.12	14 (3%)	42	39	49, 73, 128, 181	0
1	C	388/388 (100%)	0.34	21 (5%)	25	24	45, 77, 144, 210	0
2	D	2/4 (50%)	-0.39	0	100	100	20, 20, 20, 20	0
2	E	2/4 (50%)	-0.43	0	100	100	20, 20, 20, 20	0
2	F	2/4 (50%)	0.04	0	100	100	20, 20, 20, 20	0
All	All	1170/1176 (99%)	0.17	50 (4%)	35	33	20, 74, 140, 210	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	SER	12.4
1	C	225	SER	12.1
1	C	224	GLN	10.7
1	C	223	ASN	10.0
1	C	219	GLY	9.6
1	A	220	PHE	7.4
1	C	221	PRO	6.2
1	C	220	PHE	6.1
1	A	221	PRO	6.0
1	C	227	VAL	6.0
1	C	228	LEU	5.8
1	B	221	PRO	5.4
1	C	226	GLU	5.4
1	B	229	ALA	4.8
1	C	366	TYR	4.4
1	A	375	THR	4.4
1	A	226	GLU	4.3
1	B	220	PHE	4.1
1	C	222	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	229	ALA	4.0
1	A	224	GLN	3.9
1	B	226	GLU	3.6
1	A	373	VAL	3.6
1	B	230	SER	3.5
1	C	231	VAL	3.5
1	B	225	SER	3.3
1	A	225	SER	2.9
1	A	425	GLU	2.9
1	C	229	ALA	2.7
1	A	230	SER	2.6
1	B	223	ASN	2.6
1	B	112	TYR	2.5
1	B	377	GLN	2.5
1	C	69	GLY	2.5
1	A	238	GLY	2.4
1	B	228	LEU	2.4
1	B	447	ILE	2.3
1	A	376	SER	2.3
1	B	331	TRP	2.2
1	A	374	ALA	2.2
1	A	223	ASN	2.2
1	C	320	ASP	2.2
1	C	328	LEU	2.1
1	C	105	PRO	2.1
1	C	371	GLU	2.1
1	B	375	THR	2.1
1	A	426	PHE	2.1
1	C	114	GLN	2.1
1	B	113	TYR	2.1
1	C	212	SER	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, 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
2	TVA	E	4	19/19	0.69	0.40	20,20,20,20	0
2	TVA	F	4	19/19	0.75	0.36	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TIH	D	3	10/11	0.77	0.30	20,20,20,20	0
2	TVA	D	4	19/19	0.77	0.32	20,20,20,20	0
2	TIH	E	3	10/11	0.80	0.24	20,20,20,20	0
2	TIH	F	3	10/11	0.85	0.22	20,20,20,20	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.