



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:08 AM GMT

PDB ID : 3DET
Title : Structure of the E148A, Y445A doubly ungated mutant of E.coli CLC_Ec1,
Cl⁻/H⁺ antiporter
Authors : Jayaram, H.; Accardi, A.; Wu, F.; Williams, C.; Miller, C.
Deposited on : 2008-06-10
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

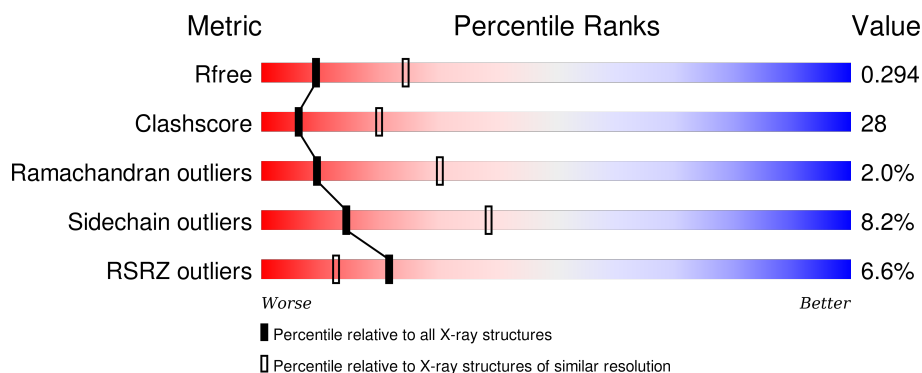
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	473	<div> <div>4%</div> <div>48% 41% 6%</div> </div>
1	B	473	<div> <div>7%</div> <div>45% 41% 7% 7%</div> </div>
2	C	221	<div> <div>5%</div> <div>63% 32% 5%</div> </div>
2	E	221	<div> <div>3%</div> <div>63% 34% .</div> </div>
3	D	211	<div> <div>9%</div> <div>52% 41% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	211	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (11%), green (53%), yellow (43%), and orange (1%). The segments are labeled with their respective percentages: 11%, 53%, 43%, and a small orange segment at the end. A small black dot is visible at the far right end of the bar.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13201 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3322	2182	560	560	20			
1	B	441	Total	C	N	O	S	0	0	0
			3293	2166	553	554	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	GLU	ENGINEERED	UNP P37019
A	445	ALA	TYR	ENGINEERED	UNP P37019
B	148	ALA	GLU	ENGINEERED	UNP P37019
B	445	ALA	TYR	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

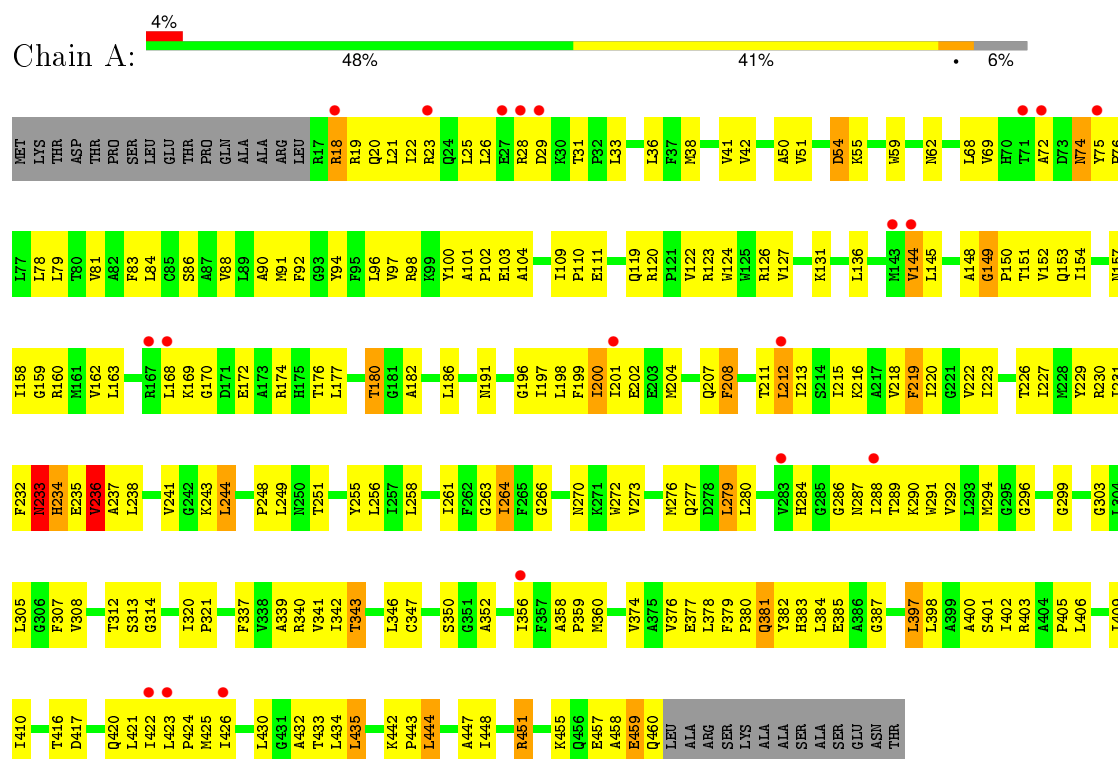
- Molecule 3 is a protein called Fab fragment, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

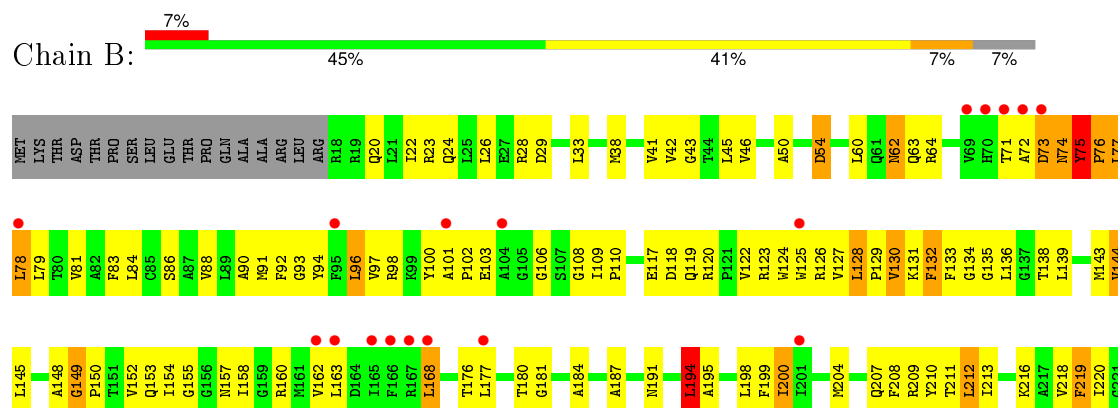
3 Residue-property plots

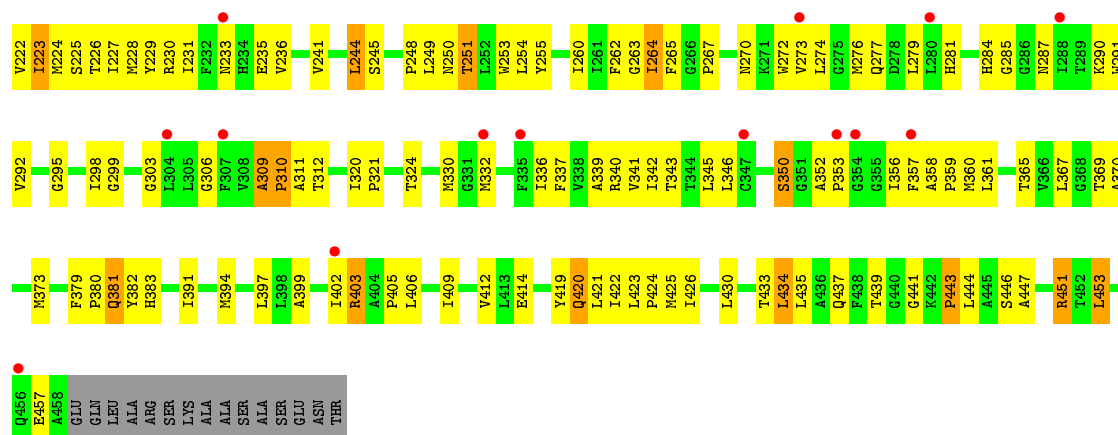
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: H(+)/Cl(-) exchange transporter clcA

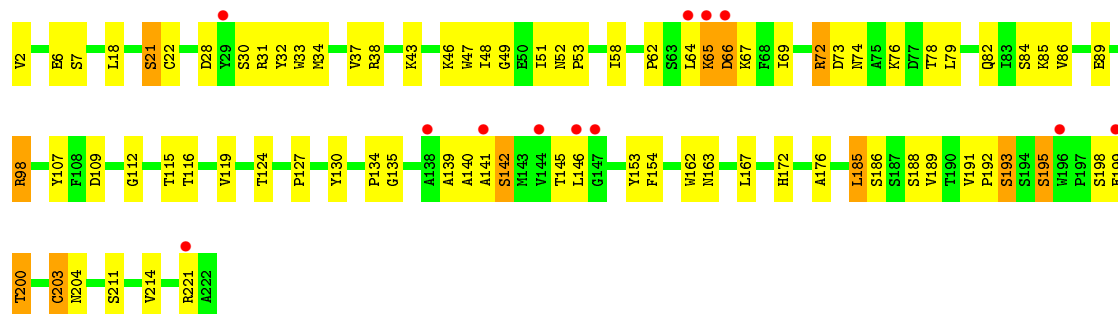


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

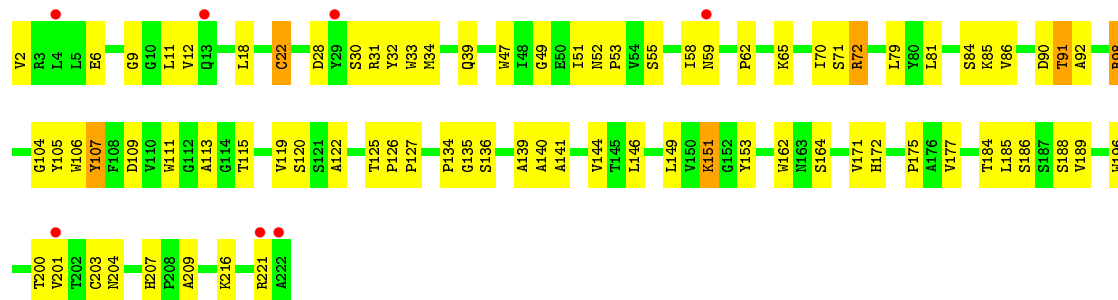




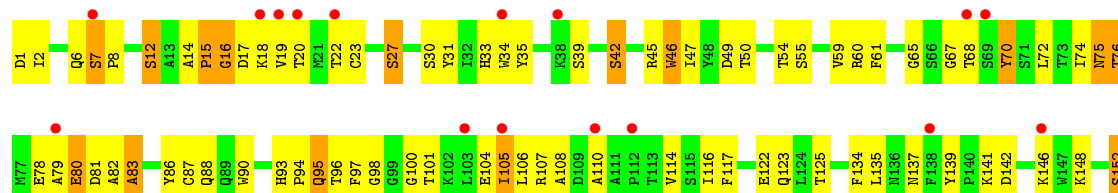
• Molecule 2: Fab fragment, Heavy chain

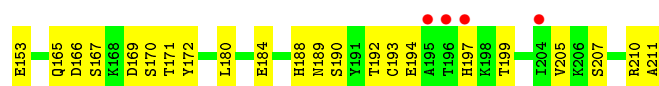


• Molecule 2: Fab fragment, Heavy chain

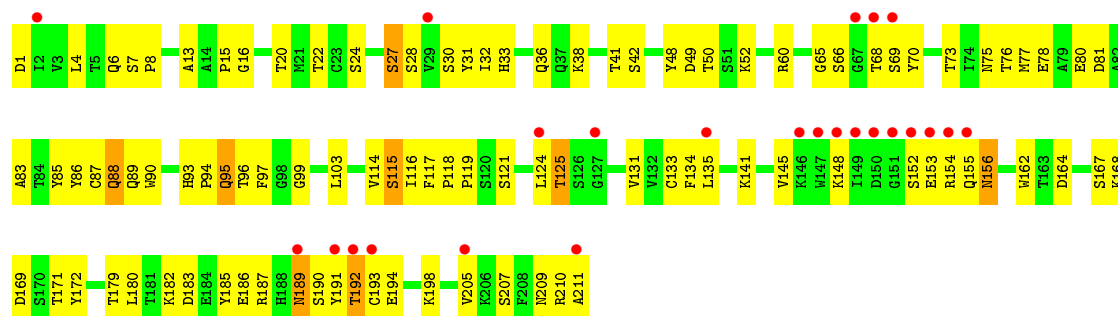


• Molecule 3: Fab fragment, Light chain





● Molecule 3: Fab fragment, Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.17Å 97.51Å 173.28Å 90.00° 132.88° 90.00°	Depositor
Resolution (Å)	59.03 – 2.80 59.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.4 (59.03-2.80) 91.5 (59.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.255 , 0.299 0.249 , 0.294	Depositor DCC
R_{free} test set	3203 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63808 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13201	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	2/3393 (0.1%)	0.84	5/4605 (0.1%)
1	B	0.76	0/3364	0.87	5/4567 (0.1%)
2	C	0.80	0/1721	0.85	0/2355
2	E	0.80	0/1721	0.82	0/2355
3	D	0.69	0/1660	0.84	1/2257 (0.0%)
3	F	0.81	0/1660	0.88	0/2257
All	All	0.77	2/13519 (0.0%)	0.85	11/18396 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	LEU	N-CA	-6.23	1.33	1.46
1	A	202	GLU	CG-CD	5.24	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	76	THR	N-CA-C	-9.00	86.70	111.00
1	B	403	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	B	75	TYR	N-CA-C	-6.45	93.59	111.00
1	A	340	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	B	194	LEU	CB-CG-CD1	-6.14	100.57	111.00
1	B	212	LEU	CA-CB-CG	-5.99	101.52	115.30
1	A	233	ASN	C-N-CA	-5.79	107.23	121.70
1	A	237	ALA	C-N-CA	-5.72	107.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ALA	CB-CA-C	-5.48	101.89	110.10
1	A	236	VAL	N-CA-C	-5.25	96.84	111.00
1	B	54	ASP	CB-CG-OD2	-5.07	113.73	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	ASN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3478	222	0
1	B	3293	0	3452	248	0
2	C	1672	0	1654	71	0
2	E	1672	0	1654	65	0
3	D	1621	0	1546	98	0
3	F	1621	0	1546	89	0
All	All	13201	0	13330	738	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 28.

All (738) 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:A:232:PHE:C	1:A:233:ASN:ND2	1.74	1.41
1:B:75:TYR:CB	1:B:76:PRO:HD3	1.53	1.37
1:A:232:PHE:O	1:A:233:ASN:ND2	1.58	1.35
1:A:235:GLU:O	1:A:236:VAL:HG23	1.19	1.28
1:B:73:ASP:O	1:B:77:LEU:HB3	1.39	1.22
1:B:77:LEU:O	1:B:77:LEU:HD12	1.40	1.22
1:A:381:GLN:NE2	1:A:381:GLN:H	1.44	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:CB	1:B:76:PRO:CD	2.25	1.14
1:B:126:ARG:O	1:B:130:VAL:HG23	1.47	1.14
1:A:381:GLN:N	1:A:381:GLN:HE21	1.46	1.11
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.28	1.11
1:B:75:TYR:HB2	1:B:76:PRO:CD	1.79	1.11
1:B:75:TYR:HB2	1:B:76:PRO:HD3	1.20	1.09
3:D:95:GLN:H	3:D:95:GLN:CD	1.51	1.08
1:B:381:GLN:N	1:B:381:GLN:HE21	1.53	1.06
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.38	1.06
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.38	1.05
1:B:381:GLN:NE2	1:B:381:GLN:H	1.55	1.05
3:F:76:THR:O	3:F:76:THR:CG2	2.03	1.03
3:F:95:GLN:H	3:F:95:GLN:CD	1.59	1.03
3:F:76:THR:O	3:F:76:THR:HG22	1.24	1.02
3:D:14:ALA:O	3:D:15:PRO:O	1.76	1.02
1:B:132:PHE:O	1:B:136:LEU:HD13	1.59	1.00
1:B:451:ARG:HH11	1:B:451:ARG:HG3	1.27	0.99
3:F:189:ASN:HD21	3:F:211:ALA:H	1.04	0.97
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.44	0.96
1:A:235:GLU:O	1:A:236:VAL:CG2	2.13	0.96
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.01	0.95
3:D:7:SER:HB2	3:D:22:THR:HB	1.51	0.93
1:B:337:PHE:O	1:B:341:VAL:HG23	1.68	0.92
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.50	0.92
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.48	0.92
3:F:95:GLN:N	3:F:95:GLN:CD	2.21	0.92
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.51	0.92
1:A:144:VAL:HG21	1:A:343:THR:HB	1.52	0.91
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.53	0.91
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.52	0.91
2:C:73:ASP:OD1	2:C:76:LYS:HD2	1.70	0.90
2:E:9:GLY:H	2:E:115:THR:HG21	1.33	0.90
1:B:126:ARG:O	1:B:130:VAL:CG2	2.20	0.90
1:A:216:LYS:HZ3	1:B:433:THR:HG22	1.35	0.90
3:D:95:GLN:N	3:D:95:GLN:CD	2.19	0.89
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.54	0.89
3:D:17:ASP:OD1	3:D:18:LYS:O	1.90	0.88
1:A:459:GLU:O	1:A:460:GLN:HG3	1.75	0.86
1:A:258:LEU:HA	1:A:261:ILE:HD12	1.57	0.86
1:A:459:GLU:O	1:A:460:GLN:CG	2.24	0.86
1:B:457:GLU:O	1:B:457:GLU:HG3	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:189:ASN:HD21	3:D:211:ALA:H	1.24	0.86
1:B:132:PHE:CD1	1:B:132:PHE:C	2.46	0.85
1:B:131:LYS:HE2	1:B:153:GLN:NE2	1.91	0.85
2:E:9:GLY:N	2:E:115:THR:HG21	1.92	0.84
3:D:2:ILE:O	3:D:96:THR:HG21	1.76	0.84
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.42	0.84
2:E:9:GLY:HA3	2:E:115:THR:HG22	1.58	0.83
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.61	0.83
1:B:131:LYS:HE2	1:B:153:GLN:HE21	1.44	0.83
3:F:31:TYR:HA	3:F:50:THR:OG1	1.78	0.83
2:C:7:SER:HA	2:C:115:THR:HG21	1.58	0.83
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.60	0.82
3:D:106:LEU:HD23	3:D:107:ARG:N	1.95	0.81
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.15	0.81
1:B:96:LEU:O	1:B:130:VAL:CG1	2.29	0.80
1:B:422:ILE:HA	1:B:425:MET:HE3	1.64	0.80
1:B:77:LEU:C	1:B:77:LEU:HD12	1.99	0.79
1:B:132:PHE:HD1	1:B:132:PHE:C	1.84	0.79
3:D:192:THR:HG22	3:D:207:SER:HB2	1.62	0.79
3:F:7:SER:HB2	3:F:22:THR:HB	1.65	0.79
1:B:98:ARG:NH2	1:B:102:PRO:HB3	1.98	0.78
3:D:95:GLN:N	3:D:95:GLN:OE1	2.16	0.78
1:B:78:LEU:HD12	1:B:79:LEU:N	1.98	0.77
2:E:30:SER:O	2:E:31:ARG:HB2	1.83	0.77
1:A:270:ASN:O	1:A:273:VAL:HG12	1.85	0.77
1:B:144:VAL:HG21	1:B:343:THR:HB	1.67	0.77
3:F:27:SER:O	3:F:68:THR:HG22	1.84	0.77
3:F:95:GLN:H	3:F:95:GLN:NE2	1.82	0.77
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.19	0.77
2:C:30:SER:O	2:C:31:ARG:HB2	1.85	0.76
3:D:192:THR:HG22	3:D:207:SER:CB	2.15	0.76
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.66	0.76
3:F:7:SER:HB3	3:F:8:PRO:CD	2.16	0.76
1:B:409:ILE:HD13	1:B:426:ILE:HA	1.69	0.75
1:A:234:HIS:ND1	1:A:234:HIS:N	2.33	0.75
2:C:32:TYR:CD2	2:C:98:ARG:HG3	2.21	0.75
3:D:31:TYR:HA	3:D:50:THR:OG1	1.86	0.75
1:A:233:ASN:ND2	1:A:233:ASN:N	2.32	0.75
1:B:279:LEU:HD23	1:B:279:LEU:O	1.87	0.74
1:A:197:ILE:HD13	1:A:219:PHE:CD1	2.23	0.74
1:A:422:ILE:HA	1:A:425:MET:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.53	0.74
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.08	0.73
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.53	0.73
1:A:356:ILE:HG23	1:A:360:MET:CE	2.18	0.73
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.53	0.73
1:A:235:GLU:C	1:A:236:VAL:HG23	2.08	0.73
2:E:9:GLY:HA3	2:E:115:THR:CG2	2.18	0.73
1:B:150:PRO:O	1:B:154:ILE:HG13	1.89	0.73
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.04	0.73
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.24	0.72
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.04	0.72
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.70	0.72
2:E:11:LEU:HD21	2:E:122:ALA:O	1.90	0.72
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.04	0.72
1:B:451:ARG:CG	1:B:451:ARG:HH11	2.02	0.71
3:F:38:LYS:O	3:F:41:THR:HG22	1.91	0.71
1:B:92:PHE:O	1:B:96:LEU:HD23	1.91	0.71
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.73	0.71
3:F:7:SER:CB	3:F:8:PRO:HD3	2.18	0.71
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.55	0.71
3:D:7:SER:HB3	3:D:8:PRO:CD	2.21	0.70
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.26	0.70
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.19	0.70
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.22	0.69
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.72	0.69
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.74	0.69
1:B:451:ARG:NH1	1:B:451:ARG:HG3	2.01	0.69
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.28	0.69
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.73	0.69
1:A:264:ILE:HG22	1:A:435:LEU:HD12	1.74	0.69
3:D:95:GLN:H	3:D:95:GLN:NE2	1.90	0.68
1:A:430:LEU:HD23	1:B:223:ILE:CD1	2.23	0.68
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.75	0.68
3:D:125:THR:HG22	3:D:125:THR:O	1.94	0.68
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.76	0.68
3:D:189:ASN:HD22	3:D:210:ARG:HB2	1.57	0.67
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.76	0.67
2:C:185:LEU:O	2:C:185:LEU:HD12	1.93	0.67
1:B:154:ILE:O	1:B:158:ILE:HG12	1.93	0.67
1:B:96:LEU:O	1:B:130:VAL:HG13	1.95	0.67
3:D:60:ARG:CZ	3:D:78:GLU:HG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD12	1:A:212:LEU:H	1.58	0.67
1:A:86:SER:OG	1:A:303:GLY:HA3	1.95	0.67
1:A:21:LEU:HD22	1:B:119:GLN:HG3	1.76	0.67
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.76	0.66
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.77	0.66
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.30	0.66
3:D:17:ASP:C	3:D:17:ASP:OD1	2.34	0.66
1:A:430:LEU:HD23	1:B:223:ILE:HD11	1.76	0.66
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.11	0.66
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.29	0.66
1:B:270:ASN:O	1:B:273:VAL:HG12	1.96	0.66
1:B:356:ILE:HG23	1:B:360:MET:CE	2.26	0.66
3:F:7:SER:CB	3:F:22:THR:HB	2.25	0.65
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.61	0.65
1:A:219:PHE:CD2	1:B:430:LEU:HD13	2.32	0.65
3:F:90:TRP:CE3	3:F:95:GLN:HG3	2.32	0.65
1:B:132:PHE:CD1	1:B:136:LEU:HD13	2.30	0.65
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.11	0.65
1:B:76:PRO:O	1:B:77:LEU:C	2.33	0.65
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.61	0.65
1:A:92:PHE:O	1:A:96:LEU:HD23	1.96	0.65
3:F:194:GLU:HG2	3:F:205:VAL:CG1	2.26	0.65
3:D:210:ARG:HH11	3:D:210:ARG:HG2	1.62	0.65
1:B:33:LEU:HD23	1:B:33:LEU:O	1.97	0.65
1:A:150:PRO:O	1:A:154:ILE:HG13	1.96	0.65
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.79	0.65
3:D:16:GLY:HA2	3:D:76:THR:HG22	1.77	0.64
1:B:176:THR:O	1:B:180:THR:HG23	1.96	0.64
3:F:13:ALA:HB3	3:F:77:MET:CE	2.27	0.64
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.79	0.64
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.29	0.64
2:C:163:ASN:HD22	2:C:167:LEU:HB2	1.63	0.64
1:B:421:LEU:O	1:B:424:PRO:HD2	1.97	0.64
1:B:306:GLY:O	1:B:310:PRO:HG3	1.97	0.64
1:B:101:ALA:CB	1:B:130:VAL:HG21	2.27	0.64
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.28	0.64
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.80	0.64
1:A:199:PHE:CE2	1:A:204:MET:SD	2.91	0.63
1:A:180:THR:HG22	1:A:218:VAL:HA	1.81	0.63
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.63	0.63
1:A:122:VAL:HB	1:A:160:ARG:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.13	0.63
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.29	0.63
3:F:30:SER:HA	3:F:70:TYR:OH	1.99	0.62
1:B:144:VAL:O	1:B:145:LEU:HG	1.99	0.62
1:A:169:LYS:HG2	1:A:170:GLY:N	2.14	0.62
1:B:274:LEU:O	1:B:277:GLN:HB2	1.99	0.62
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.81	0.62
2:C:98:ARG:HD3	2:C:109:ASP:OD2	2.00	0.62
1:A:68:LEU:HD23	1:A:81:VAL:HG23	1.81	0.62
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.34	0.62
2:E:105:TYR:N	2:E:105:TYR:CD1	2.67	0.62
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.15	0.62
2:C:7:SER:CA	2:C:115:THR:HG21	2.28	0.62
1:A:346:LEU:O	1:A:350:SER:HB3	2.00	0.62
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.82	0.62
1:A:74:ASN:HD22	1:A:76:PRO:HD2	1.63	0.62
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.81	0.62
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.82	0.62
1:A:216:LYS:NZ	1:B:433:THR:HG22	2.13	0.61
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.65	0.61
3:D:75:ASN:C	3:D:76:THR:O	2.31	0.61
3:D:12:SER:HA	3:D:104:GLU:O	2.00	0.61
1:B:409:ILE:CD1	1:B:426:ILE:HA	2.30	0.61
1:A:28:ARG:CD	1:B:207:GLN:HG2	2.29	0.61
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.99	0.61
3:D:189:ASN:ND2	3:D:210:ARG:HB2	2.16	0.61
3:F:66:SER:HA	3:F:70:TYR:CZ	2.36	0.61
3:F:191:TYR:O	3:F:207:SER:HB2	2.00	0.61
1:B:272:TRP:O	1:B:276:MET:HB2	2.01	0.61
2:C:145:THR:HG22	3:D:117:PHE:HZ	1.65	0.61
2:C:43:LYS:HB3	2:C:43:LYS:NZ	2.16	0.61
3:D:16:GLY:HA2	3:D:76:THR:CG2	2.30	0.61
2:C:163:ASN:HD21	2:C:167:LEU:HD22	1.64	0.61
1:B:241:VAL:HG13	1:B:324:THR:HG21	1.83	0.61
1:A:78:LEU:HD21	1:A:307:PHE:CZ	2.36	0.61
1:A:100:TYR:O	1:A:126:ARG:NH1	2.33	0.61
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.36	0.61
1:B:163:LEU:HD12	1:B:168:LEU:HB3	1.81	0.60
1:B:309:ALA:O	1:B:311:ALA:N	2.34	0.60
3:F:148:LYS:HA	3:F:152:SER:O	2.00	0.60
1:B:77:LEU:O	1:B:77:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.83	0.60
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.83	0.60
3:F:95:GLN:N	3:F:95:GLN:OE1	2.33	0.60
1:A:74:ASN:C	1:A:74:ASN:HD22	2.05	0.60
1:B:356:ILE:HG23	1:B:360:MET:HE1	1.83	0.60
1:A:68:LEU:CD2	1:A:81:VAL:HG23	2.32	0.60
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.66	0.60
2:E:9:GLY:H	2:E:115:THR:CG2	2.09	0.60
1:B:163:LEU:HD12	1:B:168:LEU:CB	2.32	0.60
1:A:409:ILE:HD12	1:A:426:ILE:HA	1.84	0.60
1:A:33:LEU:HD23	1:A:33:LEU:C	2.22	0.60
1:A:270:ASN:O	1:A:273:VAL:CG1	2.50	0.59
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.83	0.59
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.37	0.59
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.83	0.59
2:E:151:LYS:HB2	2:E:184:THR:OG1	2.02	0.59
3:D:17:ASP:OD1	3:D:18:LYS:N	2.36	0.59
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.84	0.59
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.85	0.59
2:C:139:ALA:O	2:C:140:ALA:C	2.40	0.59
1:A:144:VAL:O	1:A:144:VAL:HG12	2.03	0.59
1:A:458:ALA:O	1:A:460:GLN:N	2.36	0.59
1:B:93:GLY:O	1:B:97:VAL:HG23	2.02	0.59
1:B:447:ALA:O	1:B:451:ARG:HG2	2.03	0.59
3:F:192:THR:HB	3:F:207:SER:HB3	1.83	0.59
3:F:189:ASN:ND2	3:F:211:ALA:H	1.88	0.59
1:B:346:LEU:O	1:B:350:SER:HB3	2.03	0.59
1:A:200:ILE:HD12	1:A:204:MET:CG	2.26	0.58
1:B:132:PHE:HD1	1:B:133:PHE:N	2.00	0.58
3:F:183:ASP:HB3	3:F:187:ARG:NH2	2.17	0.58
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.85	0.58
2:C:6:GLU:O	2:C:115:THR:HG23	2.03	0.58
1:A:403:ARG:NH2	1:B:29:ASP:OD1	2.36	0.58
1:B:73:ASP:O	1:B:77:LEU:CB	2.32	0.58
1:B:101:ALA:HB3	1:B:130:VAL:HG21	1.83	0.58
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.85	0.58
1:B:267:PRO:O	1:B:270:ASN:HB2	2.03	0.58
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.85	0.58
2:C:185:LEU:C	2:C:185:LEU:HD12	2.24	0.58
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.84	0.58
1:B:75:TYR:HB2	1:B:76:PRO:HD2	1.78	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:GLY:CA	2:E:115:THR:CG2	2.82	0.58
3:D:189:ASN:HD21	3:D:211:ALA:N	1.98	0.58
2:C:7:SER:HA	2:C:115:THR:CG2	2.29	0.58
1:B:180:THR:HG22	1:B:218:VAL:HA	1.86	0.58
1:A:226:THR:O	1:A:230:ARG:HG2	2.04	0.58
1:B:74:ASN:O	1:B:76:PRO:HD2	2.03	0.58
1:A:200:ILE:CD1	1:A:204:MET:HG3	2.24	0.58
3:F:192:THR:CB	3:F:207:SER:HB3	2.34	0.58
3:F:141:LYS:HB3	3:F:172:TYR:CD1	2.39	0.58
3:F:7:SER:CB	3:F:8:PRO:CD	2.81	0.57
1:B:132:PHE:O	1:B:136:LEU:CD1	2.44	0.57
1:A:227:ILE:O	1:A:231:ILE:HG12	2.04	0.57
1:B:132:PHE:HE1	1:B:136:LEU:CD2	2.17	0.57
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.19	0.57
3:D:15:PRO:O	3:D:16:GLY:C	2.42	0.57
2:C:37:VAL:HG13	2:C:46:LYS:O	2.05	0.57
1:A:223:ILE:HD12	1:B:430:LEU:CD2	2.35	0.57
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.39	0.57
2:C:86:VAL:HG12	2:C:119:VAL:HG11	1.85	0.57
1:A:91:MET:CG	1:A:296:GLY:HA3	2.34	0.57
1:B:20:GLN:O	1:B:23:ARG:HB3	2.04	0.57
1:A:19:ARG:HB2	1:A:19:ARG:NH1	2.19	0.57
2:E:139:ALA:O	2:E:140:ALA:C	2.42	0.57
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.87	0.57
1:A:248:PRO:O	1:A:251:THR:HB	2.05	0.57
1:A:18:ARG:O	1:A:22:ILE:HG13	2.05	0.56
2:E:188:SER:HB3	3:F:134:PHE:CE2	2.39	0.56
2:C:189:VAL:O	2:C:189:VAL:HG13	2.03	0.56
3:D:60:ARG:NE	3:D:78:GLU:HG2	2.19	0.56
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.05	0.56
1:A:25:LEU:HD23	1:B:208:PHE:HE1	1.70	0.56
3:D:30:SER:HA	3:D:70:TYR:OH	2.06	0.56
3:F:90:TRP:CD2	3:F:95:GLN:HG3	2.40	0.56
1:B:109:ILE:N	1:B:110:PRO:CD	2.68	0.56
1:A:160:ARG:HH12	1:A:174:ARG:HD2	1.71	0.56
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.88	0.56
1:B:218:VAL:O	1:B:222:VAL:HG23	2.06	0.55
2:E:70:ILE:HG12	2:E:81:LEU:HD13	1.88	0.55
1:B:91:MET:HG2	1:B:292:VAL:O	2.06	0.55
1:B:380:PRO:HD2	1:B:381:GLN:NE2	2.21	0.55
1:A:154:ILE:O	1:A:158:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.88	0.55
3:F:6:GLN:HG3	3:F:99:GLY:H	1.71	0.55
3:F:78:GLU:O	3:F:81:ASP:HB2	2.05	0.55
2:C:28:ASP:O	2:C:30:SER:O	2.24	0.55
2:C:43:LYS:CB	2:C:43:LYS:NZ	2.69	0.55
2:E:6:GLU:HA	2:E:22:CYS:HA	1.89	0.55
2:E:113:ALA:HA	3:F:42:SER:OG	2.07	0.55
1:B:73:ASP:CB	1:B:74:ASN:HA	2.37	0.55
1:B:132:PHE:CD1	1:B:133:PHE:N	2.75	0.55
1:A:180:THR:CG2	1:A:218:VAL:HA	2.36	0.55
3:D:116:ILE:HD12	3:D:193:CYS:HB2	1.89	0.55
1:B:117:GLU:O	1:B:118:ASP:HB2	2.07	0.55
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.89	0.55
3:D:22:THR:HG22	3:D:23:CYS:N	2.22	0.55
1:B:200:ILE:HA	1:B:204:MET:HB2	1.87	0.54
1:B:187:ALA:HB2	1:B:222:VAL:HG13	1.89	0.54
1:B:248:PRO:O	1:B:251:THR:HB	2.06	0.54
1:A:381:GLN:HE21	1:A:381:GLN:H	0.68	0.54
1:A:78:LEU:HD21	1:A:307:PHE:CE2	2.42	0.54
1:B:132:PHE:O	1:B:132:PHE:CD1	2.61	0.54
1:A:459:GLU:O	1:A:460:GLN:HG2	2.03	0.54
3:F:93:HIS:CG	3:F:94:PRO:HA	2.41	0.54
1:A:457:GLU:O	1:A:458:ALA:C	2.46	0.54
3:F:116:ILE:HD12	3:F:133:CYS:HB2	1.88	0.54
1:B:73:ASP:CB	1:B:74:ASN:CA	2.85	0.54
2:C:141:ALA:O	2:C:193:SER:HB2	2.07	0.54
2:C:142:SER:O	2:C:193:SER:HB2	2.08	0.54
1:A:159:GLY:O	1:A:162:VAL:HG22	2.08	0.54
1:A:20:GLN:O	1:A:23:ARG:HB3	2.08	0.54
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.42	0.54
2:E:9:GLY:CA	2:E:115:THR:HG21	2.37	0.54
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.21	0.54
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.90	0.54
1:B:38:MET:O	1:B:41:VAL:HG13	2.08	0.53
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.89	0.53
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.90	0.53
1:B:132:PHE:HE1	1:B:136:LEU:HD21	1.72	0.53
1:B:284:HIS:O	1:B:287:ASN:HB3	2.08	0.53
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.91	0.53
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.42	0.53
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.90	0.53
1:B:106:GLY:O	1:B:131:LYS:NZ	2.42	0.53
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.91	0.53
1:B:263:GLY:HA3	1:B:435:LEU:HB2	1.91	0.53
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.44	0.53
3:D:7:SER:CB	3:D:8:PRO:CD	2.87	0.52
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.91	0.52
3:D:7:SER:CB	3:D:8:PRO:HD3	2.37	0.52
2:C:30:SER:O	2:C:31:ARG:CB	2.56	0.52
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.91	0.52
3:D:7:SER:CB	3:D:22:THR:HB	2.32	0.52
2:E:134:PRO:O	2:E:221:ARG:HG3	2.08	0.52
3:D:165:GLN:HG2	3:D:170:SER:HA	1.91	0.52
3:F:31:TYR:HB3	3:F:49:ASP:HA	1.91	0.52
2:E:11:LEU:HD11	2:E:120:SER:HB3	1.91	0.52
1:A:212:LEU:HD12	1:A:212:LEU:N	2.24	0.52
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.10	0.52
1:B:330:MET:O	1:B:330:MET:HE2	2.09	0.52
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.75	0.52
1:A:219:PHE:HD2	1:B:430:LEU:HD13	1.73	0.52
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.92	0.52
3:D:105:ILE:O	3:D:105:ILE:HG22	2.09	0.52
1:A:270:ASN:HD21	1:A:401:SER:HB3	1.75	0.52
1:A:279:LEU:HD22	1:A:279:LEU:O	2.09	0.52
1:B:144:VAL:HG21	1:B:343:THR:CB	2.39	0.52
3:D:46:TRP:HA	3:D:46:TRP:CE3	2.45	0.52
3:F:6:GLN:NE2	3:F:87:CYS:H	2.07	0.51
3:D:78:GLU:O	3:D:81:ASP:HB2	2.10	0.51
3:F:189:ASN:HA	3:F:210:ARG:HD3	1.92	0.51
3:D:194:GLU:HG2	3:D:205:VAL:CG1	2.25	0.51
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.76	0.51
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.33	0.51
1:A:241:VAL:CG1	1:A:244:LEU:HD21	2.40	0.51
1:B:155:GLY:HA3	1:B:181:GLY:O	2.09	0.51
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.11	0.51
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.43	0.51
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.40	0.51
1:A:50:ALA:O	1:A:54:ASP:HB2	2.10	0.51
1:B:122:VAL:HG11	1:B:160:ARG:HB2	1.92	0.51
3:D:106:LEU:HD23	3:D:107:ARG:H	1.72	0.51
1:A:211:THR:HG22	1:A:212:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD21	1:A:347:CYS:HB3	1.93	0.51
1:A:180:THR:HG22	1:A:218:VAL:HG22	1.93	0.51
1:A:90:ALA:O	1:A:94:TYR:HD1	1.93	0.51
3:D:14:ALA:C	3:D:15:PRO:O	2.46	0.51
1:A:38:MET:HA	1:A:41:VAL:HG12	1.93	0.51
1:B:148:ALA:O	1:B:152:VAL:HG23	2.10	0.51
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.93	0.51
1:A:91:MET:HG3	1:A:296:GLY:CA	2.40	0.51
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.77	0.50
3:D:35:TYR:CD2	3:D:45:ARG:HA	2.46	0.50
1:A:98:ARG:HA	1:A:98:ARG:NE	2.27	0.50
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.27	0.50
1:B:38:MET:O	1:B:41:VAL:CG1	2.59	0.50
1:B:41:VAL:O	1:B:45:LEU:HG	2.12	0.50
1:A:421:LEU:O	1:A:425:MET:HG3	2.10	0.50
3:D:148:LYS:HA	3:D:152:SER:O	2.11	0.50
3:F:183:ASP:HB3	3:F:187:ARG:HH22	1.75	0.50
1:B:28:ARG:HG2	1:B:29:ASP:N	2.27	0.50
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.46	0.50
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.29	0.50
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.47	0.50
1:A:251:THR:HG22	1:A:255:TYR:CE1	2.45	0.50
1:B:264:ILE:HG13	1:B:265:PHE:N	2.26	0.50
1:B:22:ILE:O	1:B:26:LEU:HD12	2.11	0.50
1:A:197:ILE:HG12	1:A:222:VAL:HG21	1.93	0.50
1:A:72:ALA:HA	1:A:78:LEU:HD12	1.94	0.50
1:A:109:ILE:N	1:A:110:PRO:CD	2.74	0.50
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.76	0.50
3:F:145:VAL:HA	3:F:194:GLU:O	2.11	0.50
1:B:38:MET:O	1:B:42:VAL:HG23	2.11	0.50
1:B:42:VAL:O	1:B:46:VAL:HG23	2.12	0.50
1:A:451:ARG:CB	1:A:451:ARG:HH11	2.22	0.50
1:B:119:GLN:O	1:B:120:ARG:HG2	2.12	0.50
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.46	0.50
2:E:139:ALA:O	2:E:141:ALA:N	2.44	0.50
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.93	0.50
2:E:185:LEU:HD12	2:E:185:LEU:C	2.32	0.50
1:A:455:LYS:O	1:A:459:GLU:HG2	2.11	0.50
1:B:267:PRO:HG2	1:B:439:THR:OG1	2.12	0.50
3:D:142:ASP:O	3:D:197:HIS:HD2	1.94	0.50
1:A:200:ILE:HA	1:A:204:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:74:ILE:O	3:D:76:THR:O	2.30	0.50
2:E:51:ILE:HG23	2:E:51:ILE:O	2.12	0.49
3:D:82:ALA:O	3:D:83:ALA:HB2	2.12	0.49
1:A:312:THR:HG22	1:A:339:ALA:HB3	1.94	0.49
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.94	0.49
1:A:447:ALA:O	1:A:451:ARG:HG2	2.11	0.49
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.27	0.49
1:A:273:VAL:HG11	1:A:444:LEU:HD21	1.94	0.49
1:B:184:ALA:HB1	1:B:225:SER:OG	2.12	0.49
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.46	0.49
3:F:189:ASN:O	3:F:209:ASN:HA	2.11	0.49
1:A:430:LEU:CD2	1:B:223:ILE:HD11	2.40	0.49
1:B:270:ASN:O	1:B:273:VAL:CG1	2.60	0.49
2:C:86:VAL:HG12	2:C:119:VAL:CG1	2.42	0.49
3:F:121:SER:O	3:F:125:THR:OG1	2.31	0.49
1:B:295:GLY:HA2	1:B:298:ILE:HD12	1.93	0.49
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.48	0.49
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.93	0.49
2:E:104:GLY:O	2:E:106:TRP:CD1	2.65	0.49
2:E:149:LEU:HD12	2:E:186:SER:HB3	1.93	0.49
1:B:78:LEU:CA	1:B:81:VAL:HG22	2.35	0.49
3:D:79:ALA:C	3:D:81:ASP:H	2.15	0.49
1:B:226:THR:O	1:B:230:ARG:HG2	2.11	0.49
1:B:73:ASP:HB3	1:B:74:ASN:HA	1.95	0.49
1:A:272:TRP:O	1:A:276:MET:HB2	2.13	0.49
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.93	0.49
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.95	0.49
1:A:416:THR:O	1:A:417:ASP:C	2.50	0.49
1:B:229:TYR:CE1	1:B:233:ASN:ND2	2.81	0.49
3:D:166:ASP:OD1	3:D:167:SER:N	2.46	0.48
3:F:80:GLU:HA	3:F:167:SER:O	2.12	0.48
1:B:78:LEU:HD12	1:B:79:LEU:H	1.76	0.48
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.16	0.48
2:C:22:CYS:O	2:C:78:THR:HG23	2.12	0.48
1:B:180:THR:CG2	1:B:218:VAL:HA	2.43	0.48
3:D:107:ARG:NE	3:D:108:ALA:O	2.35	0.48
2:E:32:TYR:O	2:E:72:ARG:NH2	2.39	0.48
1:A:42:VAL:HG23	1:A:162:VAL:HG21	1.94	0.48
3:F:186:GLU:HA	3:F:210:ARG:CZ	2.43	0.48
2:E:188:SER:HB3	3:F:134:PHE:CZ	2.48	0.48
1:B:60:LEU:O	1:B:64:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:HB2	1:B:130:VAL:HG21	1.95	0.48
2:C:43:LYS:HB3	2:C:43:LYS:HZ3	1.76	0.48
1:B:229:TYR:CD1	1:B:233:ASN:ND2	2.82	0.48
1:B:212:LEU:HD12	1:B:212:LEU:N	2.28	0.48
1:A:430:LEU:HD13	1:B:219:PHE:CD2	2.49	0.48
1:B:71:THR:O	1:B:73:ASP:N	2.47	0.48
1:A:305:LEU:C	1:A:307:PHE:H	2.18	0.48
3:F:192:THR:HG22	3:F:207:SER:CB	2.43	0.48
3:D:79:ALA:O	3:D:81:ASP:N	2.47	0.48
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.49	0.48
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.49	0.47
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.14	0.47
1:B:277:GLN:NE2	1:B:451:ARG:HH12	2.12	0.47
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.45	0.47
1:B:209:ARG:HH11	1:B:209:ARG:HG2	1.78	0.47
2:C:135:GLY:HA2	2:C:221:ARG:HD3	1.95	0.47
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.96	0.47
1:B:149:GLY:O	1:B:150:PRO:C	2.51	0.47
1:A:176:THR:HG22	1:A:177:LEU:HD23	1.96	0.47
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.96	0.47
1:B:108:GLY:HA3	1:B:153:GLN:HB2	1.96	0.47
2:E:105:TYR:HD1	2:E:105:TYR:H	1.61	0.47
1:B:109:ILE:HD13	1:B:199:PHE:HE2	1.80	0.47
1:A:148:ALA:O	1:A:152:VAL:HG23	2.15	0.47
3:D:1:ASP:OD2	3:D:1:ASP:N	2.47	0.47
1:A:78:LEU:HD22	1:A:79:LEU:HD23	1.97	0.47
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.48	0.47
3:F:179:THR:O	3:F:180:LEU:HD23	2.14	0.47
1:B:241:VAL:CG1	1:B:244:LEU:HD21	2.44	0.47
2:C:200:THR:HG22	2:C:200:THR:O	2.15	0.47
3:D:6:GLN:NE2	3:D:87:CYS:H	2.13	0.46
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.97	0.46
1:B:369:THR:O	1:B:370:ALA:C	2.52	0.46
2:C:64:LEU:N	2:C:64:LEU:HD23	2.30	0.46
1:A:98:ARG:HB3	1:A:288:ILE:HG13	1.96	0.46
2:E:30:SER:O	2:E:31:ARG:CB	2.54	0.46
1:A:78:LEU:HD23	1:A:78:LEU:C	2.36	0.46
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.43	0.46
2:C:189:VAL:O	2:C:189:VAL:CG1	2.64	0.46
1:A:90:ALA:HB2	1:A:299:GLY:HA3	1.97	0.46
1:A:131:LYS:HE2	1:A:153:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:GLU:CG	1:B:457:GLU:O	2.48	0.46
1:B:421:LEU:C	1:B:424:PRO:HD2	2.35	0.46
2:C:124:THR:HA	2:C:154:PHE:O	2.16	0.46
2:E:111:TRP:N	2:E:111:TRP:CD1	2.84	0.46
3:D:210:ARG:HH11	3:D:210:ARG:CG	2.27	0.46
1:B:132:PHE:CE1	1:B:136:LEU:CD1	2.99	0.46
1:B:358:ALA:HA	1:B:361:LEU:HD12	1.97	0.46
2:E:71:SER:O	2:E:79:LEU:HD12	2.16	0.46
2:E:2:VAL:HG23	2:E:2:VAL:O	2.16	0.46
1:A:287:ASN:ND2	1:A:290:LYS:H	2.14	0.46
2:E:39:GLN:O	2:E:92:ALA:HB1	2.16	0.46
1:A:223:ILE:HD11	1:B:430:LEU:HD22	1.98	0.46
2:C:107:TYR:HB3	3:D:33:HIS:NE2	2.30	0.46
1:A:287:ASN:HD21	1:A:289:THR:HB	1.80	0.46
1:B:287:ASN:ND2	1:B:290:LYS:H	2.14	0.46
1:B:224:MET:O	1:B:228:MET:HG2	2.15	0.46
1:B:131:LYS:HE3	1:B:150:PRO:HA	1.98	0.46
3:D:146:LYS:NZ	3:D:153:GLU:OE1	2.47	0.46
1:A:398:LEU:CD2	1:A:402:ILE:HD12	2.45	0.46
1:A:84:LEU:O	1:A:88:VAL:HG23	2.16	0.45
1:B:76:PRO:C	1:B:78:LEU:N	2.67	0.45
2:C:73:ASP:OD1	2:C:76:LYS:CD	2.55	0.45
3:D:188:HIS:O	3:D:210:ARG:NE	2.50	0.45
2:C:185:LEU:C	2:C:185:LEU:CD1	2.84	0.45
1:B:255:TYR:CE2	1:B:424:PRO:HB3	2.50	0.45
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.30	0.45
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.98	0.45
2:C:134:PRO:HD3	2:C:146:LEU:CD2	2.47	0.45
1:A:360:MET:HG2	1:A:397:LEU:CD1	2.46	0.45
1:B:341:VAL:O	1:B:345:LEU:HG	2.16	0.45
1:A:91:MET:HG2	1:A:292:VAL:O	2.16	0.45
3:F:95:GLN:O	3:F:95:GLN:OE1	2.35	0.45
1:A:422:ILE:HG23	1:A:423:LEU:N	2.31	0.45
2:E:185:LEU:O	2:E:185:LEU:HD12	2.17	0.45
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.98	0.45
3:F:75:ASN:O	3:F:76:THR:HB	2.17	0.45
1:A:430:LEU:HD23	1:B:223:ILE:HD12	1.96	0.45
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.31	0.45
3:D:169:ASP:O	3:D:170:SER:HB2	2.18	0.45
1:B:138:THR:HG22	1:B:143:MET:SD	2.57	0.45
3:F:115:SER:HB2	3:F:117:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:VAL:HG12	2:E:172:HIS:N	2.30	0.45
1:B:98:ARG:HA	1:B:98:ARG:NE	2.31	0.44
1:A:211:THR:CG2	1:A:213:ILE:HG13	2.46	0.44
3:D:22:THR:CG2	3:D:23:CYS:N	2.80	0.44
2:C:2:VAL:O	2:C:2:VAL:HG23	2.17	0.44
1:A:379:PHE:CB	1:A:382:TYR:CD1	3.00	0.44
1:A:88:VAL:HA	1:A:91:MET:HE2	1.98	0.44
3:F:124:LEU:O	3:F:182:LYS:HD2	2.16	0.44
1:A:430:LEU:CD2	1:B:223:ILE:CD1	2.94	0.44
3:D:134:PHE:C	3:D:135:LEU:HD23	2.38	0.44
3:D:180:LEU:HD13	3:D:184:GLU:HG3	1.98	0.44
1:A:28:ARG:NH1	1:B:443:PRO:CB	2.81	0.44
1:B:255:TYR:CG	1:B:424:PRO:HB3	2.52	0.44
2:C:141:ALA:O	2:C:142:SER:C	2.54	0.44
1:A:104:ALA:HB1	1:A:131:LYS:HD3	2.00	0.44
1:B:191:ASN:OD1	1:B:230:ARG:HD3	2.17	0.44
3:F:38:LYS:HG3	3:F:83:ALA:HB2	1.99	0.44
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.98	0.44
2:E:9:GLY:N	2:E:115:THR:CG2	2.69	0.44
1:A:75:TYR:CZ	1:A:79:LEU:HD11	2.52	0.44
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.48	0.44
2:E:216:LYS:HE2	2:E:216:LYS:HB2	1.63	0.44
1:B:124:TRP:CE3	1:B:125:TRP:N	2.86	0.44
1:A:360:MET:HG2	1:A:397:LEU:HD12	1.98	0.44
1:A:33:LEU:HD23	1:A:33:LEU:O	2.17	0.44
1:B:253:TRP:CZ2	1:B:254:LEU:HD21	2.53	0.44
3:F:154:ARG:HD2	3:F:155:GLN:H	1.82	0.44
1:B:195:ALA:N	1:B:414:GLU:OE2	2.50	0.44
1:A:22:ILE:HD11	1:B:453:LEU:HB3	2.00	0.44
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.53	0.44
2:E:144:VAL:O	2:E:144:VAL:HG13	2.17	0.44
1:B:77:LEU:CD1	1:B:77:LEU:C	2.70	0.43
1:A:444:LEU:HD13	1:A:448:ILE:HD12	1.99	0.43
1:B:312:THR:HG22	1:B:339:ALA:CB	2.49	0.43
3:D:137:ASN:HA	3:D:171:THR:HB	1.99	0.43
3:D:54:THR:O	3:D:55:SER:C	2.56	0.43
1:B:135:GLY:O	1:B:139:LEU:HB2	2.18	0.43
3:D:79:ALA:C	3:D:81:ASP:N	2.69	0.43
2:E:135:GLY:HA2	2:E:221:ARG:CD	2.48	0.43
3:D:93:HIS:CG	3:D:94:PRO:HA	2.53	0.43
3:D:60:ARG:HB2	3:D:75:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:TYR:CB	3:F:33:HIS:CD2	2.88	0.43
2:C:112:GLY:O	3:D:42:SER:HB3	2.18	0.43
2:C:195:SER:O	2:C:199:GLU:CB	2.67	0.43
1:B:227:ILE:O	1:B:231:ILE:HG13	2.19	0.43
2:E:28:ASP:O	2:E:30:SER:O	2.36	0.43
3:F:4:LEU:HA	3:F:24:SER:O	2.18	0.43
1:A:241:VAL:HG12	1:A:244:LEU:CD2	2.48	0.43
3:F:32:ILE:HB	3:F:88:GLN:O	2.18	0.43
1:A:78:LEU:CD2	1:A:79:LEU:HD23	2.48	0.43
1:B:94:TYR:CZ	1:B:295:GLY:HA3	2.53	0.43
1:A:374:VAL:HG12	1:A:378:LEU:HD12	2.01	0.43
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.53	0.43
1:A:376:VAL:HG22	1:A:384:LEU:HB2	2.01	0.43
1:B:100:TYR:O	1:B:126:ARG:NH1	2.52	0.43
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.54	0.43
1:A:284:HIS:C	1:A:286:GLY:H	2.22	0.43
2:C:172:HIS:HB2	2:C:188:SER:OG	2.19	0.43
1:B:123:ARG:HH21	1:B:126:ARG:HD3	1.83	0.43
2:E:51:ILE:CD1	2:E:72:ARG:HG2	2.42	0.43
1:A:69:VAL:HA	1:A:72:ALA:HB2	2.01	0.43
1:B:235:GLU:O	1:B:236:VAL:HG22	2.19	0.43
1:A:18:ARG:CZ	1:B:457:GLU:HB3	2.48	0.43
1:A:198:LEU:HG	1:A:410:ILE:HD13	2.00	0.43
2:C:84:SER:O	2:C:85:LYS:C	2.55	0.43
1:A:223:ILE:CD1	1:B:430:LEU:CD2	2.95	0.43
1:A:19:ARG:HB2	1:A:19:ARG:HH11	1.84	0.43
1:B:231:ILE:O	1:B:231:ILE:HG22	2.19	0.43
3:D:110:ALA:C	3:D:199:THR:HG21	2.38	0.43
2:E:177:VAL:HG23	2:E:177:VAL:O	2.19	0.43
1:A:249:LEU:HA	1:A:249:LEU:HD23	1.80	0.43
3:F:20:THR:HG23	3:F:73:THR:OG1	2.18	0.43
1:A:381:GLN:N	1:A:381:GLN:NE2	2.27	0.43
3:F:60:ARG:NH2	3:F:81:ASP:CG	2.72	0.43
2:C:6:GLU:HA	2:C:21:SER:O	2.19	0.43
2:C:6:GLU:HA	2:C:22:CYS:HA	2.00	0.43
1:B:42:VAL:HG22	1:B:162:VAL:HG21	2.00	0.43
1:A:211:THR:HG22	1:A:212:LEU:H	1.84	0.43
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.49	0.43
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.83	0.43
1:A:31:THR:HB	1:A:36:LEU:HD21	2.01	0.43
1:B:78:LEU:CD1	1:B:79:LEU:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:LEU:HA	3:D:139:TYR:OH	2.19	0.42
3:D:34:TRP:CG	3:D:72:LEU:HD12	2.53	0.42
3:F:6:GLN:HE22	3:F:87:CYS:H	1.66	0.42
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.54	0.42
2:E:189:VAL:HG13	2:E:189:VAL:O	2.18	0.42
1:A:379:PHE:HA	1:A:381:GLN:NE2	2.34	0.42
1:A:459:GLU:O	1:A:459:GLU:HG3	2.19	0.42
3:F:89:GLN:HE21	3:F:96:THR:N	2.17	0.42
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.83	0.42
1:B:132:PHE:CE1	1:B:136:LEU:CD2	3.00	0.42
3:F:77:MET:HG2	3:F:78:GLU:N	2.33	0.42
2:E:86:VAL:HG13	2:E:90:ASP:HB2	2.02	0.42
3:D:34:TRP:N	3:D:47:ILE:O	2.43	0.42
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.54	0.42
3:F:6:GLN:HG3	3:F:99:GLY:N	2.35	0.42
1:A:42:VAL:CG2	1:A:162:VAL:HG21	2.49	0.42
1:A:51:VAL:O	1:A:55:LYS:HG2	2.19	0.42
1:B:379:PHE:HA	1:B:381:GLN:NE2	2.35	0.42
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.87	0.42
1:B:78:LEU:HA	1:B:81:VAL:CG2	2.35	0.42
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.54	0.42
1:B:187:ALA:CB	1:B:222:VAL:HG13	2.49	0.42
1:B:272:TRP:CD1	1:B:272:TRP:N	2.87	0.42
1:A:241:VAL:HG12	1:A:241:VAL:O	2.19	0.42
1:B:62:ASN:HB3	1:B:63:GLN:HE21	1.84	0.42
2:E:146:LEU:HD12	2:E:201:VAL:HG11	2.02	0.42
3:D:8:PRO:O	3:D:101:THR:HG23	2.20	0.42
1:B:399:ALA:O	1:B:403:ARG:HA	2.19	0.42
1:A:97:VAL:HG13	1:A:101:ALA:O	2.19	0.42
1:B:74:ASN:O	1:B:75:TYR:HB2	2.20	0.42
1:B:132:PHE:O	1:B:132:PHE:HD1	1.98	0.42
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.17	0.42
1:A:22:ILE:O	1:A:26:LEU:HD12	2.20	0.42
1:B:43:GLY:O	1:B:225:SER:HB3	2.20	0.42
3:F:13:ALA:CB	3:F:77:MET:HE3	2.37	0.42
2:C:66:ASP:O	2:C:67:LYS:C	2.59	0.42
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.55	0.42
1:A:385:GLU:O	1:A:387:GLY:N	2.53	0.42
1:A:83:PHE:C	1:A:83:PHE:CD1	2.93	0.42
1:B:420:GLN:HG3	1:B:420:GLN:H	1.13	0.42
1:B:86:SER:OG	1:B:303:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:O	1:A:222:VAL:HG23	2.19	0.41
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.55	0.41
3:F:185:TYR:HA	3:F:191:TYR:OH	2.20	0.41
1:B:332:MET:O	1:B:336:ILE:HG13	2.20	0.41
2:C:191:VAL:HB	2:C:192:PRO:HD2	2.02	0.41
1:B:394:MET:HG2	1:B:412:VAL:HG22	2.02	0.41
2:E:125:THR:HA	2:E:126:PRO:HD2	1.95	0.41
1:B:211:THR:CG2	1:B:213:ILE:HG13	2.50	0.41
1:B:148:ALA:O	1:B:149:GLY:C	2.58	0.41
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.35	0.41
3:F:24:SER:HA	3:F:68:THR:O	2.21	0.41
3:F:153:GLU:HG3	3:F:154:ARG:N	2.35	0.41
1:B:419:TYR:O	1:B:419:TYR:CG	2.74	0.41
1:B:405:PRO:O	1:B:406:LEU:C	2.57	0.41
1:A:172:GLU:HA	1:A:212:LEU:O	2.21	0.41
1:A:231:ILE:HD13	1:B:249:LEU:CD1	2.48	0.41
3:D:70:TYR:CD1	3:D:70:TYR:N	2.88	0.41
1:A:383:HIS:HB3	2:C:33:TRP:CZ2	2.55	0.41
1:A:421:LEU:O	1:A:424:PRO:HD2	2.20	0.41
1:A:305:LEU:HA	1:A:308:VAL:HG22	2.03	0.41
1:B:33:LEU:HD23	1:B:33:LEU:C	2.41	0.41
1:A:148:ALA:O	1:A:149:GLY:C	2.58	0.41
1:B:250:ASN:ND2	1:B:382:TYR:HE2	2.18	0.41
1:B:358:ALA:HB3	1:B:359:PRO:CD	2.47	0.41
2:C:51:ILE:HG23	2:C:51:ILE:O	2.21	0.41
1:A:342:ILE:O	1:A:346:LEU:HB2	2.20	0.41
1:A:382:TYR:HB3	1:A:384:LEU:CD2	2.51	0.41
1:A:270:ASN:HA	1:A:273:VAL:HG12	2.01	0.41
1:A:313:SER:OG	1:A:314:GLY:N	2.51	0.41
1:B:144:VAL:O	1:B:145:LEU:CG	2.68	0.41
1:A:74:ASN:ND2	1:A:74:ASN:C	2.72	0.41
1:A:201:ILE:HD13	1:A:201:ILE:HG21	1.74	0.41
3:D:17:ASP:O	3:D:19:VAL:HG23	2.21	0.41
1:B:131:LYS:CE	1:B:153:GLN:NE2	2.73	0.41
3:F:49:ASP:O	3:F:50:THR:HB	2.21	0.41
3:D:116:ILE:HD13	3:D:207:SER:HA	2.03	0.41
1:A:222:VAL:O	1:A:223:ILE:C	2.58	0.41
2:C:163:ASN:ND2	2:C:167:LEU:HB2	2.31	0.41
1:B:284:HIS:CB	1:B:290:LYS:HB2	2.51	0.41
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.36	0.41
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:OD1	1:B:403:ARG:NE	2.48	0.41
1:A:280:LEU:HD22	1:A:294:MET:SD	2.61	0.41
1:B:84:LEU:O	1:B:88:VAL:HG23	2.20	0.41
2:C:107:TYR:CE1	3:D:45:ARG:NE	2.89	0.41
1:A:434:LEU:HD23	1:B:216:LYS:HD3	2.03	0.41
2:E:86:VAL:HG12	2:E:119:VAL:CG1	2.50	0.41
1:B:109:ILE:HD13	1:B:199:PHE:CE2	2.56	0.41
2:C:89:GLU:CD	2:C:89:GLU:H	2.25	0.41
2:E:175:PRO:HG2	3:F:162:TRP:O	2.21	0.41
1:B:130:VAL:O	1:B:134:GLY:N	2.54	0.40
1:A:180:THR:HG22	1:A:218:VAL:CA	2.50	0.40
1:A:405:PRO:O	1:A:406:LEU:C	2.59	0.40
1:B:309:ALA:N	1:B:310:PRO:HD3	2.37	0.40
2:C:86:VAL:CG1	2:C:119:VAL:CG2	3.00	0.40
1:B:194:LEU:HB2	1:B:414:GLU:CD	2.42	0.40
2:C:195:SER:O	2:C:199:GLU:HB3	2.21	0.40
1:A:59:TRP:O	1:A:62:ASN:HB3	2.21	0.40
2:C:65:LYS:HB3	2:C:65:LYS:HE3	1.61	0.40
1:B:83:PHE:C	1:B:83:PHE:CD1	2.94	0.40
1:A:216:LYS:HE2	1:B:433:THR:HG21	2.04	0.40
3:D:146:LYS:HE3	3:D:148:LYS:HE3	2.02	0.40
3:D:31:TYR:HA	3:D:50:THR:HG1	1.83	0.40
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.21	0.40
1:A:241:VAL:CG1	1:A:241:VAL:O	2.69	0.40
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.52	0.40
2:E:85:LYS:HD3	2:E:85:LYS:N	2.36	0.40
1:A:98:ARG:HH21	1:A:102:PRO:HA	1.87	0.40
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.57	0.40
1:B:50:ALA:O	1:B:54:ASP:HB2	2.22	0.40
1:A:337:PHE:O	1:A:341:VAL:HG23	2.21	0.40
1:A:459:GLU:C	1:A:460:GLN:HG3	2.38	0.40
3:D:6:GLN:NE2	3:D:100:GLY:H	2.19	0.40
2:E:196:TRP:HD1	2:E:201:VAL:HG23	1.86	0.40
3:D:59:VAL:C	3:D:61:PHE:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/473 (93%)	387 (88%)	49 (11%)	6 (1%)	14	42
1	B	439/473 (93%)	361 (82%)	60 (14%)	18 (4%)	3	11
2	C	219/221 (99%)	191 (87%)	27 (12%)	1 (0%)	34	69
2	E	219/221 (99%)	199 (91%)	18 (8%)	2 (1%)	21	55
3	D	209/211 (99%)	179 (86%)	23 (11%)	7 (3%)	5	16
3	F	209/211 (99%)	188 (90%)	20 (10%)	1 (0%)	34	69
All	All	1737/1810 (96%)	1505 (87%)	197 (11%)	35 (2%)	9	30

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL
1	B	75	TYR
1	B	144	VAL
3	D	15	PRO
1	B	72	ALA
1	B	310	PRO
3	D	16	GLY
1	B	96	LEU
2	E	62	PRO
3	F	198	LYS
1	A	144	VAL
1	B	128	LEU
1	B	210	TYR
1	B	365	THR
1	B	443	PRO
3	D	80	GLU
1	A	443	PRO
1	A	459	GLU
1	B	76	PRO
1	B	285	GLY

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Mol	Chain	Res	Type
1	B	309	ALA
1	B	373	MET
3	D	83	ALA
2	E	65	LYS
1	B	350	SER
3	D	67	GLY
3	D	105	ILE
1	A	149	GLY
1	B	149	GLY
2	C	62	PRO
1	B	342	ILE
1	A	266	GLY
1	B	223	ILE
1	B	441	GLY
3	D	7	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/356 (94%)	304 (91%)	29 (9%)	13	35
1	B	330/356 (93%)	304 (92%)	26 (8%)	15	40
2	C	181/181 (100%)	163 (90%)	18 (10%)	10	28
2	E	181/181 (100%)	168 (93%)	13 (7%)	18	45
3	D	185/185 (100%)	171 (92%)	14 (8%)	16	42
3	F	185/185 (100%)	171 (92%)	14 (8%)	16	42
All	All	1395/1444 (97%)	1281 (92%)	114 (8%)	14	38

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	54	ASP
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	151	THR
1	A	180	THR
1	A	200	ILE
1	A	208	PHE
1	A	212	LEU
1	A	215	ILE
1	A	219	PHE
1	A	233	ASN
1	A	234	HIS
1	A	243	LYS
1	A	244	LEU
1	A	256	LEU
1	A	264	ILE
1	A	277	GLN
1	A	279	LEU
1	A	343	THR
1	A	377	GLU
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	433	THR
1	A	435	LEU
1	A	442	LYS
1	A	444	LEU
1	A	451	ARG
1	B	62	ASN
1	B	73	ASP
1	B	77	LEU
1	B	78	LEU
1	B	103	GLU
1	B	130	VAL
1	B	132	PHE
1	B	168	LEU
1	B	177	LEU
1	B	194	LEU
1	B	200	ILE
1	B	219	PHE
1	B	244	LEU
1	B	245	SER
1	B	251	THR
1	B	264	ILE

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Mol	Chain	Res	Type
1	B	340	ARG
1	B	357	PHE
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	434	LEU
1	B	444	LEU
1	B	451	ARG
1	B	453	LEU
2	C	18	LEU
2	C	21	SER
2	C	65	LYS
2	C	66	ASP
2	C	72	ARG
2	C	98	ARG
2	C	116	THR
2	C	142	SER
2	C	185	LEU
2	C	186	SER
2	C	193	SER
2	C	195	SER
2	C	198	SER
2	C	200	THR
2	C	203	CYS
2	C	204	ASN
2	C	211	SER
2	C	214	VAL
3	D	12	SER
3	D	20	THR
3	D	27	SER
3	D	39	SER
3	D	42	SER
3	D	46	TRP
3	D	68	THR
3	D	70	TYR
3	D	75	ASN
3	D	80	GLU
3	D	95	GLN
3	D	122	GLU
3	D	152	SER
3	D	190	SER

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Mol	Chain	Res	Type
2	E	22	CYS
2	E	55	SER
2	E	59	ASN
2	E	72	ARG
2	E	84	SER
2	E	91	THR
2	E	98	ARG
2	E	107	TYR
2	E	136	SER
2	E	151	LYS
2	E	164	SER
2	E	200	THR
2	E	204	ASN
3	F	15	PRO
3	F	27	SER
3	F	28	SER
3	F	69	SER
3	F	88	GLN
3	F	95	GLN
3	F	115	SER
3	F	125	THR
3	F	156	ASN
3	F	164	ASP
3	F	168	LYS
3	F	189	ASN
3	F	190	SER
3	F	192	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	119	GLN
1	A	153	GLN
1	A	157	ASN
1	A	270	ASN
1	A	277	GLN
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	62	ASN

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Mol	Chain	Res	Type
1	B	63	GLN
1	B	153	GLN
1	B	157	ASN
1	B	270	ASN
1	B	277	GLN
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
2	C	163	ASN
3	D	6	GLN
3	D	36	GLN
3	D	136	ASN
3	D	189	ASN
2	E	39	GLN
2	E	172	HIS
3	F	6	GLN
3	F	37	GLN
3	F	89	GLN
3	F	136	ASN
3	F	137	ASN
3	F	189	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 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	444/473 (93%)	0.46	20 (4%)	37	26	80, 99, 129, 147	0
1	B	441/473 (93%)	0.54	32 (7%)	18	10	72, 105, 140, 156	0
2	C	221/221 (100%)	0.30	12 (5%)	29	19	69, 95, 121, 145	0
2	E	221/221 (100%)	0.14	7 (3%)	51	39	70, 94, 116, 132	0
3	D	211/211 (100%)	0.45	20 (9%)	10	5	82, 107, 125, 129	0
3	F	211/211 (100%)	0.48	24 (11%)	7	3	64, 87, 126, 131	0
All	All	1749/1810 (96%)	0.42	115 (6%)	22	13	64, 99, 129, 156	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	10.1
1	A	168	LEU	7.4
1	B	104	ALA	6.8
3	F	147	TRP	6.7
1	B	73	ASP	6.4
1	B	307	PHE	6.3
1	B	70	HIS	6.3
3	F	211	ALA	5.7
1	B	168	LEU	5.6
1	B	71	THR	5.3
2	C	147	GLY	5.2
3	F	149	ILE	5.2
3	F	151	GLY	4.2
3	F	189	ASN	4.1
3	F	148	LYS	4.1
3	F	152	SER	4.0
1	B	353	PRO	3.9
1	A	288	ILE	3.8
1	A	29	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	3.7
1	B	456	GLN	3.7
2	E	13	GLN	3.7
2	E	59	ASN	3.6
3	D	68	THR	3.5
1	A	144	VAL	3.5
3	D	138	PHE	3.4
3	F	153	GLU	3.4
2	E	29	TYR	3.3
3	D	18	LYS	3.3
1	A	71	THR	3.3
3	F	2	ILE	3.2
1	A	75	TYR	3.2
1	B	304	LEU	3.2
1	B	288	ILE	3.2
1	B	78	LEU	3.2
3	D	196	THR	3.2
3	D	22	THR	3.2
3	D	7	SER	3.2
3	F	150	ASP	3.2
3	F	191	TYR	3.1
1	B	273	VAL	3.1
2	E	201	VAL	3.1
3	D	19	VAL	3.0
2	C	196	TRP	2.9
2	C	29	TYR	2.9
1	B	69	VAL	2.9
3	F	192	THR	2.9
2	E	222	ALA	2.9
1	B	332	MET	2.8
2	C	138	ALA	2.8
3	F	29	VAL	2.8
3	D	20	THR	2.8
3	D	105	ILE	2.8
1	A	143	MET	2.8
1	B	233	ASN	2.8
3	D	197	HIS	2.7
1	A	27	GLU	2.7
3	D	204	ILE	2.7
3	D	69	SER	2.7
1	B	162	VAL	2.7
1	B	177	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	95	PHE	2.6
3	D	79	ALA	2.6
2	C	64	LEU	2.6
3	F	205	VAL	2.6
2	C	66	ASP	2.6
1	B	166	PHE	2.6
2	C	146	LEU	2.6
1	A	283	VAL	2.5
3	F	68	THR	2.5
1	B	163	LEU	2.5
3	F	124	LEU	2.5
2	C	199	GLU	2.4
2	C	221	ARG	2.4
1	B	335	PHE	2.4
2	C	65	LYS	2.4
2	E	4	LEU	2.4
1	B	165	ILE	2.4
1	A	28	ARG	2.4
2	C	144	VAL	2.4
3	D	110	ALA	2.4
3	F	146	LYS	2.4
1	A	423	LEU	2.3
3	F	67	GLY	2.3
1	A	426	ILE	2.3
3	D	146	LYS	2.3
1	B	280	LEU	2.3
1	A	201	ILE	2.3
1	A	212	LEU	2.3
3	F	155	GLN	2.3
3	F	127	GLY	2.2
1	B	167	ARG	2.2
1	A	422	ILE	2.2
1	A	167	ARG	2.2
3	F	154	ARG	2.2
3	F	193	CYS	2.1
1	B	125	TRP	2.1
3	D	38	LYS	2.1
3	D	195	ALA	2.1
1	A	23	ARG	2.1
1	A	18	ARG	2.1
3	D	34	TRP	2.1
3	F	135	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	402	ILE	2.1
3	D	112	PRO	2.1
1	B	101	ALA	2.1
1	B	347	CYS	2.1
1	B	357	PHE	2.0
3	F	69	SER	2.0
3	D	103	LEU	2.0
2	C	141	ALA	2.0
2	E	221	ARG	2.0
1	A	356	ILE	2.0
1	B	201	ILE	2.0
1	B	354	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.