Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 AM GMT

PDB ID	:	3EJZ
Title	:	Structure of E203V mutant E.coli Cl-/H+ exchanger, CLC-ec1
Authors	:	Lim, H.-H.; Miller, C.
Deposited on	:	2008-09-18
Resolution	:	2.90 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:

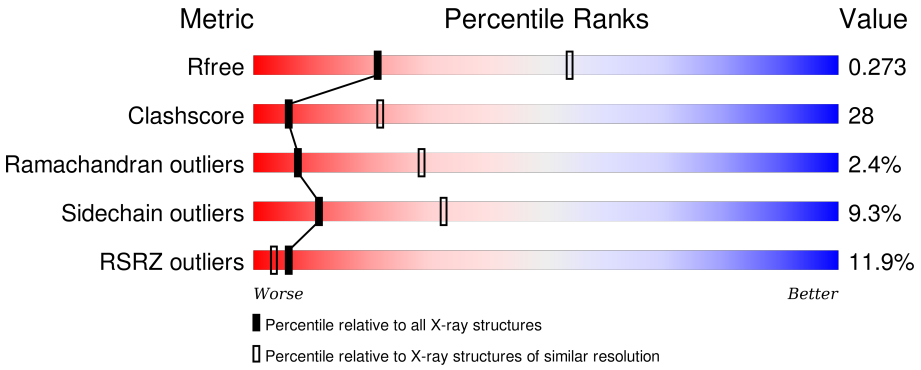
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 <=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	9% 53% 34% 7% 6%
1	B	473	11% 52% 34% 7% 7%
2	C	221	7% 63% 32% 5%
2	E	221	9% 65% 31% .
3	D	211	20% 45% 45% 9%

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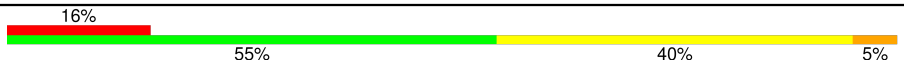
Mol	Chain	Length	Quality of chain
3	F	211	

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
4	BR	A	474	-	-	X	-
4	BR	A	475	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13223 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
			3331	2190	560	561	20			
1	B	441	Total	C	N	O	S	0	0	0
			3302	2174	553	555	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	VAL	GLU	ENGINEERED	UNP P37019
B	203	VAL	GLU	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			

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Br	0	0
			2	2		

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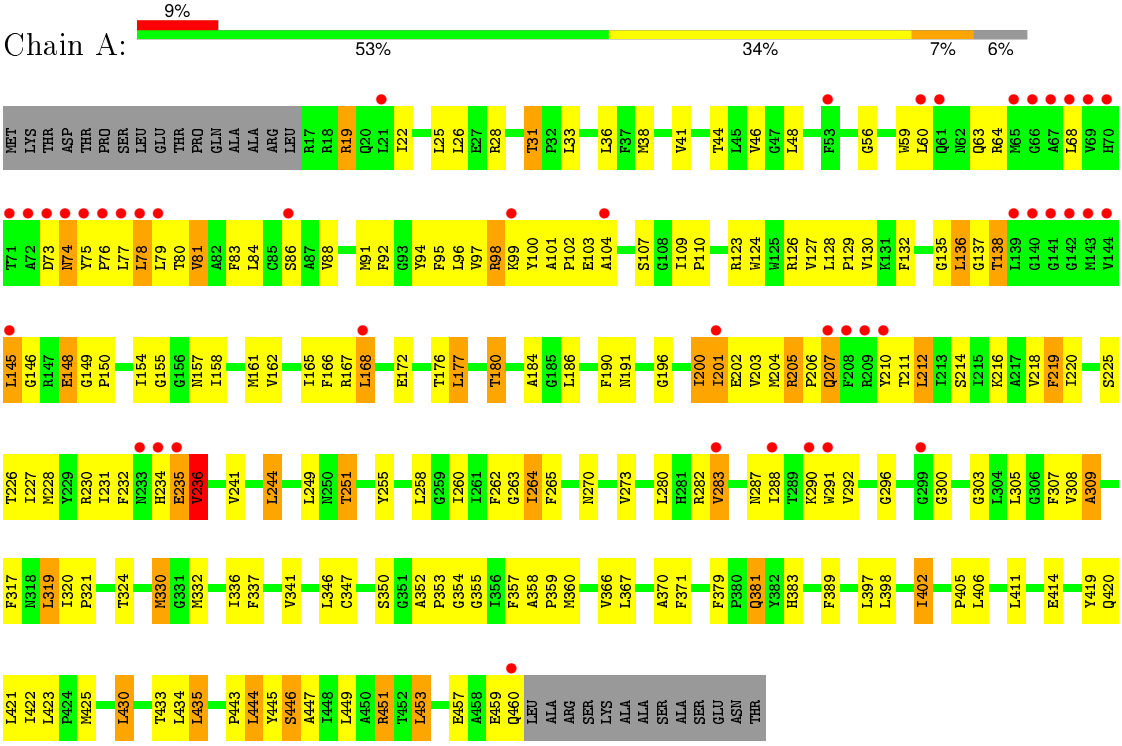
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Br		
4	A	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

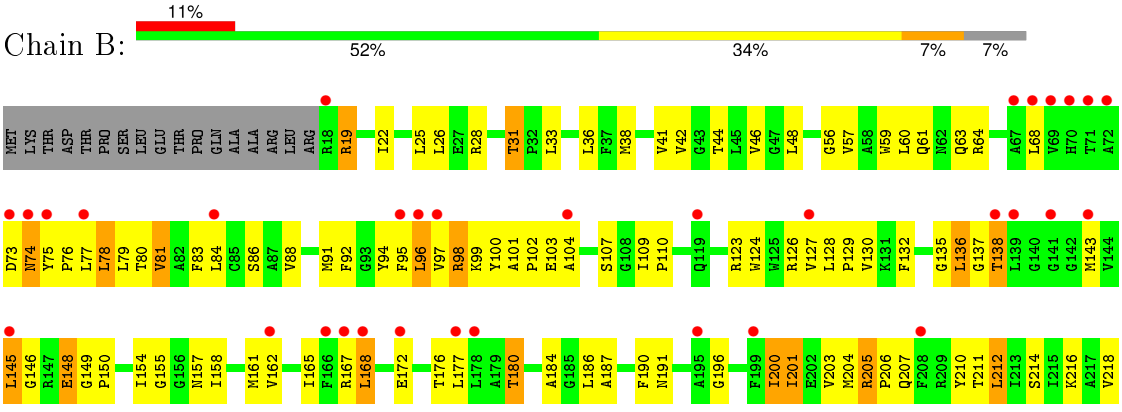
- Molecule 1: H(+)/Cl(-) exchange transporter clcA

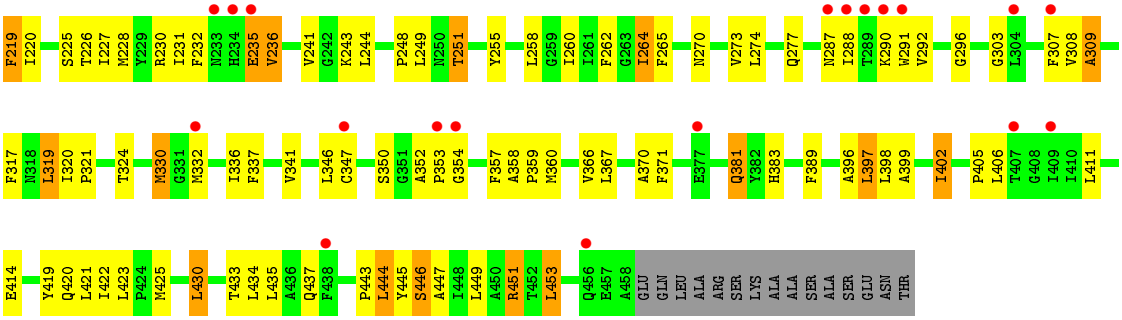
Chain A:



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

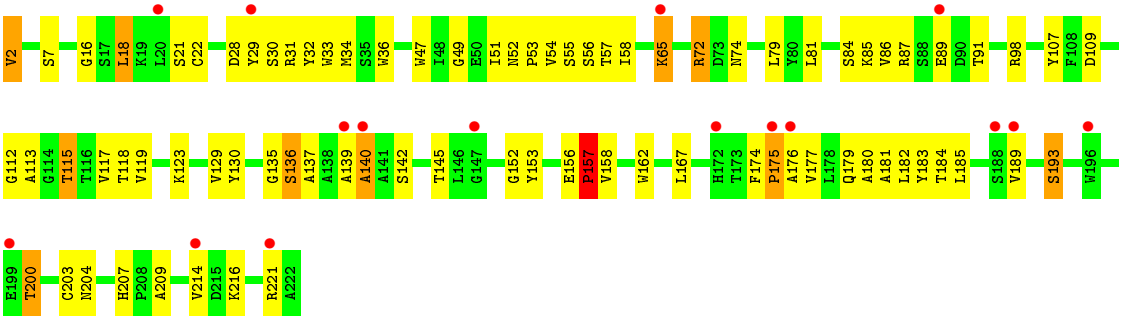
Chain B:





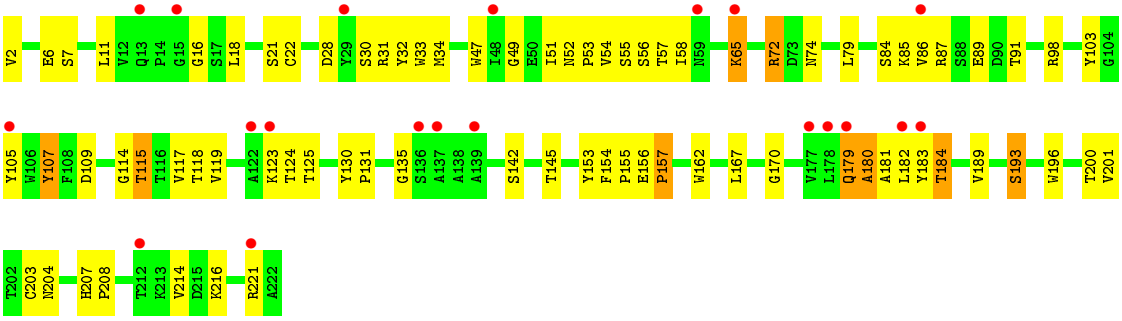
• Molecule 2: Fab fragment, Heavy chain

Chain C:



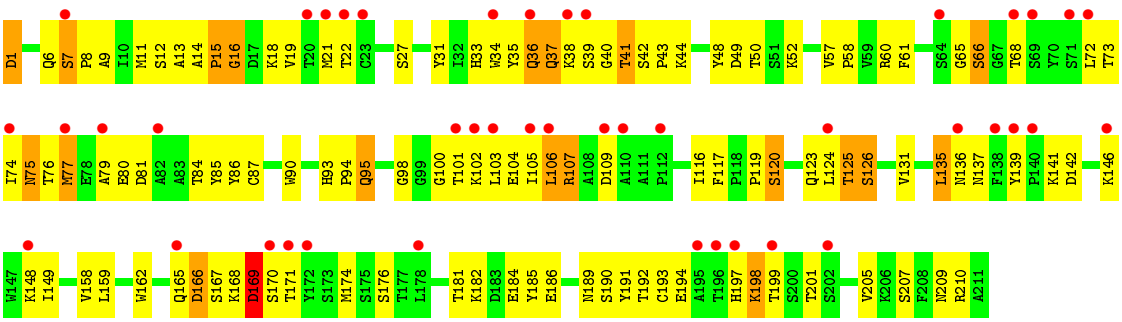
• Molecule 2: Fab fragment, Heavy chain

Chain E:



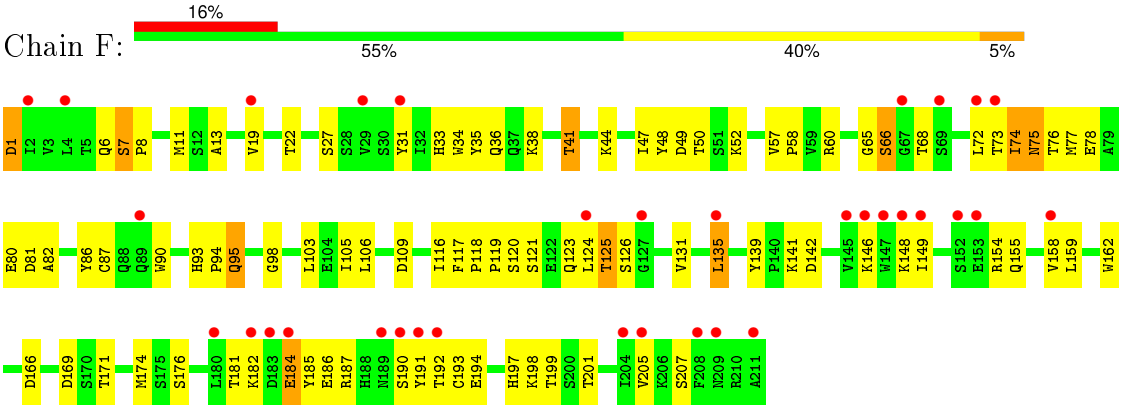
• Molecule 3: Fab fragment, Light chain

Chain D:



• Molecule 3: Fab fragment, Light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.26Å 96.42Å 170.15Å 90.00° 131.78° 90.00°	Depositor
Resolution (Å)	58.76 – 2.90 58.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (58.76-2.90) 99.3 (58.76-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.252 , 0.281 0.246 , 0.273	Depositor DCC
R_{free} test set	3094 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	89.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 80.0	EDS
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 61700 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.40	0/3403	0.55	0/4619
1	B	0.40	0/3374	0.54	0/4581
2	C	0.52	0/1721	0.73	2/2355 (0.1%)
2	E	0.53	0/1721	0.68	0/2355
3	D	0.46	0/1660	0.69	1/2257 (0.0%)
3	F	0.53	0/1660	0.67	0/2257
All	All	0.46	0/13539	0.63	3/18424 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	140	ALA	CB-CA-C	8.01	122.11	110.10
3	D	169	ASP	CB-CA-C	7.16	124.73	110.40
2	C	136	SER	CB-CA-C	6.77	122.97	110.10

There are no chirality outliers.

There are no planarity outliers.

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	3331	0	3486	209	0
1	B	3302	0	3459	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1672	0	1654	73	0
2	E	1672	0	1654	65	0
3	D	1621	0	1546	151	0
3	F	1621	0	1546	110	0
4	A	2	0	0	3	0
4	B	2	0	0	1	0
All	All	13223	0	13345	754	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 (754) 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)
3:D:105:ILE:HB	3:D:170:SER:OG	1.43	1.18
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.11	1.14
1:B:235:GLU:O	1:B:236:VAL:HG23	1.46	1.14
3:D:36:GLN:HG3	3:D:37:GLN:N	1.69	1.08
1:B:19:ARG:HH11	1:B:19:ARG:HG2	1.09	1.07
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.38	1.06
3:D:95:GLN:H	3:D:95:GLN:CD	1.59	1.04
3:F:34:TRP:CG	3:F:72:LEU:HD12	1.92	1.04
3:F:95:GLN:H	3:F:95:GLN:CD	1.62	1.03
3:D:36:GLN:HG3	3:D:37:GLN:H	1.21	1.03
3:D:80:GLU:O	3:D:81:ASP:OD2	1.78	1.00
3:D:19:VAL:O	3:D:73:THR:HG23	1.60	1.00
1:A:176:THR:O	1:A:180:THR:HG23	1.62	1.00
3:D:13:ALA:HB3	3:D:77:MET:HE3	1.44	0.99
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.45	0.97
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.47	0.96
3:D:14:ALA:HA	3:D:106:LEU:HB2	1.47	0.96
3:D:6:GLN:NE2	3:D:100:GLY:H	1.65	0.95
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.46	0.94
1:A:154:ILE:O	1:A:158:ILE:HG12	1.69	0.93
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.48	0.92
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.47	0.92
1:B:154:ILE:O	1:B:158:ILE:HG12	1.69	0.92
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.49	0.91
3:D:86:TYR:CD2	3:D:100:GLY:HA3	2.07	0.90
1:A:381:GLN:N	1:A:381:GLN:HE21	1.70	0.90
3:D:105:ILE:CB	3:D:170:SER:OG	2.18	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLN:HE21	1:B:381:GLN:H	0.94	0.89
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.53	0.89
1:A:381:GLN:NE2	1:A:381:GLN:H	1.71	0.87
3:F:73:THR:HG22	3:F:74:ILE:N	1.90	0.87
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.54	0.87
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.57	0.87
3:D:168:LYS:O	3:D:169:ASP:HB3	1.71	0.86
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.57	0.86
3:D:95:GLN:N	3:D:95:GLN:CD	2.29	0.85
1:B:235:GLU:O	1:B:236:VAL:CG2	2.25	0.85
3:D:15:PRO:HA	3:D:77:MET:O	1.77	0.85
3:F:73:THR:CG2	3:F:74:ILE:N	2.39	0.85
1:B:381:GLN:NE2	1:B:381:GLN:H	1.75	0.84
1:B:381:GLN:N	1:B:381:GLN:HE21	1.74	0.83
2:C:135:GLY:HA2	2:C:221:ARG:HD3	1.62	0.82
1:A:381:GLN:HE21	1:A:381:GLN:H	0.88	0.82
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.62	0.82
3:D:14:ALA:CA	3:D:106:LEU:HB2	2.10	0.81
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.15	0.81
3:D:36:GLN:CG	3:D:37:GLN:N	2.43	0.81
3:D:192:THR:HG22	3:D:207:SER:CB	2.11	0.81
3:F:73:THR:CG2	3:F:74:ILE:H	1.94	0.80
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.64	0.80
3:F:76:THR:O	3:F:76:THR:HG22	1.82	0.80
2:E:32:TYR:CE2	2:E:98:ARG:HD3	2.17	0.80
1:A:205:ARG:HG3	1:A:205:ARG:O	1.81	0.80
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.64	0.79
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.64	0.79
3:F:34:TRP:CG	3:F:72:LEU:CD1	2.66	0.79
1:B:19:ARG:NH1	1:B:19:ARG:HG2	1.89	0.78
3:D:80:GLU:C	3:D:81:ASP:OD2	2.21	0.78
3:F:95:GLN:N	3:F:95:GLN:CD	2.29	0.78
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.64	0.78
3:D:107:ARG:HD3	3:D:139:TYR:HB2	1.64	0.78
2:C:153:TYR:CZ	2:C:183:TYR:HB3	2.18	0.77
1:B:243:LYS:HG2	2:E:31:ARG:HH21	1.48	0.77
3:F:125:THR:O	3:F:125:THR:HG22	1.84	0.77
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.00	0.77
3:D:77:MET:HE2	3:D:103:LEU:HD21	1.65	0.77
3:F:7:SER:HB2	3:F:22:THR:HB	1.67	0.77
1:A:98:ARG:HE	1:A:98:ARG:HA	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:GLN:H	3:F:95:GLN:NE2	1.82	0.76
2:C:174:PHE:O	2:C:175:PRO:O	2.04	0.76
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.68	0.76
3:F:192:THR:HG22	3:F:207:SER:CB	2.15	0.76
1:B:19:ARG:CG	1:B:19:ARG:HH11	1.96	0.76
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.21	0.76
3:D:125:THR:HG22	3:D:125:THR:O	1.86	0.75
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.68	0.75
3:F:7:SER:HB3	3:F:8:PRO:CD	2.15	0.75
1:B:98:ARG:HA	1:B:98:ARG:HE	1.52	0.75
3:D:38:LYS:O	3:D:40:GLY:N	2.19	0.75
3:D:6:GLN:NE2	3:D:100:GLY:N	2.34	0.74
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.68	0.74
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.67	0.74
3:F:106:LEU:HD23	3:F:139:TYR:OH	1.88	0.74
1:A:19:ARG:CG	1:A:19:ARG:HH11	1.97	0.74
1:B:212:LEU:H	1:B:212:LEU:HD12	1.53	0.74
3:D:95:GLN:H	3:D:95:GLN:NE2	1.87	0.73
3:D:86:TYR:CD2	3:D:100:GLY:CA	2.71	0.73
3:D:7:SER:HB2	3:D:22:THR:HB	1.71	0.73
3:F:34:TRP:CD2	3:F:72:LEU:HD12	2.24	0.72
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.72	0.72
3:D:105:ILE:HG22	3:D:106:LEU:N	2.05	0.72
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.05	0.72
1:B:422:ILE:HA	1:B:425:MET:HE2	1.71	0.71
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.25	0.71
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.57	0.71
2:E:30:SER:O	2:E:31:ARG:HB2	1.89	0.71
2:C:174:PHE:O	2:C:175:PRO:C	2.28	0.71
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.74	0.70
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.27	0.70
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.27	0.70
3:D:13:ALA:HB3	3:D:77:MET:CE	2.19	0.70
2:C:30:SER:O	2:C:31:ARG:HB2	1.92	0.70
1:A:212:LEU:HD12	1:A:212:LEU:H	1.55	0.70
3:D:21:MET:SD	3:D:101:THR:HG21	2.32	0.70
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.73	0.70
3:D:21:MET:CB	3:D:101:THR:HG21	2.21	0.70
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.74	0.69
3:D:19:VAL:O	3:D:73:THR:CG2	2.41	0.69
3:D:192:THR:HG22	3:D:207:SER:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.27	0.69
3:D:61:PHE:CE2	3:D:74:ILE:HG12	2.28	0.68
2:E:124:THR:HG22	2:E:125:THR:N	2.08	0.68
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.74	0.68
3:D:105:ILE:HB	3:D:170:SER:HG	1.55	0.68
3:F:34:TRP:CD2	3:F:72:LEU:CD1	2.77	0.68
3:F:34:TRP:CD1	3:F:72:LEU:HD12	2.29	0.68
1:B:243:LYS:CG	2:E:31:ARG:NH2	2.57	0.68
3:F:192:THR:HG22	3:F:207:SER:HB2	1.74	0.68
3:D:7:SER:HB3	3:D:8:PRO:CD	2.22	0.68
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.75	0.68
1:A:422:ILE:HA	1:A:425:MET:HE2	1.75	0.68
2:C:174:PHE:C	2:C:175:PRO:O	2.32	0.67
3:F:73:THR:HG23	3:F:74:ILE:H	1.58	0.67
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.28	0.67
1:A:172:GLU:HA	1:A:212:LEU:HB2	1.77	0.67
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.76	0.67
1:B:91:MET:HG2	1:B:292:VAL:O	1.94	0.67
1:B:212:LEU:HD12	1:B:212:LEU:N	2.09	0.67
2:E:52:ASN:ND2	2:E:57:THR:HB	2.09	0.67
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.29	0.67
3:D:6:GLN:HE21	3:D:100:GLY:H	1.42	0.67
1:B:172:GLU:HA	1:B:212:LEU:HB2	1.77	0.67
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.77	0.67
2:C:177:VAL:CG2	2:C:184:THR:O	2.43	0.66
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.77	0.66
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.63	0.66
3:D:166:ASP:CG	3:D:167:SER:N	2.49	0.66
3:D:19:VAL:O	3:D:73:THR:HA	1.96	0.66
3:F:7:SER:CB	3:F:22:THR:HB	2.25	0.66
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.78	0.65
1:A:212:LEU:HD12	1:A:212:LEU:N	2.12	0.65
1:A:211:THR:HG22	1:A:212:LEU:H	1.61	0.65
1:A:19:ARG:HG2	1:A:19:ARG:NH1	1.91	0.65
1:B:44:THR:O	1:B:48:LEU:HG	1.97	0.65
3:D:105:ILE:CG2	3:D:170:SER:OG	2.44	0.65
3:F:7:SER:CB	3:F:8:PRO:HD3	2.21	0.65
2:E:105:TYR:CE1	3:F:31:TYR:CD1	2.85	0.65
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.61	0.65
3:D:84:THR:HG21	3:D:86:TYR:CZ	2.32	0.64
1:B:264:ILE:HG13	1:B:265:PHE:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:HG22	1:B:212:LEU:H	1.60	0.64
3:D:158:VAL:O	3:D:159:LEU:HD23	1.97	0.64
3:D:109:ASP:HB3	3:D:199:THR:HG22	1.79	0.64
2:C:145:THR:HG22	3:D:117:PHE:HZ	1.62	0.64
1:A:124:TRP:CZ3	1:A:161:MET:HG3	2.32	0.64
1:A:176:THR:O	1:A:180:THR:CG2	2.42	0.64
1:A:56:GLY:HA3	1:A:136:LEU:HD11	1.80	0.64
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.33	0.63
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.65	0.63
1:A:264:ILE:HG13	1:A:265:PHE:N	2.13	0.63
3:F:116:ILE:HD12	3:F:193:CYS:HB2	1.81	0.63
1:A:91:MET:HG2	1:A:292:VAL:O	1.98	0.63
3:D:86:TYR:HA	3:D:100:GLY:HA2	1.81	0.63
1:B:124:TRP:CZ3	1:B:161:MET:HG3	2.34	0.63
3:D:7:SER:CB	3:D:22:THR:HB	2.27	0.63
3:D:135:LEU:HD23	3:D:135:LEU:N	2.14	0.63
3:D:169:ASP:O	3:D:170:SER:HB2	1.98	0.63
1:A:414:GLU:HG2	1:B:419:TYR:OH	1.98	0.63
3:D:79:ALA:O	3:D:81:ASP:N	2.28	0.63
1:A:249:LEU:HD13	1:B:231:ILE:HD13	1.80	0.63
1:A:459:GLU:O	1:A:459:GLU:HG3	1.99	0.62
2:C:177:VAL:HG22	2:C:184:THR:O	1.99	0.62
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.63	0.62
3:D:107:ARG:HD3	3:D:139:TYR:CB	2.29	0.62
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.82	0.62
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.98	0.62
3:F:1:ASP:OD2	3:F:1:ASP:N	2.30	0.62
1:A:204:MET:O	1:A:205:ARG:C	2.37	0.62
1:B:56:GLY:HA3	1:B:136:LEU:HD11	1.80	0.62
3:D:182:LYS:HE2	3:D:186:GLU:OE1	1.99	0.62
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.82	0.62
1:A:330:MET:HA	1:A:330:MET:HE2	1.82	0.62
1:B:357:PHE:CE2	1:B:398:LEU:HD11	2.35	0.61
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.33	0.61
2:C:52:ASN:ND2	2:C:57:THR:HB	2.14	0.61
3:D:60:ARG:HB2	3:D:75:ASN:H	1.65	0.61
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.35	0.61
1:A:124:TRP:CE3	1:A:161:MET:HG3	2.35	0.61
2:C:153:TYR:CE1	2:C:183:TYR:CB	2.83	0.61
1:B:124:TRP:CE3	1:B:161:MET:HG3	2.35	0.61
3:D:36:GLN:O	3:D:37:GLN:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:O	1:B:127:VAL:HG23	2.00	0.60
1:A:98:ARG:HA	1:A:98:ARG:NE	2.15	0.60
1:B:148:GLU:CD	1:B:148:GLU:H	2.04	0.60
1:A:270:ASN:O	1:A:273:VAL:HG12	2.01	0.60
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.83	0.60
3:D:14:ALA:N	3:D:106:LEU:HG	2.16	0.60
3:D:166:ASP:OD1	3:D:168:LYS:N	2.34	0.60
3:D:194:GLU:HG2	3:D:205:VAL:CG1	2.27	0.60
2:E:16:GLY:O	2:E:86:VAL:HG23	2.01	0.60
3:D:107:ARG:CZ	3:D:107:ARG:HB2	2.32	0.60
3:D:1:ASP:OD2	3:D:1:ASP:N	2.29	0.60
3:D:7:SER:CB	3:D:8:PRO:HD3	2.28	0.60
2:C:153:TYR:CE1	2:C:183:TYR:HB3	2.36	0.60
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.02	0.60
1:A:330:MET:HE1	1:A:370:ALA:HA	1.81	0.60
1:A:148:GLU:H	1:A:148:GLU:CD	2.05	0.60
1:B:243:LYS:CG	2:E:31:ARG:HH21	2.14	0.60
1:B:75:TYR:CE2	1:B:79:LEU:HD11	2.37	0.60
3:D:166:ASP:OD1	3:D:167:SER:N	2.35	0.60
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.83	0.60
1:A:123:ARG:O	1:A:127:VAL:HG23	2.02	0.60
3:D:19:VAL:CG2	3:D:77:MET:HB2	2.32	0.60
1:A:357:PHE:CE2	1:A:398:LEU:HD11	2.37	0.59
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.84	0.59
3:F:182:LYS:HE2	3:F:186:GLU:OE1	2.01	0.59
3:D:19:VAL:HG23	3:D:77:MET:HB2	1.83	0.59
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.38	0.59
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.84	0.59
3:D:86:TYR:CE2	3:D:100:GLY:HA3	2.36	0.59
3:D:95:GLN:N	3:D:95:GLN:OE1	2.35	0.59
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.37	0.59
3:F:27:SER:O	3:F:68:THR:HG22	2.03	0.59
1:A:109:ILE:HG23	1:A:204:MET:CE	2.32	0.59
2:E:153:TYR:HD1	2:E:155:PRO:O	1.84	0.59
3:D:27:SER:O	3:D:68:THR:HG22	2.02	0.59
3:D:11:MET:HG3	3:D:103:LEU:HD12	1.84	0.59
3:D:36:GLN:HA	3:D:85:TYR:HA	1.85	0.59
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.69	0.59
1:A:132:PHE:O	1:A:136:LEU:HB2	2.03	0.59
3:D:105:ILE:CG2	3:D:106:LEU:N	2.66	0.59
1:A:126:ARG:O	1:A:129:PRO:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:GLN:O	3:D:43:PRO:HA	2.03	0.58
2:E:105:TYR:CE1	3:F:31:TYR:HD1	2.20	0.58
1:A:44:THR:O	1:A:48:LEU:HG	2.03	0.58
3:D:146:LYS:HB3	3:D:194:GLU:HB2	1.85	0.58
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.36	0.58
1:B:330:MET:HE1	1:B:370:ALA:HA	1.83	0.58
1:A:235:GLU:O	1:A:236:VAL:HG23	2.03	0.58
2:E:52:ASN:HD22	2:E:57:THR:HB	1.69	0.58
1:A:180:THR:HB	1:A:218:VAL:HA	1.85	0.58
2:E:91:THR:HG23	2:E:118:THR:HA	1.85	0.58
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.36	0.58
1:A:330:MET:CE	1:A:330:MET:HA	2.34	0.58
1:A:234:HIS:CD2	1:A:235:GLU:HG3	2.38	0.58
3:F:72:LEU:HD23	3:F:72:LEU:O	2.04	0.57
3:F:6:GLN:HE21	3:F:98:GLY:C	2.07	0.57
1:B:98:ARG:HA	1:B:98:ARG:NE	2.17	0.57
1:B:227:ILE:O	1:B:231:ILE:HG12	2.04	0.57
1:B:451:ARG:HH11	1:B:451:ARG:CG	2.17	0.57
1:A:453:LEU:HB3	1:B:22:ILE:HD11	1.85	0.57
2:C:18:LEU:HD11	2:C:117:VAL:HG22	1.86	0.57
2:C:153:TYR:CD2	2:C:183:TYR:O	2.56	0.57
2:E:145:THR:HG22	3:F:117:PHE:HZ	1.69	0.57
2:C:16:GLY:O	2:C:86:VAL:HG23	2.03	0.57
2:E:124:THR:CG2	2:E:125:THR:N	2.67	0.57
2:E:124:THR:O	2:E:125:THR:OG1	2.17	0.57
1:A:38:MET:HG3	1:A:168:LEU:CD1	2.33	0.57
3:D:116:ILE:HD12	3:D:193:CYS:HB2	1.85	0.57
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.86	0.57
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.34	0.57
1:A:78:LEU:HD13	1:A:79:LEU:N	2.19	0.57
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.70	0.57
3:F:90:TRP:CE2	3:F:95:GLN:NE2	2.67	0.57
1:B:127:VAL:HB	1:B:157:ASN:HD21	1.69	0.57
1:A:86:SER:OG	1:A:303:GLY:HA3	2.04	0.57
2:C:181:ALA:O	2:C:182:LEU:HD23	2.05	0.57
1:B:48:LEU:HD21	1:B:228:MET:SD	2.45	0.56
2:C:91:THR:HG23	2:C:118:THR:HA	1.86	0.56
3:D:61:PHE:HA	3:D:73:THR:O	2.05	0.56
3:D:79:ALA:C	3:D:81:ASP:H	2.09	0.56
3:D:192:THR:HG22	3:D:207:SER:HB3	1.85	0.56
1:B:204:MET:O	1:B:205:ARG:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:O	1:B:205:ARG:HG3	2.05	0.56
1:B:78:LEU:HD13	1:B:79:LEU:N	2.19	0.56
3:F:135:LEU:N	3:F:135:LEU:HD23	2.20	0.56
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.06	0.56
3:F:158:VAL:O	3:F:159:LEU:HD23	2.05	0.56
3:F:95:GLN:N	3:F:95:GLN:OE1	2.39	0.56
3:F:125:THR:CG2	3:F:125:THR:O	2.54	0.56
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.88	0.56
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.86	0.56
3:D:79:ALA:C	3:D:81:ASP:N	2.59	0.56
3:F:194:GLU:HG2	3:F:205:VAL:CG1	2.29	0.56
2:C:139:ALA:O	2:C:140:ALA:C	2.44	0.56
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.86	0.56
1:B:38:MET:HG3	1:B:168:LEU:CD1	2.36	0.56
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.41	0.55
3:D:169:ASP:OD1	3:D:171:THR:HG23	2.06	0.55
3:F:75:ASN:O	3:F:76:THR:HB	2.06	0.55
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.88	0.55
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.41	0.55
1:B:132:PHE:O	1:B:136:LEU:HB2	2.06	0.55
3:D:65:GLY:O	3:D:66:SER:HB3	2.06	0.55
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.42	0.55
3:D:37:GLN:HG3	3:D:41:THR:O	2.06	0.55
1:A:98:ARG:CA	1:A:98:ARG:HE	2.18	0.55
1:B:75:TYR:HA	1:B:78:LEU:HD12	1.89	0.55
1:A:145:LEU:HD21	1:A:347:CYS:HB3	1.89	0.55
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.89	0.55
1:B:19:ARG:NH1	1:B:19:ARG:CG	2.63	0.55
2:C:113:ALA:HA	3:D:42:SER:OG	2.07	0.55
1:A:419:TYR:CZ	1:B:414:GLU:HG2	2.41	0.55
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.37	0.55
1:B:109:ILE:N	1:B:110:PRO:CD	2.69	0.55
1:A:447:ALA:O	1:A:451:ARG:HG2	2.06	0.54
1:B:180:THR:HB	1:B:218:VAL:HA	1.88	0.54
1:B:243:LYS:HG2	2:E:31:ARG:NH2	2.16	0.54
1:B:176:THR:O	1:B:180:THR:HG23	2.08	0.54
1:B:126:ARG:O	1:B:129:PRO:HG2	2.07	0.54
3:D:72:LEU:HD23	3:D:73:THR:N	2.23	0.54
1:B:235:GLU:O	1:B:236:VAL:CB	2.55	0.54
1:A:459:GLU:O	1:A:460:GLN:HG2	2.08	0.54
3:D:125:THR:O	3:D:125:THR:CG2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:CG	1:A:451:ARG:HH11	2.20	0.54
3:F:197:HIS:CE1	3:F:199:THR:HG23	2.43	0.54
3:D:124:LEU:HD22	3:D:182:LYS:HG3	1.88	0.54
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.07	0.54
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.43	0.54
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.43	0.54
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.29	0.54
1:B:83:PHE:C	1:B:83:PHE:CD1	2.80	0.54
3:D:6:GLN:NE2	3:D:100:GLY:CA	2.71	0.54
3:F:38:LYS:O	3:F:41:THR:HG22	2.08	0.54
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.08	0.53
1:A:75:TYR:HA	1:A:78:LEU:HD12	1.89	0.53
2:C:179:GLN:O	2:C:180:ALA:C	2.46	0.53
3:D:34:TRP:CG	3:D:72:LEU:HD12	2.44	0.53
3:F:124:LEU:C	3:F:126:SER:H	2.11	0.53
1:B:330:MET:HA	1:B:330:MET:CE	2.37	0.53
3:D:6:GLN:HE21	3:D:98:GLY:CA	2.22	0.53
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.90	0.53
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.44	0.53
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.91	0.53
1:A:433:THR:HG21	1:B:216:LYS:HE2	1.91	0.53
1:A:214:SER:O	1:A:218:VAL:HG23	2.09	0.53
1:A:48:LEU:HD21	1:A:228:MET:SD	2.49	0.53
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.44	0.53
3:D:168:LYS:O	3:D:169:ASP:CB	2.45	0.53
1:A:449:LEU:HD23	1:B:25:LEU:HD11	1.90	0.53
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.37	0.53
2:C:153:TYR:CE1	2:C:183:TYR:HB2	2.43	0.53
1:A:419:TYR:OH	1:B:414:GLU:HG2	2.09	0.53
3:D:9:ALA:O	3:D:102:LYS:HB3	2.08	0.53
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.91	0.53
3:F:77:MET:CE	3:F:103:LEU:HD21	2.36	0.52
3:F:192:THR:HG22	3:F:207:SER:HB3	1.90	0.52
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.42	0.52
1:B:98:ARG:HE	1:B:98:ARG:CA	2.21	0.52
1:B:100:TYR:O	1:B:126:ARG:HD3	2.09	0.52
1:A:204:MET:O	1:A:205:ARG:O	2.26	0.52
3:D:197:HIS:CE1	3:D:199:THR:HG23	2.44	0.52
3:D:104:GLU:CB	3:D:165:GLN:OE1	2.57	0.52
3:D:104:GLU:HB3	3:D:165:GLN:OE1	2.08	0.52
1:A:100:TYR:O	1:A:126:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.09	0.52
1:B:270:ASN:O	1:B:273:VAL:HG12	2.09	0.52
3:D:14:ALA:HB2	3:D:106:LEU:HD12	1.91	0.52
2:C:153:TYR:CD1	2:C:183:TYR:HB2	2.45	0.52
1:B:145:LEU:HD21	1:B:347:CYS:HB3	1.92	0.52
3:F:7:SER:CB	3:F:8:PRO:CD	2.86	0.52
1:B:158:ILE:O	1:B:162:VAL:HG13	2.10	0.52
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.92	0.52
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.92	0.52
1:A:219:PHE:HB3	1:B:430:LEU:CD1	2.40	0.52
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.91	0.52
3:F:60:ARG:HG3	3:F:74:ILE:CG2	2.40	0.52
1:A:109:ILE:N	1:A:110:PRO:CD	2.72	0.52
2:E:125:THR:N	2:E:154:PHE:O	2.43	0.52
2:C:7:SER:HA	2:C:115:THR:HG21	1.92	0.52
2:C:32:TYR:CD2	2:C:98:ARG:HD3	2.45	0.51
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.40	0.51
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.92	0.51
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.46	0.51
3:F:194:GLU:CG	3:F:205:VAL:HG12	2.32	0.51
3:F:191:TYR:O	3:F:207:SER:HB2	2.10	0.51
2:C:130:TYR:HB3	3:D:120:SER:OG	2.10	0.51
2:C:177:VAL:HG23	2:C:184:THR:O	2.09	0.51
2:C:156:GLU:OE2	2:C:176:ALA:HB3	2.11	0.51
1:A:227:ILE:O	1:A:231:ILE:HG12	2.10	0.51
1:A:107:SER:N	4:A:475:BR:BR	2.95	0.51
1:B:86:SER:OG	1:B:303:GLY:HA3	2.10	0.51
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.45	0.51
1:B:332:MET:O	1:B:336:ILE:HG13	2.11	0.51
3:D:35:TYR:HA	3:D:44:LYS:O	2.11	0.51
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.92	0.51
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.14	0.51
1:B:78:LEU:HD13	1:B:79:LEU:H	1.75	0.51
1:B:447:ALA:O	1:B:451:ARG:HG2	2.10	0.51
3:D:60:ARG:O	3:D:75:ASN:N	2.44	0.50
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.10	0.50
3:F:11:MET:CE	3:F:19:VAL:HG13	2.41	0.50
1:A:83:PHE:C	1:A:83:PHE:CD1	2.84	0.50
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.11	0.50
1:A:22:ILE:HD11	1:B:453:LEU:HB3	1.93	0.50
3:D:181:THR:OG1	3:D:184:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:13:ALA:C	3:D:106:LEU:HG	2.32	0.50
1:A:78:LEU:HD13	1:A:79:LEU:H	1.77	0.50
1:B:260:ILE:O	1:B:264:ILE:HG23	2.11	0.50
1:B:451:ARG:HH11	1:B:451:ARG:HG3	1.76	0.50
1:A:73:ASP:N	1:A:73:ASP:OD1	2.41	0.50
1:A:109:ILE:HG23	1:A:204:MET:HE2	1.92	0.50
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.93	0.50
1:B:138:THR:HG22	1:B:143:MET:SD	2.51	0.50
1:A:59:TRP:O	1:A:63:GLN:HG2	2.11	0.50
1:B:68:LEU:HD22	1:B:78:LEU:HD23	1.94	0.50
1:A:22:ILE:O	1:A:26:LEU:HD12	2.12	0.50
1:A:127:VAL:HB	1:A:157:ASN:HD21	1.74	0.50
3:F:77:MET:HG2	3:F:78:GLU:N	2.26	0.50
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.42	0.50
2:C:52:ASN:HD22	2:C:57:THR:HB	1.75	0.50
3:D:105:ILE:CG2	3:D:106:LEU:H	2.24	0.49
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.47	0.49
1:A:184:ALA:HB1	1:A:225:SER:HB3	1.95	0.49
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.48	0.49
3:F:73:THR:C	3:F:74:ILE:HG13	2.30	0.49
3:F:19:VAL:HG21	3:F:77:MET:CE	2.42	0.49
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.47	0.49
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.47	0.49
1:B:73:ASP:OD1	1:B:73:ASP:N	2.41	0.49
2:C:153:TYR:O	2:C:183:TYR:N	2.39	0.49
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.46	0.49
3:D:84:THR:HG22	3:D:86:TYR:CE1	2.46	0.49
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.27	0.49
3:D:34:TRP:CD2	3:D:72:LEU:HD12	2.48	0.49
3:D:19:VAL:O	3:D:73:THR:CA	2.60	0.49
3:D:6:GLN:HE21	3:D:98:GLY:C	2.15	0.49
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.32	0.49
2:E:52:ASN:ND2	2:E:57:THR:H	2.11	0.49
1:A:91:MET:HG3	1:A:296:GLY:CA	2.43	0.49
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.95	0.49
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.47	0.49
1:A:158:ILE:O	1:A:162:VAL:HG13	2.12	0.49
3:D:191:TYR:O	3:D:207:SER:HB2	2.12	0.49
2:E:52:ASN:ND2	2:E:57:THR:N	2.60	0.49
1:A:83:PHE:HD1	1:A:84:LEU:HD23	1.77	0.49
1:A:216:LYS:HE2	1:B:433:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:34:TRP:CD2	3:F:72:LEU:HD13	2.46	0.49
2:E:11:LEU:HD23	2:E:124:THR:OG1	2.13	0.49
3:D:90:TRP:CE2	3:D:95:GLN:NE2	2.67	0.49
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.42	0.49
3:F:124:LEU:HD22	3:F:182:LYS:HG3	1.93	0.49
1:B:92:PHE:C	1:B:92:PHE:CD1	2.86	0.49
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.94	0.48
2:C:87:ARG:HE	2:C:89:GLU:HB2	1.78	0.48
1:B:346:LEU:O	1:B:350:SER:HB3	2.13	0.48
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.95	0.48
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.44	0.48
1:A:148:GLU:OE1	1:A:357:PHE:CB	2.61	0.48
3:D:84:THR:CG2	3:D:86:TYR:CE1	2.95	0.48
3:F:34:TRP:CZ2	3:F:72:LEU:HB2	2.48	0.48
1:A:203:VAL:HA	1:B:28:ARG:NH2	2.28	0.48
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.48	0.48
3:D:12:SER:HA	3:D:104:GLU:O	2.13	0.48
3:D:166:ASP:C	3:D:166:ASP:OD1	2.51	0.48
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.13	0.48
1:B:451:ARG:NH1	1:B:451:ARG:HG3	2.28	0.48
3:F:181:THR:OG1	3:F:184:GLU:HB3	2.13	0.48
1:A:355:GLY:HA2	4:A:474:BR:BR	2.68	0.48
1:A:430:LEU:HD11	1:B:219:PHE:HB3	1.94	0.48
1:B:91:MET:HG3	1:B:296:GLY:CA	2.44	0.48
1:A:234:HIS:HD2	1:A:235:GLU:HG3	1.78	0.48
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.44	0.48
1:A:355:GLY:CA	4:A:474:BR:BR	3.17	0.48
1:A:346:LEU:O	1:A:350:SER:HB3	2.14	0.48
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.61	0.48
1:B:109:ILE:HG23	1:B:204:MET:CE	2.43	0.48
1:B:214:SER:O	1:B:218:VAL:HG23	2.14	0.48
1:A:38:MET:HA	1:A:41:VAL:HG13	1.95	0.48
1:B:201:ILE:HG13	1:B:201:ILE:O	2.13	0.48
2:C:32:TYR:O	2:C:72:ARG:NH2	2.41	0.48
2:E:181:ALA:O	2:E:182:LEU:HD23	2.13	0.48
1:B:402:ILE:HD13	1:B:445:TYR:CD1	2.49	0.48
3:D:6:GLN:HE22	3:D:100:GLY:HA2	1.79	0.48
1:B:91:MET:CG	1:B:296:GLY:HA3	2.44	0.48
1:A:91:MET:CG	1:A:296:GLY:HA3	2.43	0.48
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.48	0.48
1:B:38:MET:HA	1:B:41:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:31:TYR:HA	3:F:50:THR:OG1	2.13	0.48
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.49	0.47
2:C:185:LEU:C	2:C:185:LEU:HD12	2.35	0.47
1:A:92:PHE:C	1:A:92:PHE:CD1	2.87	0.47
1:A:219:PHE:HB3	1:B:430:LEU:HD11	1.96	0.47
3:D:18:LYS:HE3	3:D:75:ASN:OD1	2.14	0.47
1:A:205:ARG:HD3	1:A:207:GLN:OE1	2.14	0.47
3:F:35:TYR:CD1	3:F:35:TYR:N	2.82	0.47
3:F:73:THR:O	3:F:74:ILE:HG12	2.14	0.47
3:F:11:MET:HE2	3:F:19:VAL:HG13	1.97	0.47
1:A:109:ILE:HG23	1:A:204:MET:HE1	1.95	0.47
1:A:68:LEU:HD22	1:A:78:LEU:HD23	1.96	0.47
3:D:124:LEU:C	3:D:126:SER:H	2.16	0.47
3:D:14:ALA:O	3:D:16:GLY:N	2.42	0.47
3:D:36:GLN:O	3:D:37:GLN:CB	2.63	0.47
3:D:84:THR:CG2	3:D:86:TYR:CZ	2.97	0.47
3:F:73:THR:C	3:F:74:ILE:CG1	2.82	0.47
3:D:21:MET:HB3	3:D:101:THR:HG21	1.93	0.47
1:A:249:LEU:C	1:A:251:THR:H	2.17	0.47
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.30	0.47
1:B:249:LEU:C	1:B:251:THR:H	2.17	0.47
1:B:184:ALA:HB1	1:B:225:SER:HB3	1.97	0.47
2:C:84:SER:O	2:C:85:LYS:C	2.53	0.47
2:E:107:TYR:C	2:E:107:TYR:CD1	2.89	0.47
2:E:7:SER:HA	2:E:115:THR:HG21	1.97	0.47
1:B:107:SER:HB3	4:B:475:BR:BR	2.70	0.47
1:A:421:LEU:O	1:A:425:MET:HG3	2.14	0.47
1:B:200:ILE:HA	1:B:204:MET:HB2	1.96	0.47
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.97	0.47
2:E:32:TYR:O	2:E:72:ARG:NH2	2.44	0.46
1:A:98:ARG:CA	1:A:98:ARG:NE	2.78	0.46
2:C:107:TYR:HB3	3:D:33:HIS:NE2	2.30	0.46
1:A:148:GLU:OE1	1:A:357:PHE:HB3	2.15	0.46
1:B:22:ILE:O	1:B:26:LEU:HD12	2.15	0.46
2:E:32:TYR:CD2	2:E:98:ARG:HD3	2.50	0.46
1:B:38:MET:O	1:B:42:VAL:HG23	2.16	0.46
1:B:88:VAL:HA	1:B:91:MET:HE2	1.96	0.46
1:B:148:GLU:OE1	1:B:357:PHE:CB	2.63	0.46
3:F:65:GLY:O	3:F:66:SER:HB3	2.15	0.46
2:E:153:TYR:O	2:E:183:TYR:HB2	2.15	0.46
1:B:83:PHE:HD1	1:B:84:LEU:HD23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG21	1:B:353:PRO:HG3	1.98	0.46
2:C:87:ARG:HG3	2:C:89:GLU:OE1	2.15	0.46
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.96	0.46
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.63	0.46
2:E:130:TYR:CE2	3:F:123:GLN:HG3	2.51	0.46
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.81	0.46
1:A:405:PRO:HG2	1:A:406:LEU:H	1.80	0.46
1:A:260:ILE:O	1:A:264:ILE:HG23	2.16	0.46
1:A:357:PHE:HE2	1:A:411:LEU:HD22	1.81	0.46
3:D:21:MET:HB2	3:D:101:THR:HG21	1.96	0.46
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.51	0.46
1:A:201:ILE:HG13	1:A:201:ILE:O	2.16	0.46
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.98	0.46
2:E:52:ASN:HD21	2:E:57:THR:N	2.13	0.46
1:A:234:HIS:CD2	1:A:235:GLU:CG	2.99	0.46
2:C:86:VAL:HG12	2:C:119:VAL:HG21	1.98	0.46
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.98	0.46
3:D:36:GLN:HA	3:D:84:THR:O	2.16	0.45
1:B:330:MET:HA	1:B:330:MET:HE2	1.97	0.45
2:E:156:GLU:HB3	2:E:157:PRO:HA	1.98	0.45
1:B:31:THR:HB	1:B:36:LEU:HD21	1.98	0.45
1:B:77:LEU:O	1:B:80:THR:HB	2.17	0.45
1:A:234:HIS:HD2	1:A:235:GLU:CG	2.30	0.45
1:A:31:THR:HB	1:A:36:LEU:HD21	1.98	0.45
1:A:33:LEU:HD23	1:A:33:LEU:C	2.37	0.45
1:A:337:PHE:O	1:A:341:VAL:HG23	2.17	0.45
3:D:98:GLY:C	3:D:100:GLY:H	2.19	0.45
3:F:34:TRP:CE3	3:F:72:LEU:HD13	2.51	0.45
1:A:200:ILE:HA	1:A:204:MET:HB2	1.99	0.45
3:F:106:LEU:HD23	3:F:139:TYR:HH	1.82	0.45
1:A:28:ARG:NH2	1:B:203:VAL:HA	2.31	0.45
3:F:49:ASP:O	3:F:50:THR:HB	2.15	0.45
2:E:6:GLU:CD	2:E:114:GLY:H	2.19	0.45
1:A:332:MET:O	1:A:336:ILE:HG13	2.17	0.45
3:F:103:LEU:HA	3:F:103:LEU:HD12	1.61	0.45
1:A:88:VAL:HA	1:A:91:MET:HE2	1.98	0.45
3:F:197:HIS:HE1	3:F:199:THR:HG23	1.81	0.45
1:A:241:VAL:CG2	1:A:324:THR:HG21	2.47	0.45
1:A:99:LYS:HB3	1:A:100:TYR:CD1	2.52	0.45
1:A:226:THR:O	1:A:230:ARG:HG2	2.17	0.45
3:F:109:ASP:HB3	3:F:199:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:ARG:HD2	3:F:155:GLN:H	1.81	0.45
1:B:59:TRP:O	1:B:63:GLN:HG2	2.17	0.45
3:D:7:SER:CB	3:D:8:PRO:CD	2.91	0.45
1:A:457:GLU:C	1:A:459:GLU:H	2.19	0.45
3:D:21:MET:SD	3:D:101:THR:CG2	3.05	0.45
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.99	0.45
3:D:31:TYR:HA	3:D:50:THR:OG1	2.17	0.44
1:B:165:ILE:O	1:B:165:ILE:CG2	2.65	0.44
1:A:135:GLY:O	1:A:137:GLY:N	2.50	0.44
1:A:75:TYR:HE2	1:A:79:LEU:HD11	1.80	0.44
2:E:153:TYR:HE1	2:E:156:GLU:HA	1.83	0.44
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.82	0.44
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.98	0.44
1:B:319:LEU:HD11	1:B:366:VAL:CG2	2.47	0.44
1:B:308:VAL:O	1:B:309:ALA:HB2	2.16	0.44
3:F:6:GLN:HE21	3:F:98:GLY:CA	2.30	0.44
1:A:402:ILE:HD13	1:A:445:TYR:CD1	2.52	0.44
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.64	0.44
1:A:124:TRP:HA	1:A:157:ASN:ND2	2.33	0.44
1:B:422:ILE:HG23	1:B:423:LEU:N	2.33	0.44
1:B:75:TYR:HE2	1:B:79:LEU:HD11	1.80	0.44
1:A:78:LEU:HD21	1:A:307:PHE:CZ	2.53	0.44
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.82	0.44
3:F:124:LEU:O	3:F:126:SER:N	2.45	0.44
1:B:95:PHE:O	1:B:97:VAL:N	2.50	0.44
3:D:210:ARG:HH11	3:D:210:ARG:HG2	1.83	0.44
2:C:135:GLY:C	2:C:137:ALA:H	2.21	0.44
2:E:207:HIS:HA	2:E:208:PRO:HD2	1.69	0.44
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.34	0.44
1:B:405:PRO:HG2	1:B:406:LEU:H	1.82	0.44
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.00	0.44
3:F:105:ILE:HG22	3:F:106:LEU:N	2.32	0.44
1:A:330:MET:O	1:A:330:MET:HG3	2.17	0.44
2:C:112:GLY:O	3:D:42:SER:OG	2.25	0.44
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.73	0.44
1:B:444:LEU:HD22	1:B:444:LEU:O	2.18	0.44
2:E:179:GLN:O	2:E:180:ALA:HB3	2.17	0.44
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.83	0.44
1:A:451:ARG:HG3	1:A:451:ARG:NH1	2.32	0.44
3:F:38:LYS:HE2	3:F:80:GLU:O	2.18	0.44
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:HG22	1:B:212:LEU:N	2.31	0.44
2:E:87:ARG:HE	2:E:89:GLU:HB2	1.83	0.44
1:A:444:LEU:HD22	1:A:444:LEU:O	2.18	0.43
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.81	0.43
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.82	0.43
3:F:36:GLN:NE2	3:F:38:LYS:HG3	2.33	0.43
1:A:135:GLY:C	1:A:137:GLY:N	2.70	0.43
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.83	0.43
1:A:60:LEU:O	1:A:64:ARG:HG3	2.18	0.43
3:F:82:ALA:HB2	3:F:105:ILE:CG1	2.49	0.43
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.33	0.43
1:A:451:ARG:CB	1:A:451:ARG:HH11	2.31	0.43
2:C:54:VAL:HG23	2:C:56:SER:HB3	2.01	0.43
3:D:168:LYS:HD3	3:D:168:LYS:HA	1.92	0.43
3:F:31:TYR:HB3	3:F:49:ASP:HA	2.00	0.43
1:A:19:ARG:CG	1:A:19:ARG:NH1	2.64	0.43
1:A:422:ILE:HG23	1:A:423:LEU:N	2.32	0.43
3:D:136:ASN:O	3:D:137:ASN:HB2	2.18	0.43
1:A:308:VAL:O	1:A:309:ALA:HB2	2.18	0.43
3:F:35:TYR:HA	3:F:44:LYS:O	2.18	0.43
1:B:60:LEU:O	1:B:64:ARG:HG3	2.18	0.43
1:A:95:PHE:O	1:A:97:VAL:N	2.52	0.43
1:B:241:VAL:HG21	1:B:324:THR:HG21	2.01	0.43
3:F:47:ILE:HD12	3:F:72:LEU:HG	1.99	0.43
3:D:149:ILE:HG12	3:D:191:TYR:CE2	2.54	0.43
1:B:148:GLU:OE1	1:B:357:PHE:HB3	2.18	0.43
1:A:231:ILE:HB	1:A:232:PHE:CD1	2.54	0.43
3:F:93:HIS:CG	3:F:94:PRO:HA	2.54	0.43
2:E:189:VAL:HG13	2:E:189:VAL:O	2.18	0.43
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.49	0.43
1:A:319:LEU:HD11	1:A:366:VAL:CG2	2.48	0.43
1:A:210:TYR:HB2	1:B:210:TYR:N	2.32	0.43
1:A:210:TYR:N	1:B:210:TYR:HB2	2.33	0.43
3:D:185:TYR:CE1	3:D:191:TYR:CE1	3.07	0.43
2:C:153:TYR:CE1	2:C:158:VAL:HG13	2.54	0.43
2:C:107:TYR:C	2:C:107:TYR:CD1	2.92	0.43
1:B:212:LEU:H	1:B:212:LEU:CD1	2.27	0.43
1:A:74:ASN:HD22	1:A:76:PRO:HD2	1.82	0.43
1:A:77:LEU:O	1:A:81:VAL:HG13	2.19	0.43
1:A:200:ILE:HA	1:A:200:ILE:HD12	1.74	0.43
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HD21	1:B:307:PHE:CZ	2.54	0.43
1:A:282:ARG:O	1:A:283:VAL:C	2.57	0.43
3:F:187:ARG:HG3	3:F:187:ARG:O	2.19	0.43
3:F:60:ARG:HG3	3:F:74:ILE:HG22	2.01	0.42
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.34	0.42
1:A:166:PHE:O	1:A:168:LEU:N	2.52	0.42
1:A:421:LEU:HA	1:A:421:LEU:HD23	1.78	0.42
2:E:86:VAL:HG12	2:E:119:VAL:HG21	2.00	0.42
2:C:200:THR:HG22	2:C:200:THR:O	2.18	0.42
2:C:189:VAL:O	2:C:189:VAL:HG13	2.19	0.42
1:B:74:ASN:HD22	1:B:76:PRO:HD2	1.83	0.42
1:B:398:LEU:HA	1:B:398:LEU:HD23	1.93	0.42
1:B:109:ILE:HG23	1:B:204:MET:HE2	2.01	0.42
1:B:186:LEU:O	1:B:187:ALA:C	2.57	0.42
1:A:184:ALA:HB1	1:A:225:SER:CB	2.49	0.42
2:C:142:SER:O	2:C:193:SER:HB2	2.19	0.42
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.37	0.42
1:B:421:LEU:O	1:B:425:MET:HG3	2.19	0.42
3:D:197:HIS:HE1	3:D:199:THR:HG23	1.84	0.42
2:E:11:LEU:HD12	2:E:11:LEU:HA	1.86	0.42
3:D:124:LEU:O	3:D:126:SER:N	2.46	0.42
1:B:451:ARG:NH1	1:B:451:ARG:CG	2.80	0.42
2:E:84:SER:O	2:E:85:LYS:C	2.57	0.42
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.53	0.42
1:A:172:GLU:N	1:A:212:LEU:HD22	2.35	0.42
3:F:57:VAL:HA	3:F:58:PRO:HD2	1.82	0.42
3:D:14:ALA:N	3:D:106:LEU:HB2	2.35	0.42
1:B:150:PRO:O	1:B:154:ILE:HG13	2.20	0.42
2:E:30:SER:C	2:E:32:TYR:H	2.22	0.42
1:B:78:LEU:C	1:B:78:LEU:HD22	2.39	0.42
1:A:25:LEU:HD11	1:B:449:LEU:HD23	2.02	0.42
1:B:46:VAL:HG22	1:B:155:GLY:HA2	2.01	0.42
2:C:2:VAL:HG22	2:C:2:VAL:O	2.18	0.42
3:D:35:TYR:O	3:D:85:TYR:HA	2.20	0.42
1:B:99:LYS:HB3	1:B:100:TYR:CD1	2.55	0.42
3:F:185:TYR:CE1	3:F:191:TYR:CE1	3.07	0.42
1:B:422:ILE:HA	1:B:425:MET:CE	2.46	0.42
2:E:170:GLY:O	2:E:189:VAL:HA	2.20	0.42
1:A:126:ARG:HH11	1:A:126:ARG:HG2	1.85	0.42
1:B:77:LEU:O	1:B:81:VAL:HG13	2.19	0.42
1:B:248:PRO:O	1:B:251:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:TYR:CE1	2:C:34:MET:HG3	2.55	0.42
2:C:52:ASN:ND2	2:C:57:THR:H	2.17	0.42
2:E:196:TRP:HD1	2:E:201:VAL:HG23	1.85	0.42
3:F:34:TRP:CB	3:F:72:LEU:CD1	2.97	0.42
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.55	0.42
2:E:87:ARG:HG3	2:E:89:GLU:OE1	2.20	0.42
1:A:457:GLU:OE1	1:B:19:ARG:HG3	2.21	0.41
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.84	0.41
1:B:135:GLY:C	1:B:137:GLY:N	2.73	0.41
1:A:150:PRO:O	1:A:154:ILE:HG13	2.20	0.41
2:E:28:ASP:O	2:E:30:SER:O	2.38	0.41
1:B:337:PHE:O	1:B:341:VAL:HG23	2.19	0.41
2:E:142:SER:O	2:E:193:SER:HB2	2.19	0.41
1:A:77:LEU:O	1:A:80:THR:HB	2.20	0.41
1:B:396:ALA:O	1:B:399:ALA:HB3	2.20	0.41
3:D:93:HIS:CG	3:D:94:PRO:HA	2.56	0.41
2:E:107:TYR:HB3	3:F:33:HIS:NE2	2.35	0.41
1:B:135:GLY:O	1:B:137:GLY:N	2.54	0.41
1:B:201:ILE:O	1:B:201:ILE:CG1	2.68	0.41
1:B:184:ALA:HB1	1:B:225:SER:CB	2.50	0.41
1:B:236:VAL:HG12	1:B:236:VAL:O	2.19	0.41
2:C:28:ASP:O	2:C:30:SER:O	2.38	0.41
1:B:231:ILE:HG22	1:B:231:ILE:O	2.21	0.41
2:C:52:ASN:ND2	2:C:57:THR:N	2.68	0.41
2:E:131:PRO:HD3	2:E:216:LYS:HG2	2.03	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.80	0.41
2:C:153:TYR:CE2	2:C:183:TYR:O	2.74	0.41
1:A:33:LEU:HD23	1:A:33:LEU:O	2.20	0.41
1:A:244:LEU:N	1:A:244:LEU:CD2	2.84	0.41
3:D:6:GLN:HA	3:D:22:THR:O	2.21	0.41
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.50	0.41
2:E:103:TYR:HD2	3:F:31:TYR:CE2	2.39	0.41
1:B:241:VAL:CG2	1:B:324:THR:HG21	2.51	0.41
1:B:255:TYR:CE2	1:B:389:PHE:CD2	3.09	0.41
1:B:33:LEU:C	1:B:33:LEU:HD23	2.40	0.41
1:B:126:ARG:HG2	1:B:126:ARG:HH11	1.85	0.41
2:C:30:SER:C	2:C:32:TYR:H	2.24	0.41
3:F:73:THR:O	3:F:74:ILE:CG1	2.68	0.41
2:C:174:PHE:HA	2:C:175:PRO:HD2	1.95	0.41
3:F:149:ILE:HG12	3:F:191:TYR:CE2	2.55	0.41
1:A:212:LEU:H	1:A:212:LEU:CD1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:HG22	1:A:212:LEU:N	2.33	0.41
2:E:125:THR:HB	2:E:154:PHE:H	1.85	0.41
1:A:422:ILE:HA	1:A:422:ILE:HD12	1.96	0.41
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.84	0.41
1:B:57:VAL:HG12	1:B:61:GLN:OE1	2.21	0.41
1:A:165:ILE:O	1:A:165:ILE:CG2	2.68	0.41
3:D:6:GLN:NE2	3:D:100:GLY:HA2	2.36	0.41
1:A:255:TYR:CE2	1:A:389:PHE:CD2	3.10	0.41
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.70	0.41
3:D:189:ASN:O	3:D:209:ASN:HA	2.21	0.41
3:D:57:VAL:HA	3:D:58:PRO:HD2	1.85	0.41
3:D:12:SER:HB3	3:D:106:LEU:HD23	2.02	0.40
1:B:136:LEU:HA	1:B:136:LEU:HD12	1.76	0.40
2:E:183:TYR:HB3	2:E:184:THR:H	1.75	0.40
1:B:451:ARG:HH11	1:B:451:ARG:CB	2.34	0.40
2:C:7:SER:HA	2:C:115:THR:CG2	2.51	0.40
1:A:216:LYS:NZ	1:B:437:GLN:NE2	2.69	0.40
1:B:59:TRP:CZ3	1:B:63:GLN:HG3	2.56	0.40
2:C:129:VAL:O	2:C:216:LYS:HE3	2.21	0.40
3:F:19:VAL:HG21	3:F:77:MET:HE3	2.03	0.40
1:A:176:THR:HG22	1:A:177:LEU:N	2.37	0.40
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.03	0.40
1:A:434:LEU:HA	1:A:434:LEU:HD23	1.65	0.40
1:B:274:LEU:O	1:B:277:GLN:HB3	2.22	0.40
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.86	0.40
2:E:22:CYS:HB3	2:E:79:LEU:HB3	2.04	0.40
1:A:423:LEU:HD11	1:B:226:THR:HG21	2.04	0.40
1:A:78:LEU:HD22	1:A:78:LEU:C	2.42	0.40
1:A:74:ASN:C	1:A:74:ASN:HD22	2.25	0.40
3:F:124:LEU:C	3:F:126:SER:N	2.75	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	442/473 (93%)	382 (86%)	50 (11%)	10 (2%)	8 30
1	B	439/473 (93%)	382 (87%)	48 (11%)	9 (2%)	9 32
2	C	219/221 (99%)	197 (90%)	18 (8%)	4 (2%)	11 37
2	E	219/221 (99%)	195 (89%)	21 (10%)	3 (1%)	14 44
3	D	209/211 (99%)	173 (83%)	26 (12%)	10 (5%)	3 10
3	F	209/211 (99%)	184 (88%)	20 (10%)	5 (2%)	7 29
All	All	1737/1810 (96%)	1513 (87%)	183 (10%)	41 (2%)	7 29

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	A	205	ARG
1	A	236	VAL
1	B	236	VAL
2	C	157	PRO
2	C	175	PRO
3	D	7	SER
3	D	37	GLN
3	D	39	SER
2	E	184	THR
3	F	7	SER
1	A	96	LEU
1	B	96	LEU
1	B	136	LEU
1	B	167	ARG
2	C	65	LYS
3	D	125	THR
3	D	169	ASP
3	F	74	ILE
3	F	125	THR
3	F	198	LYS
2	C	136	SER
3	D	66	SER
2	E	65	LYS
2	E	180	ALA
3	F	66	SER
1	A	136	LEU

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Mol	Chain	Res	Type
1	A	149	GLY
1	B	309	ALA
3	D	198	LYS
1	A	309	ALA
1	B	205	ARG
3	D	16	GLY
3	D	126	SER
1	A	201	ILE
1	A	206	PRO
1	B	149	GLY
1	B	201	ILE
1	B	206	PRO
3	D	15	PRO
1	A	283	VAL

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	335/358 (94%)	299 (89%)	36 (11%)	8 24
1	B	332/358 (93%)	297 (90%)	35 (10%)	8 25
2	C	181/181 (100%)	167 (92%)	14 (8%)	16 42
2	E	181/181 (100%)	166 (92%)	15 (8%)	14 38
3	D	185/185 (100%)	169 (91%)	16 (9%)	13 36
3	F	185/185 (100%)	171 (92%)	14 (8%)	16 43
All	All	1399/1448 (97%)	1269 (91%)	130 (9%)	11 32

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	31	THR
1	A	74	ASN
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	98	ARG
1	A	103	GLU
1	A	138	THR
1	A	145	LEU
1	A	148	GLU
1	A	168	LEU
1	A	177	LEU
1	A	180	THR
1	A	200	ILE
1	A	202	GLU
1	A	207	GLN
1	A	212	LEU
1	A	219	PHE
1	A	235	GLU
1	A	236	VAL
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	288	ILE
1	A	319	LEU
1	A	330	MET
1	A	381	GLN
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	430	LEU
1	A	435	LEU
1	A	444	LEU
1	A	446	SER
1	A	451	ARG
1	A	453	LEU
1	B	19	ARG
1	B	31	THR
1	B	74	ASN
1	B	78	LEU
1	B	81	VAL
1	B	96	LEU
1	B	98	ARG
1	B	103	GLU
1	B	138	THR
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	148	GLU
1	B	168	LEU
1	B	177	LEU
1	B	180	THR
1	B	200	ILE
1	B	207	GLN
1	B	212	LEU
1	B	219	PHE
1	B	235	GLU
1	B	244	LEU
1	B	251	THR
1	B	264	ILE
1	B	288	ILE
1	B	319	LEU
1	B	330	MET
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	430	LEU
1	B	435	LEU
1	B	444	LEU
1	B	446	SER
1	B	451	ARG
1	B	453	LEU
2	C	2	VAL
2	C	18	LEU
2	C	21	SER
2	C	55	SER
2	C	65	LYS
2	C	72	ARG
2	C	115	THR
2	C	123	LYS
2	C	157	PRO
2	C	167	LEU
2	C	193	SER
2	C	200	THR
2	C	204	ASN
2	C	214	VAL
3	D	1	ASP
3	D	36	GLN
3	D	41	THR

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Mol	Chain	Res	Type
3	D	75	ASN
3	D	77	MET
3	D	95	GLN
3	D	106	LEU
3	D	107	ARG
3	D	120	SER
3	D	135	LEU
3	D	141	LYS
3	D	142	ASP
3	D	166	ASP
3	D	176	SER
3	D	190	SER
3	D	201	THR
2	E	2	VAL
2	E	21	SER
2	E	55	SER
2	E	65	LYS
2	E	72	ARG
2	E	107	TYR
2	E	115	THR
2	E	123	LYS
2	E	157	PRO
2	E	167	LEU
2	E	179	GLN
2	E	193	SER
2	E	200	THR
2	E	204	ASN
2	E	214	VAL
3	F	1	ASP
3	F	41	THR
3	F	75	ASN
3	F	95	GLN
3	F	120	SER
3	F	121	SER
3	F	135	LEU
3	F	141	LYS
3	F	142	ASP
3	F	166	ASP
3	F	176	SER
3	F	184	GLU
3	F	190	SER
3	F	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	153	GLN
1	A	157	ASN
1	A	270	ASN
1	A	284	HIS
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	270	ASN
1	B	284	HIS
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
3	D	6	GLN
3	D	136	ASN
3	F	6	GLN
3	F	36	GLN
3	F	136	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	444/473 (93%)	0.79	44 (9%) 9 5	61, 93, 155, 219	0
1	B	441/473 (93%)	0.86	52 (11%) 6 4	58, 96, 168, 244	0
2	C	221/221 (100%)	0.47	16 (7%) 18 12	49, 83, 136, 237	0
2	E	221/221 (100%)	0.56	20 (9%) 12 7	55, 86, 154, 215	0
3	D	211/211 (100%)	1.00	43 (20%) 1 1	63, 101, 148, 189	0
3	F	211/211 (100%)	1.00	34 (16%) 3 1	54, 77, 136, 186	0
All	All	1749/1810 (96%)	0.79	209 (11%) 6 3	49, 91, 155, 244	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	PHE	10.7
1	A	72	ALA	10.3
1	B	73	ASP	9.0
3	F	211	ALA	8.6
2	E	178	LEU	8.6
1	B	72	ALA	8.0
1	B	70	HIS	7.9
1	B	353	PRO	7.7
1	B	307	PHE	6.7
1	B	71	THR	6.2
1	A	73	ASP	5.4
1	B	104	ALA	5.3
1	B	74	ASN	5.3
1	B	143	MET	5.3
1	A	235	GLU	5.2
1	A	71	THR	5.0
3	D	170	SER	4.9
3	F	209	ASN	4.8
1	B	177	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	234	HIS	4.7
1	B	168	LEU	4.6
3	D	172	TYR	4.4
3	D	23	CYS	4.4
3	F	124	LEU	4.4
1	B	288	ILE	4.3
3	F	2	ILE	4.3
2	C	139	ALA	4.3
3	F	153	GLU	4.2
3	F	152	SER	4.2
1	B	75	TYR	4.2
1	A	78	LEU	4.2
3	D	39	SER	4.1
1	A	288	ILE	4.1
3	D	138	PHE	4.1
3	D	82	ALA	4.1
2	E	15	GLY	4.0
3	D	22	THR	4.0
1	B	304	LEU	4.0
1	B	234	HIS	4.0
1	A	75	TYR	3.9
3	D	20	THR	3.8
1	A	69	VAL	3.8
3	D	101	THR	3.8
3	D	110	ALA	3.7
3	D	197	HIS	3.7
2	E	13	GLN	3.7
1	A	291	TRP	3.7
1	B	138	THR	3.6
1	A	283	VAL	3.6
1	A	76	PRO	3.6
2	E	182	LEU	3.6
1	A	208	PHE	3.6
2	E	86	VAL	3.5
3	F	190	SER	3.5
2	C	140	ALA	3.5
1	B	68	LEU	3.5
1	B	354	GLY	3.5
1	B	67	ALA	3.5
1	B	167	ARG	3.4
1	A	74	ASN	3.4
3	F	189	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	69	SER	3.4
1	B	290	LYS	3.4
3	D	171	THR	3.4
1	B	69	VAL	3.4
3	D	140	PRO	3.4
3	F	147	TRP	3.3
1	A	144	VAL	3.3
1	A	67	ALA	3.3
2	C	65	LYS	3.2
2	C	199	GLU	3.2
3	F	149	ILE	3.2
3	D	165	GLN	3.2
1	A	68	LEU	3.2
1	A	207	GLN	3.1
1	A	209	ARG	3.1
1	B	291	TRP	3.1
1	B	456	GLN	3.1
3	F	89	GLN	3.1
1	A	65	MET	3.1
2	E	179	GLN	3.0
1	B	119	GLN	3.0
1	A	99	LYS	3.0
3	D	109	ASP	3.0
2	C	29	TYR	2.9
2	E	65	LYS	2.9
1	A	290	LYS	2.8
3	D	38	LYS	2.8
1	B	235	GLU	2.8
3	D	103	LEU	2.8
1	B	145	LEU	2.8
3	D	105	ILE	2.8
1	B	347	CYS	2.8
3	D	146	LYS	2.7
1	A	168	LEU	2.7
1	B	172	GLU	2.7
1	A	60	LEU	2.7
1	B	95	PHE	2.7
1	B	139	LEU	2.7
3	F	192	THR	2.7
1	A	143	MET	2.7
1	B	178	LEU	2.7
2	E	59	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	72	LEU	2.7
1	B	287	ASN	2.7
3	F	148	LYS	2.7
1	A	299	GLY	2.7
2	E	183	TYR	2.7
3	D	36	GLN	2.6
1	A	139	LEU	2.6
1	B	18	ARG	2.6
3	F	4	LEU	2.6
1	A	21	LEU	2.6
1	B	141	GLY	2.6
2	E	105	TYR	2.6
1	B	84	LEU	2.6
1	A	70	HIS	2.6
3	D	77	MET	2.6
2	C	176	ALA	2.5
3	F	127	GLY	2.5
3	D	71	SER	2.5
3	F	180	LEU	2.5
1	A	77	LEU	2.5
1	B	332	MET	2.5
3	D	7	SER	2.5
3	F	145	VAL	2.5
3	F	29	VAL	2.5
1	A	104	ALA	2.5
3	D	196	THR	2.5
1	A	140	GLY	2.5
3	D	72	LEU	2.5
3	D	69	SER	2.5
2	C	175	PRO	2.5
3	F	191	TYR	2.5
3	D	68	THR	2.4
1	A	233	ASN	2.4
1	B	409	ILE	2.4
3	F	158	VAL	2.4
2	C	188	SER	2.4
1	B	162	VAL	2.4
1	B	233	ASN	2.4
3	F	208	PHE	2.4
2	C	189	VAL	2.4
2	E	177	VAL	2.4
2	E	29	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	31	TYR	2.4
3	F	205	VAL	2.3
3	F	184	GLU	2.3
3	D	64	SER	2.3
1	A	53	PHE	2.3
1	B	166	PHE	2.3
2	C	214	VAL	2.3
2	E	136	SER	2.3
1	B	195	ALA	2.3
3	F	146	LYS	2.3
1	A	145	LEU	2.3
1	B	96	LEU	2.3
3	D	79	ALA	2.3
3	D	202	SER	2.3
1	A	66	GLY	2.3
1	B	438	PHE	2.3
1	B	289	THR	2.3
3	D	34	TRP	2.3
3	D	195	ALA	2.2
2	C	172	HIS	2.2
1	B	77	LEU	2.2
1	B	407	THR	2.2
3	D	112	PRO	2.2
1	A	142	GLY	2.2
3	D	21	MET	2.2
1	A	141	GLY	2.2
1	B	377	GLU	2.2
2	C	89	GLU	2.2
2	E	139	ALA	2.2
2	E	48	ILE	2.2
1	B	199	PHE	2.2
1	A	201	ILE	2.2
2	E	221	ARG	2.2
1	A	86	SER	2.1
2	C	196	TRP	2.1
2	C	20	LEU	2.1
3	D	106	LEU	2.1
3	D	124	LEU	2.1
3	F	73	THR	2.1
3	D	136	ASN	2.1
3	D	139	TYR	2.1
3	F	183	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	135	LEU	2.1
2	E	137	ALA	2.1
3	D	74	ILE	2.1
3	F	204	ILE	2.1
1	A	210	TYR	2.1
3	D	102	LYS	2.1
1	A	460	GLN	2.1
3	D	148	LYS	2.1
2	E	123	LYS	2.1
3	F	19	VAL	2.1
2	E	122	ALA	2.1
3	F	67	GLY	2.1
1	A	61	GLN	2.1
2	C	221	ARG	2.1
2	C	147	GLY	2.0
3	D	199	THR	2.0
3	D	178	LEU	2.0
2	E	212	THR	2.0
1	B	127	VAL	2.0
1	A	79	LEU	2.0
3	F	182	LYS	2.0
1	B	97	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BR	A	475	1/1	0.92	0.68	7.69	100,100,100,100	0
4	BR	B	475	1/1	0.93	0.29	1.66	100,100,100,100	0
4	BR	A	474	1/1	0.97	0.18	-1.13	100,100,100,100	0
4	BR	B	474	1/1	0.93	0.16	-1.30	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.