Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:07 PM GMT

PDB ID	:	4KK9
Title	:	Structure of the E148A mutant of CLC-ec1 deltaNC construct in 100mM fluoride and 2mM Bromide
Authors	:	Lim, H.-H.; Miller, C.
Deposited on	:	2013-05-05
Resolution	:	3.00 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 (i) symbol.

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

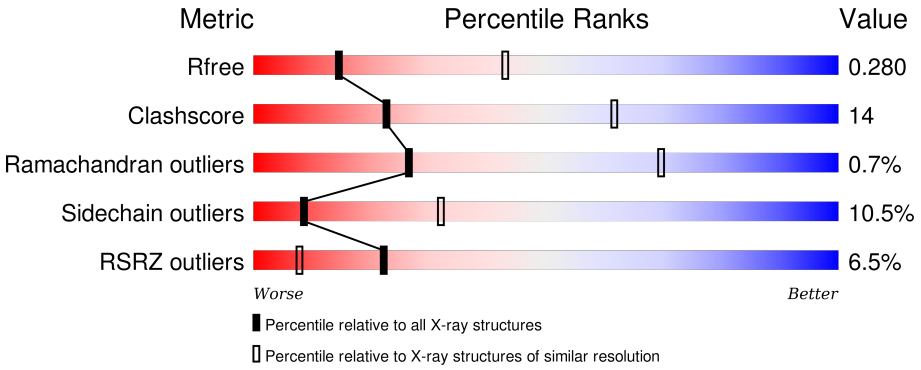
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	446	7% 68% 28%
1	B	446	6% 63% 31%
2	C	222	8% 68% 26% 5%
2	E	222	% 71% 23% 5%
3	D	211	7% 58% 36% 5%

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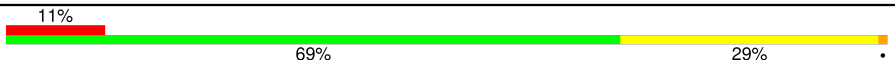
Mol	Chain	Length	Quality of chain
3	F	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13206 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	443	Total	C	N	O	S	0	0	0
			3320	2183	558	559	20			
1	B	441	Total	C	N	O	S	0	0	0
			3300	2172	553	555	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP P37019
A	148	ALA	GLU	ENGINEERED MUTATION	UNP P37019
A	461	LYS	-	EXPRESSION TAG	UNP P37019
B	16	MET	-	EXPRESSION TAG	UNP P37019
B	148	ALA	GLU	ENGINEERED MUTATION	UNP P37019
B	461	LYS	-	EXPRESSION TAG	UNP P37019

- Molecule 2 is a protein called Fab, 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, light chain.

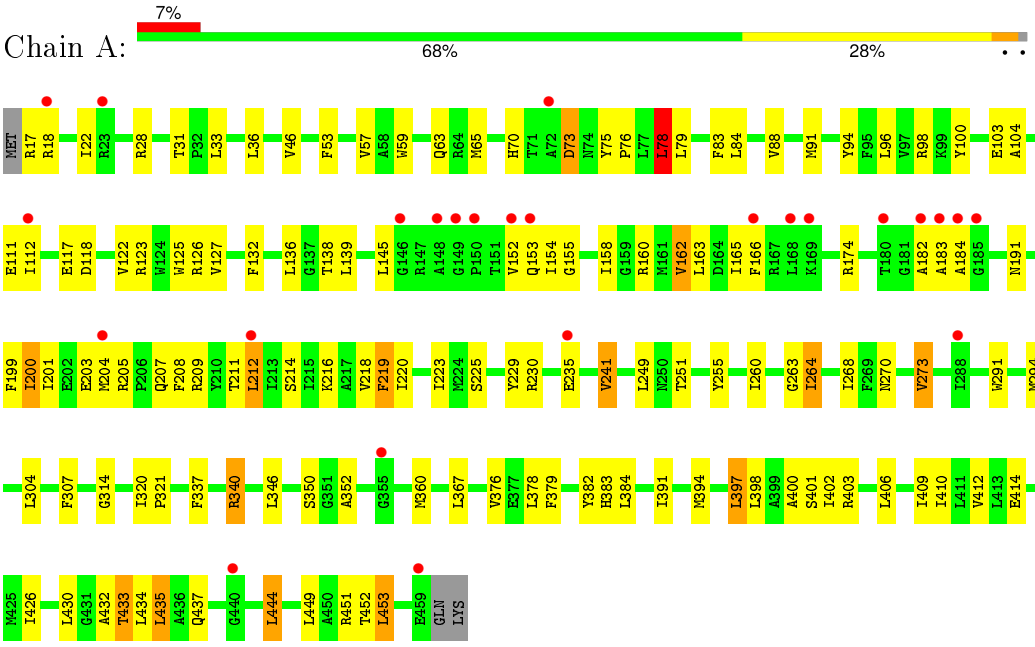
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

3 Residue-property plots (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.

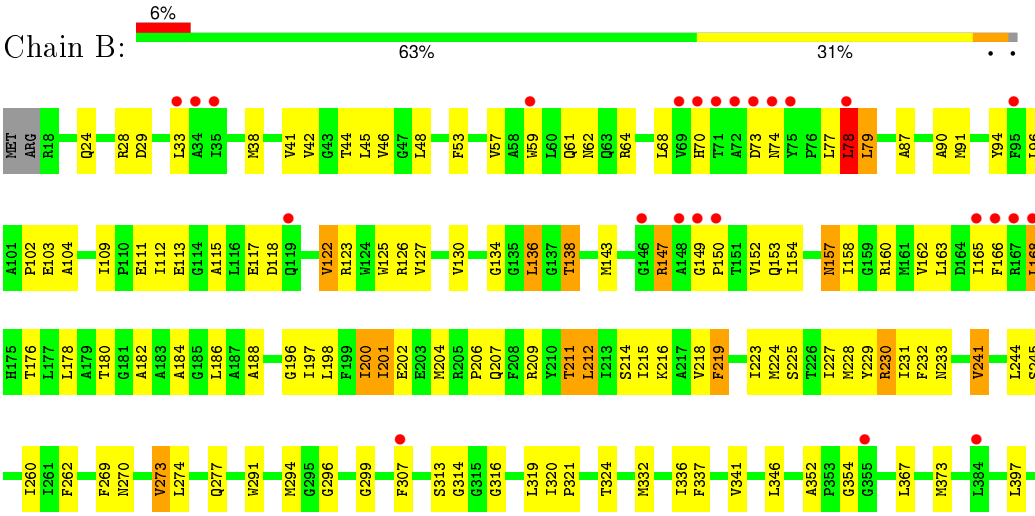
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

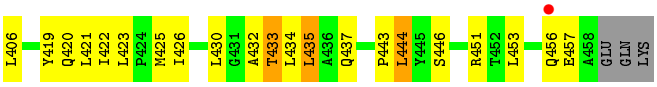
Chain A:



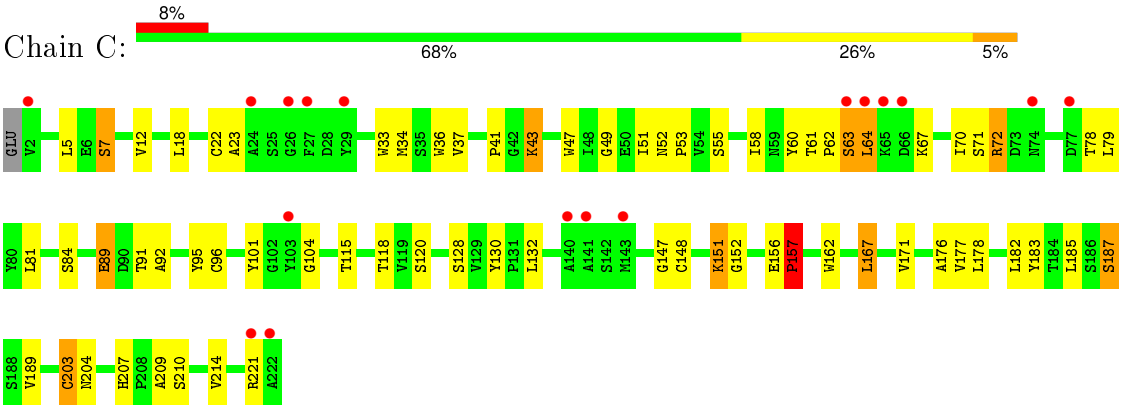
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:

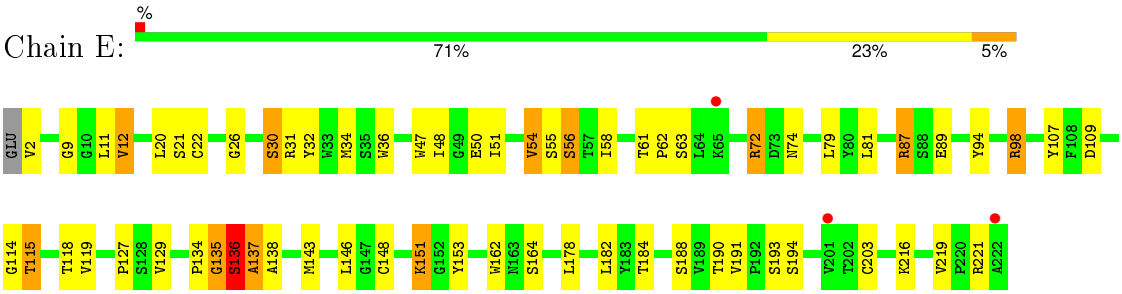




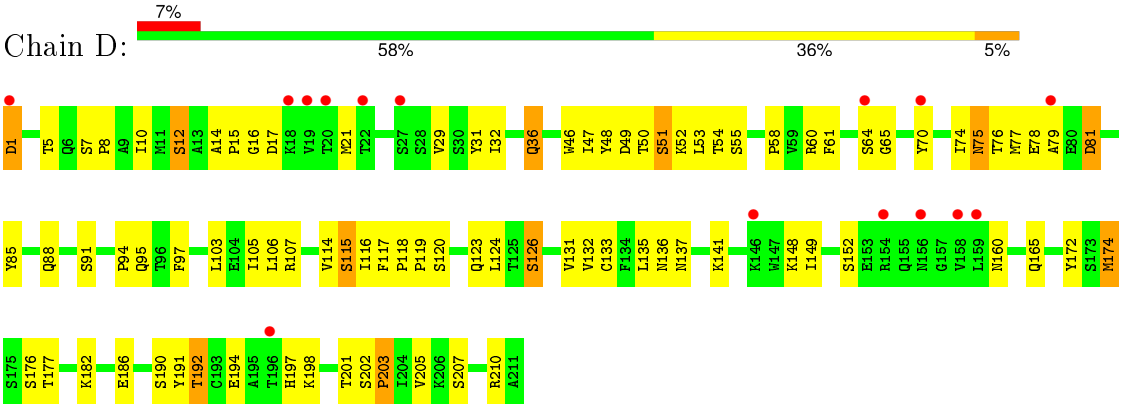
• Molecule 2: Fab, heavy chain



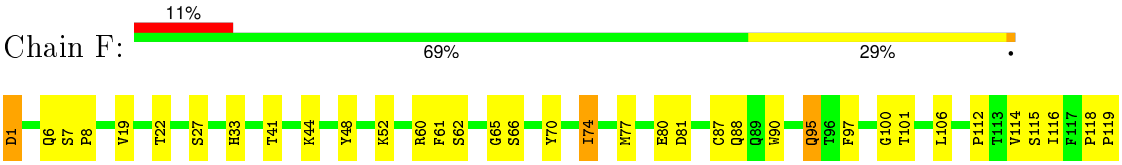
• Molecule 2: Fab, heavy chain

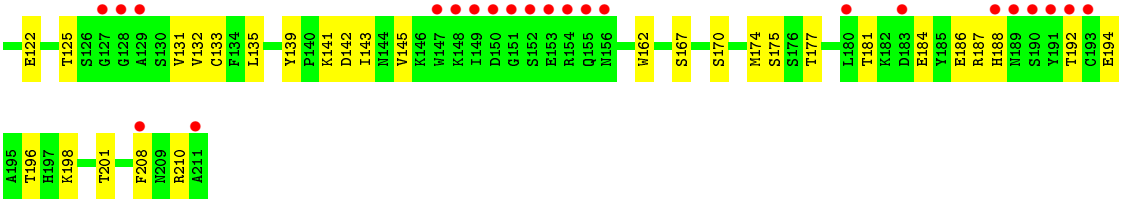


• Molecule 3: Fab, light chain



• Molecule 3: Fab, light chain




E122
T125
S126
G127
G128
A129
S130
V131
Y132
C133
F134
L135
Y139
P140
K141
D142
I143
N144
V145
K146
W147
K148
I149
D150
G151
S152
E153
R154
Q155
N156
W162
S167
S170
M174
S175
S176
T177
L180
T181
K182
D183
E184
Y185
E186
R187
H188
N189
S190
Y191
T192
C193
E194
A195
T196
H197
K198
T201
F208
M209
R210
A211

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.62Å 98.86Å 170.39Å 90.00° 131.88° 90.00°	Depositor
Resolution (Å)	39.93 – 3.00 39.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.93-3.00) 99.8 (39.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.217 , 0.270 0.229 , 0.280	Depositor DCC
R_{free} test set	2925 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	80.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.5	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 57654 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13206	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

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	0.44	0/3392	0.61	1/4604 (0.0%)
1	B	0.42	0/3372	0.62	1/4578 (0.0%)
2	C	0.52	0/1721	0.66	0/2355
2	E	0.46	0/1721	0.63	1/2355 (0.0%)
3	D	0.45	0/1660	0.63	0/2257
3	F	0.44	0/1660	0.66	0/2257
All	All	0.45	0/13526	0.63	3/18406 (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})
1	B	78	LEU	CA-CB-CG	6.06	129.23	115.30
1	A	78	LEU	CA-CB-CG	5.71	128.43	115.30
2	E	138	ALA	CB-CA-C	5.56	118.44	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	3320	0	3475	103	0
1	B	3300	0	3456	123	0
2	C	1672	0	1654	38	0
2	E	1672	0	1654	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1621	0	1546	57	0
3	F	1621	0	1546	43	0
All	All	13206	0	13331	361	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 14.

All (361) 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:95:GLN:N	3:D:95:GLN:OE1	2.03	0.90
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.43	0.81
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.63	0.80
3:F:1:ASP:OD2	3:F:1:ASP:N	2.15	0.79
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.65	0.79
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.18	0.78
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.48	0.77
2:E:136:SER:O	2:E:137:ALA:CB	2.35	0.74
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.53	0.74
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.68	0.73
2:E:136:SER:O	2:E:137:ALA:HB2	1.88	0.73
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.71	0.72
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.73	0.70
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.73	0.69
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.75	0.69
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.75	0.68
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.76	0.68
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.09	0.68
3:D:76:THR:HG22	3:D:76:THR:O	1.93	0.67
1:A:73:ASP:OD1	1:A:73:ASP:N	2.27	0.67
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.26	0.67
3:F:95:GLN:N	3:F:95:GLN:OE1	2.27	0.67
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.76	0.67
1:A:394:MET:HE2	1:A:412:VAL:HG13	1.76	0.67
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.75	0.67
1:A:200:ILE:HA	1:A:204:MET:HB2	1.76	0.67
2:E:32:TYR:O	2:E:72:ARG:NH2	2.27	0.67
2:E:30:SER:O	2:E:31:ARG:HB2	1.95	0.67
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.76	0.66
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.77	0.66
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.78	0.65
1:B:150:PRO:HG3	1:B:354:GLY:HA2	1.79	0.65
1:B:157:ASN:N	1:B:157:ASN:HD22	1.94	0.64
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.33	0.64
1:B:157:ASN:H	1:B:157:ASN:HD22	1.44	0.64
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.34	0.63
2:E:87:ARG:HE	2:E:89:GLU:HB2	1.63	0.62
1:A:403:ARG:HE	1:A:433:THR:HG22	1.64	0.62
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.80	0.62
1:B:422:ILE:HA	1:B:425:MET:HE3	1.80	0.61
1:A:414:GLU:OE1	1:B:419:TYR:OH	2.19	0.61
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.82	0.61
3:F:95:GLN:CD	3:F:95:GLN:H	2.03	0.61
3:F:95:GLN:N	3:F:95:GLN:CD	2.54	0.60
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.36	0.60
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.67	0.60
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.84	0.60
1:A:403:ARG:NH2	1:B:29:ASP:OD1	2.35	0.60
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.84	0.60
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.17	0.60
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.83	0.59
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.38	0.59
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.37	0.59
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.84	0.59
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.85	0.59
1:B:38:MET:O	1:B:42:VAL:HG23	2.03	0.59
1:B:212:LEU:H	1:B:212:LEU:HD12	1.66	0.59
1:A:314:GLY:O	1:A:340:ARG:NH2	2.35	0.59
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.37	0.59
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.18	0.59
2:C:207:HIS:ND1	2:C:210:SER:OG	2.28	0.58
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.34	0.58
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.39	0.58
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.38	0.58
1:B:337:PHE:O	1:B:341:VAL:HG23	2.04	0.57
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.86	0.57
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.87	0.57
1:A:337:PHE:CE1	1:A:367:LEU:HB2	2.40	0.57
1:A:88:VAL:HA	1:A:91:MET:HE2	1.87	0.57
2:C:5:LEU:HB3	2:C:23:ALA:HB3	1.85	0.57
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:78:GLU:O	3:D:81:ASP:HB2	2.05	0.56
2:E:9:GLY:H	2:E:115:THR:HG21	1.68	0.56
3:F:6:GLN:HG3	3:F:100:GLY:N	2.20	0.56
1:A:406:LEU:HB2	1:B:219:PHE:HE1	1.70	0.56
3:D:1:ASP:N	3:D:1:ASP:OD2	2.20	0.56
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.87	0.56
3:F:19:VAL:HB	3:F:74:ILE:HG13	1.88	0.56
1:B:78:LEU:HD13	1:B:79:LEU:HD23	1.88	0.56
2:C:101:TYR:HB2	2:C:104:GLY:HA2	1.88	0.55
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.87	0.55
1:A:214:SER:O	1:A:218:VAL:HG23	2.07	0.55
3:F:66:SER:HA	3:F:70:TYR:CZ	2.41	0.55
1:B:42:VAL:O	1:B:46:VAL:HG23	2.07	0.54
1:B:180:THR:HA	1:B:218:VAL:HG13	1.89	0.54
3:F:188:HIS:O	3:F:210:ARG:HD3	2.06	0.54
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.42	0.54
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.90	0.54
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.23	0.54
1:B:53:PHE:O	1:B:57:VAL:HG23	2.07	0.54
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.43	0.54
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.90	0.54
1:A:152:VAL:HG13	1:A:182:ALA:HB1	1.89	0.54
3:F:6:GLN:NE2	3:F:100:GLY:H	2.06	0.54
1:A:212:LEU:HD12	1:A:212:LEU:H	1.73	0.53
1:B:109:ILE:HG23	1:B:204:MET:SD	2.48	0.53
3:D:160:ASN:OD1	3:D:176:SER:OG	2.10	0.53
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.89	0.53
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.89	0.53
1:B:176:THR:O	1:B:180:THR:HG23	2.08	0.53
1:B:64:ARG:O	1:B:68:LEU:HG	2.09	0.53
1:B:154:ILE:O	1:B:158:ILE:HG12	2.09	0.53
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.23	0.53
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.74	0.53
3:F:7:SER:HB2	3:F:22:THR:HB	1.91	0.53
1:A:122:VAL:HB	1:A:160:ARG:HD3	1.91	0.53
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.77	0.52
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.89	0.52
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.92	0.52
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.44	0.52
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.44	0.52
1:B:38:MET:HA	1:B:41:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:THR:HB	3:D:207:SER:HB3	1.91	0.52
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.24	0.52
3:F:184:GLU:O	3:F:187:ARG:HG2	2.10	0.52
3:D:116:ILE:HD13	3:D:207:SER:HA	1.92	0.52
2:E:94:TYR:O	2:E:114:GLY:HA2	2.09	0.52
3:F:6:GLN:HG3	3:F:100:GLY:H	1.73	0.52
2:E:151:LYS:HB3	2:E:184:THR:HG23	1.92	0.52
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.36	0.51
1:B:150:PRO:O	1:B:154:ILE:HG13	2.11	0.51
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.45	0.51
1:B:241:VAL:HG22	1:B:324:THR:HG21	1.93	0.51
1:B:332:MET:O	1:B:336:ILE:HG13	2.10	0.51
3:D:186:GLU:O	3:D:210:ARG:NH2	2.44	0.51
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.45	0.51
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.92	0.51
3:D:29:VAL:O	3:D:70:TYR:OH	2.15	0.51
2:C:37:VAL:O	2:C:95:TYR:HB2	2.11	0.50
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.93	0.50
2:C:41:PRO:HD3	2:C:92:ALA:HA	1.94	0.50
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.93	0.50
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.93	0.50
3:F:61:PHE:CE2	3:F:74:ILE:HD13	2.47	0.50
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.92	0.50
3:D:12:SER:HB3	3:D:106:LEU:HD12	1.93	0.50
2:C:132:LEU:HB2	2:C:147:GLY:HA3	1.94	0.50
2:C:63:SER:O	2:C:64:LEU:O	2.30	0.50
1:A:294:MET:O	1:A:298:ILE:HG13	2.12	0.50
1:A:154:ILE:O	1:A:158:ILE:HG12	2.11	0.50
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.94	0.50
1:B:227:ILE:O	1:B:231:ILE:HG12	2.12	0.50
1:A:100:TYR:O	1:A:126:ARG:NH1	2.45	0.49
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.94	0.49
3:D:115:SER:HB3	3:D:117:PHE:CE1	2.48	0.49
1:A:264:ILE:O	1:A:268:ILE:HG13	2.12	0.49
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.94	0.49
2:C:167:LEU:HD23	2:C:189:VAL:HG21	1.94	0.49
3:D:106:LEU:HD23	3:D:107:ARG:N	2.28	0.49
2:E:12:VAL:HG23	2:E:119:VAL:HA	1.93	0.49
1:B:313:SER:OG	1:B:314:GLY:N	2.46	0.49
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.76	0.49
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.10	0.49
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.47	0.49
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.94	0.49
1:B:44:THR:O	1:B:48:LEU:HG	2.12	0.49
1:B:171:ASP:OD2	1:B:174:ARG:NH1	2.34	0.49
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.45	0.49
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.28	0.49
2:E:129:VAL:O	2:E:216:LYS:HE3	2.12	0.49
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.93	0.49
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.48	0.49
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.33	0.49
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.48	0.49
1:A:437:GLN:HE21	1:B:216:LYS:NZ	2.11	0.48
1:B:229:TYR:O	1:B:233:ASN:HB2	2.13	0.48
1:B:316:GLY:O	1:B:319:LEU:HG	2.11	0.48
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.48	0.48
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.13	0.48
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.49	0.48
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.95	0.48
1:B:165:ILE:HG22	1:B:166:PHE:CD2	2.49	0.48
1:A:78:LEU:HD13	1:A:79:LEU:HD23	1.94	0.48
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.49	0.48
1:B:274:LEU:O	1:B:277:GLN:HB2	2.14	0.48
2:E:135:GLY:HA2	2:E:221:ARG:CD	2.44	0.48
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.49	0.48
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.82	0.47
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.49	0.47
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.50	0.47
2:E:47:TRP:HZ2	2:E:50:GLU:HG2	1.78	0.47
1:B:157:ASN:ND2	1:B:157:ASN:N	2.61	0.47
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.18	0.47
1:A:430:LEU:HD11	1:B:219:PHE:CG	2.49	0.47
1:A:270:ASN:O	1:A:273:VAL:HG13	2.14	0.47
1:B:214:SER:O	1:B:218:VAL:HG23	2.13	0.47
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.50	0.47
3:F:188:HIS:O	3:F:210:ARG:CD	2.63	0.47
1:A:220:ILE:HD11	1:B:434:LEU:HD21	1.97	0.47
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.97	0.47
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.50	0.47
3:F:7:SER:CB	3:F:22:THR:HB	2.45	0.47
1:B:197:ILE:O	1:B:201:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.60	0.47
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.97	0.47
1:B:138:THR:HG22	1:B:143:MET:SD	2.55	0.46
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.97	0.46
3:D:197:HIS:CD2	3:D:198:LYS:H	2.33	0.46
1:B:269:PHE:O	1:B:273:VAL:HG12	2.16	0.46
2:E:2:VAL:HA	2:E:26:GLY:HA3	1.97	0.46
3:D:46:TRP:O	3:D:47:ILE:HG13	2.15	0.46
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.80	0.46
1:B:130:VAL:O	1:B:134:GLY:N	2.39	0.46
3:F:186:GLU:HA	3:F:210:ARG:NH1	2.31	0.46
1:A:199:PHE:CE1	1:A:203:GLU:HG2	2.51	0.46
1:A:449:LEU:HG	1:A:453:LEU:HD22	1.97	0.46
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.98	0.46
1:B:147:ARG:C	1:B:150:PRO:HD2	2.36	0.46
1:B:112:ILE:HG13	1:B:153:GLN:HA	1.97	0.46
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.97	0.46
1:A:249:LEU:HD13	1:B:231:ILE:HD13	1.97	0.46
1:B:188:ALA:HB2	1:B:225:SER:OG	2.16	0.46
3:D:31:TYR:HA	3:D:50:THR:OG1	2.15	0.46
2:E:143:MET:HB3	2:E:190:THR:HG23	1.98	0.46
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.80	0.45
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.98	0.45
3:D:165:GLN:HG3	3:D:172:TYR:CZ	2.51	0.45
3:D:14:ALA:O	3:D:17:ASP:HB2	2.16	0.45
1:B:294:MET:HE2	1:B:294:MET:HB3	1.90	0.45
3:D:1:ASP:HB3	3:D:94:PRO:HD2	1.99	0.45
3:F:8:PRO:O	3:F:101:THR:HG23	2.16	0.45
3:D:124:LEU:O	3:D:126:SER:N	2.50	0.45
1:B:59:TRP:O	1:B:62:ASN:HB3	2.16	0.45
1:A:195:ALA:N	1:A:414:GLU:OE2	2.47	0.45
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.99	0.45
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.98	0.45
1:A:437:GLN:HE21	1:B:216:LYS:HZ2	1.62	0.45
1:B:41:VAL:O	1:B:45:LEU:HG	2.16	0.45
3:D:141:LYS:HB3	3:D:172:TYR:CZ	2.52	0.45
1:A:59:TRP:O	1:A:63:GLN:HG2	2.15	0.45
1:A:346:LEU:O	1:A:350:SER:HB3	2.16	0.45
2:E:61:THR:O	2:E:63:SER:N	2.50	0.45
3:F:145:VAL:HA	3:F:194:GLU:O	2.17	0.45
3:F:6:GLN:HE22	3:F:87:CYS:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:60:ARG:HG3	3:F:74:ILE:HG22	1.99	0.45
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.52	0.45
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.98	0.44
3:D:47:ILE:HG12	3:D:53:LEU:CD2	2.47	0.44
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.17	0.44
3:F:106:LEU:HA	3:F:139:TYR:OH	2.17	0.44
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.99	0.44
3:D:141:LYS:HB3	3:D:172:TYR:CE2	2.52	0.44
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.67	0.44
1:B:73:ASP:OD1	1:B:73:ASP:N	2.49	0.44
1:B:202:GLU:OE2	1:B:405:PRO:HD2	2.17	0.44
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.99	0.44
1:A:401:SER:O	1:A:444:LEU:HB2	2.17	0.44
2:C:60:TYR:HE2	2:C:70:ILE:H	1.66	0.44
1:A:200:ILE:HG22	1:A:201:ILE:HG23	1.99	0.44
2:C:203:CYS:O	2:C:203:CYS:SG	2.76	0.44
1:B:200:ILE:HD12	1:B:204:MET:HG3	2.00	0.44
1:B:118:ASP:OD1	1:B:174:ARG:NH2	2.34	0.44
2:E:48:ILE:HD13	2:E:48:ILE:HA	1.86	0.44
2:C:151:LYS:HE3	2:C:151:LYS:HB2	1.67	0.44
1:B:149:GLY:N	1:B:150:PRO:CD	2.80	0.44
1:B:319:LEU:HG	1:B:319:LEU:H	1.74	0.44
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.53	0.44
3:D:174:MET:HB3	3:D:174:MET:HE2	1.74	0.44
1:B:224:MET:O	1:B:228:MET:HG2	2.17	0.44
3:D:54:THR:HG22	3:D:55:SER:N	2.33	0.44
3:D:76:THR:CG2	3:D:76:THR:O	2.64	0.43
1:B:53:PHE:CE2	1:B:147:ARG:HB3	2.53	0.43
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.17	0.43
1:A:53:PHE:O	1:A:57:VAL:HG23	2.18	0.43
2:E:178:LEU:HD12	2:E:182:LEU:O	2.18	0.43
1:B:53:PHE:HE2	1:B:147:ARG:HB3	1.83	0.43
1:A:433:THR:HB	1:B:216:LYS:HE2	2.00	0.43
2:C:162:TRP:HE1	2:C:187:SER:HG	1.66	0.43
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.54	0.43
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.53	0.43
1:A:158:ILE:O	1:A:162:VAL:HG13	2.19	0.43
2:C:91:THR:HG23	2:C:118:THR:HA	2.00	0.43
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.51	0.43
1:B:201:ILE:HG12	1:B:201:ILE:H	1.46	0.43
1:B:202:GLU:OE1	1:B:404:ALA:HB1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ILE:HD13	1:A:426:ILE:HA	2.01	0.43
1:A:31:THR:HB	1:A:36:LEU:HD21	2.00	0.43
1:B:346:LEU:HD12	1:B:346:LEU:HA	1.74	0.43
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.00	0.43
3:D:77:MET:SD	3:D:103:LEU:HD21	2.59	0.43
3:D:95:GLN:H	3:D:95:GLN:CD	2.05	0.43
2:C:22:CYS:O	2:C:78:THR:HG23	2.19	0.43
1:B:270:ASN:HA	1:B:270:ASN:HD22	1.55	0.43
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.54	0.43
1:A:398:LEU:O	1:A:402:ILE:HB	2.19	0.43
1:A:183:ALA:HB2	1:A:200:ILE:HG12	2.01	0.42
1:B:200:ILE:HA	1:B:204:MET:HB2	2.00	0.42
3:D:148:LYS:HA	3:D:152:SER:O	2.19	0.42
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.54	0.42
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.49	0.42
1:B:87:ALA:O	1:B:91:MET:HG3	2.19	0.42
2:C:37:VAL:HG22	2:C:47:TRP:HA	2.00	0.42
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.54	0.42
1:B:260:ILE:HG23	1:B:435:LEU:HG	2.01	0.42
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.53	0.42
3:D:49:ASP:O	3:D:51:SER:N	2.51	0.42
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.83	0.42
1:B:123:ARG:O	1:B:127:VAL:HG23	2.19	0.42
3:D:79:ALA:O	3:D:105:ILE:HD11	2.20	0.42
3:F:143:ILE:HG13	3:F:196:THR:O	2.19	0.42
2:E:134:PRO:HD3	2:E:146:LEU:HD23	2.00	0.42
1:A:216:LYS:HE2	1:B:433:THR:HB	2.02	0.42
1:B:90:ALA:HB3	1:B:296:GLY:HA2	2.02	0.42
1:B:100:TYR:O	1:B:126:ARG:HD3	2.20	0.42
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.55	0.42
1:B:248:PRO:HB2	1:B:251:THR:HB	2.01	0.42
1:B:136:LEU:HA	1:B:136:LEU:HD12	1.74	0.42
3:D:75:ASN:O	3:D:76:THR:HB	2.20	0.42
1:A:410:ILE:O	1:A:414:GLU:HG3	2.19	0.42
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.02	0.42
1:A:91:MET:HG3	1:A:296:GLY:CA	2.50	0.42
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.91	0.42
3:F:115:SER:O	3:F:133:CYS:HA	2.20	0.41
1:B:273:VAL:O	1:B:277:GLN:HG3	2.19	0.41
3:F:80:GLU:HA	3:F:167:SER:O	2.20	0.41
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HE3	1:A:216:LYS:HB2	1.78	0.41
1:A:160:ARG:O	1:A:163:LEU:HB3	2.20	0.41
2:C:7:SER:HA	2:C:115:THR:HG21	2.03	0.41
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.47	0.41
1:A:83:PHE:HD1	1:A:84:LEU:HD23	1.85	0.41
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.56	0.41
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.50	0.41
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.38	0.41
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.55	0.41
1:B:74:ASN:HB3	1:B:77:LEU:HB3	2.01	0.41
1:A:18:ARG:O	1:A:22:ILE:HG13	2.20	0.41
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.55	0.41
3:D:36:GLN:HB2	3:D:85:TYR:HE2	1.84	0.41
3:D:65:GLY:HA3	3:D:70:TYR:HA	2.01	0.41
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.56	0.41
3:D:114:VAL:HG22	3:D:135:LEU:HD22	2.01	0.41
3:F:112:PRO:HG3	3:F:143:ILE:HD11	2.01	0.41
3:D:136:ASN:HB3	3:D:137:ASN:ND2	2.35	0.41
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.55	0.41
3:D:202:SER:HA	3:D:203:PRO:HD2	1.67	0.41
1:B:104:ALA:HB2	1:B:127:VAL:HG13	2.02	0.41
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.50	0.41
2:E:11:LEU:HD12	2:E:11:LEU:HA	1.88	0.41
1:B:160:ARG:O	1:B:163:LEU:HB3	2.21	0.41
1:B:197:ILE:HG22	1:B:201:ILE:HD11	2.03	0.41
1:A:360:MET:HG2	1:A:397:LEU:HD13	2.03	0.41
3:D:132:VAL:HG22	3:D:177:THR:HG23	2.01	0.41
3:F:119:PRO:HD3	3:F:131:VAL:HG22	2.02	0.41
3:F:141:LYS:HB2	3:F:141:LYS:HE3	1.84	0.41
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.56	0.41
1:B:231:ILE:HB	1:B:232:PHE:HD1	1.85	0.41
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.56	0.41
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.91	0.41
1:B:115:ALA:HB1	1:B:178:LEU:HD21	2.02	0.40
3:D:182:LYS:HE2	3:D:186:GLU:OE1	2.20	0.40
2:C:89:GLU:OE2	2:C:89:GLU:N	2.53	0.40
3:D:149:ILE:HG23	3:D:191:TYR:CE2	2.56	0.40
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.22	0.40
1:A:184:ALA:HB1	1:A:225:SER:CB	2.48	0.40
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.86	0.40
3:F:6:GLN:CG	3:F:100:GLY:H	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:162:TRP:CE2	3:F:174:MET:HG3	2.56	0.40
1:A:132:PHE:O	1:A:136:LEU:HB2	2.22	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	441/446 (99%)	409 (93%)	32 (7%)	0	100 100
1	B	439/446 (98%)	403 (92%)	36 (8%)	0	100 100
2	C	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	14 51
2	E	219/222 (99%)	191 (87%)	22 (10%)	6 (3%)	6 32
3	D	209/211 (99%)	183 (88%)	23 (11%)	3 (1%)	14 51
3	F	209/211 (99%)	187 (90%)	22 (10%)	0	100 100
All	All	1736/1758 (99%)	1570 (90%)	154 (9%)	12 (1%)	26 70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
3	D	126	SER
2	E	137	ALA
2	E	62	PRO
2	E	136	SER
3	D	15	PRO
2	E	55	SER
2	C	62	PRO
3	D	203	PRO
2	E	54	VAL

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Mol	Chain	Res	Type
2	E	135	GLY
2	C	157	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	333/336 (99%)	300 (90%)	33 (10%)	10 35
1	B	331/336 (98%)	295 (89%)	36 (11%)	8 30
2	C	181/182 (100%)	158 (87%)	23 (13%)	5 23
2	E	181/182 (100%)	163 (90%)	18 (10%)	10 35
3	D	185/185 (100%)	166 (90%)	19 (10%)	9 33
3	F	185/185 (100%)	167 (90%)	18 (10%)	10 37
All	All	1396/1406 (99%)	1249 (90%)	147 (10%)	8 32

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	33	LEU
1	A	65	MET
1	A	70	HIS
1	A	73	ASP
1	A	78	LEU
1	A	96	LEU
1	A	103	GLU
1	A	111	GLU
1	A	162	VAL
1	A	200	ILE
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	235	GLU

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Mol	Chain	Res	Type
1	A	241	VAL
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
1	A	304	LEU
1	A	340	ARG
1	A	378	LEU
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
1	A	433	THR
1	A	434	LEU
1	A	435	LEU
1	A	444	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	33	LEU
1	B	70	HIS
1	B	78	LEU
1	B	79	LEU
1	B	96	LEU
1	B	103	GLU
1	B	111	GLU
1	B	113	GLU
1	B	122	VAL
1	B	136	LEU
1	B	138	THR
1	B	147	ARG
1	B	157	ASN
1	B	162	VAL
1	B	168	LEU
1	B	200	ILE
1	B	201	ILE
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	230	ARG
1	B	241	VAL
1	B	244	LEU
1	B	245	SER

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Mol	Chain	Res	Type
1	B	251	THR
1	B	273	VAL
1	B	373	MET
1	B	397	LEU
1	B	420	GLN
1	B	433	THR
1	B	435	LEU
1	B	444	LEU
1	B	451	ARG
1	B	453	LEU
1	B	456	GLN
2	C	7	SER
2	C	12	VAL
2	C	18	LEU
2	C	43	LYS
2	C	55	SER
2	C	61	THR
2	C	63	SER
2	C	71	SER
2	C	72	ARG
2	C	84	SER
2	C	89	GLU
2	C	96	CYS
2	C	120	SER
2	C	128	SER
2	C	148	CYS
2	C	151	LYS
2	C	157	PRO
2	C	167	LEU
2	C	177	VAL
2	C	187	SER
2	C	203	CYS
2	C	204	ASN
2	C	214	VAL
3	D	1	ASP
3	D	5	THR
3	D	10	ILE
3	D	12	SER
3	D	21	MET
3	D	32	ILE
3	D	36	GLN
3	D	51	SER

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Mol	Chain	Res	Type
3	D	64	SER
3	D	75	ASN
3	D	81	ASP
3	D	91	SER
3	D	115	SER
3	D	120	SER
3	D	133	CYS
3	D	174	MET
3	D	190	SER
3	D	192	THR
3	D	201	THR
2	E	12	VAL
2	E	21	SER
2	E	30	SER
2	E	56	SER
2	E	72	ARG
2	E	87	ARG
2	E	98	ARG
2	E	115	THR
2	E	118	THR
2	E	136	SER
2	E	148	CYS
2	E	151	LYS
2	E	164	SER
2	E	188	SER
2	E	191	VAL
2	E	193	SER
2	E	194	SER
2	E	219	VAL
3	F	1	ASP
3	F	27	SER
3	F	41	THR
3	F	44	LYS
3	F	62	SER
3	F	74	ILE
3	F	77	MET
3	F	95	GLN
3	F	116	ILE
3	F	122	GLU
3	F	125	THR
3	F	142	ASP
3	F	170	SER

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Mol	Chain	Res	Type
3	F	175	SER
3	F	181	THR
3	F	192	THR
3	F	198	LYS
3	F	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	270	ASN
1	A	420	GLN
1	A	437	GLN
1	B	153	GLN
1	B	157	ASN
1	B	270	ASN
1	B	284	HIS
1	B	437	GLN
2	C	39	GLN
3	D	37	GLN
3	D	136	ASN
3	D	137	ASN
3	F	6	GLN
3	F	36	GLN
3	F	137	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

There are no ligands in this entry.

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	443/446 (99%)	0.18	29 (6%) 22 8	34, 52, 82, 115	0
1	B	441/446 (98%)	0.21	26 (5%) 26 10	33, 58, 93, 131	0
2	C	221/222 (99%)	0.13	17 (7%) 16 6	24, 51, 87, 125	0
2	E	221/222 (99%)	-0.29	3 (1%) 78 51	30, 51, 82, 119	0
3	D	211/211 (100%)	0.07	15 (7%) 19 7	34, 59, 83, 94	0
3	F	211/211 (100%)	0.25	23 (10%) 7 3	29, 46, 95, 114	0
All	All	1748/1758 (99%)	0.12	113 (6%) 22 8	24, 53, 88, 131	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	29	TYR	6.7
2	C	2	VAL	6.6
1	B	72	ALA	6.5
2	C	222	ALA	5.7
1	B	73	ASP	5.6
3	D	20	THR	5.3
1	B	307	PHE	4.8
3	F	152	SER	4.6
3	F	155	GLN	4.6
1	A	235	GLU	4.6
2	C	64	LEU	4.4
3	F	180	LEU	4.4
1	B	168	LEU	4.4
3	F	153	GLU	4.4
1	A	288	ILE	4.2
2	C	65	LYS	4.1
1	A	168	LEU	4.0
1	B	74	ASN	4.0
1	B	71	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	70	HIS	3.9
3	F	149	ILE	3.9
1	B	33	LEU	3.8
3	F	154	ARG	3.8
3	F	191	TYR	3.8
3	F	156	ASN	3.7
2	C	27	PHE	3.7
3	F	127	GLY	3.6
3	D	79	ALA	3.6
1	A	149	GLY	3.5
2	E	222	ALA	3.4
3	D	158	VAL	3.4
2	C	143	MET	3.4
1	B	95	PHE	3.4
3	D	22	THR	3.4
3	F	151	GLY	3.3
1	A	182	ALA	3.3
1	B	166	PHE	3.2
1	B	75	TYR	3.2
3	F	128	GLY	3.2
2	C	140	ALA	3.2
1	A	108	GLY	3.2
1	A	72	ALA	3.1
3	D	196	THR	3.0
3	F	150	ASP	2.9
3	D	156	ASN	2.9
3	F	147	TRP	2.9
2	C	63	SER	2.9
1	B	35	ILE	2.9
1	A	107	SER	2.8
1	B	119	GLN	2.8
3	D	18	LYS	2.8
1	A	166	PHE	2.8
1	A	184	ALA	2.8
1	B	34	ALA	2.8
1	A	152	VAL	2.8
1	A	148	ALA	2.8
2	C	141	ALA	2.8
2	C	221	ARG	2.8
2	E	65	LYS	2.8
3	D	154	ARG	2.7
1	B	78	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	146	GLY	2.6
3	D	146	LYS	2.5
3	F	192	THR	2.5
1	B	69	VAL	2.5
1	B	150	PRO	2.5
3	F	211	ALA	2.5
1	A	204	MET	2.5
1	A	212	LEU	2.4
1	A	183	ALA	2.4
3	F	148	LYS	2.4
1	B	149	GLY	2.4
3	F	208	PHE	2.4
1	A	180	THR	2.4
3	F	129	ALA	2.4
1	A	109	ILE	2.4
3	F	190	SER	2.4
2	C	66	ASP	2.4
1	A	18	ARG	2.4
1	A	185	GLY	2.4
2	C	74	ASN	2.3
3	D	27	SER	2.3
1	A	355	GLY	2.3
3	F	193	CYS	2.3
1	A	459	GLU	2.3
3	D	19	VAL	2.3
1	B	165	ILE	2.3
1	A	153	GLN	2.3
3	D	1	ASP	2.3
3	F	189	ASN	2.3
1	B	384	LEU	2.3
2	C	24	ALA	2.2
1	B	456	GLN	2.2
2	C	26	GLY	2.2
1	A	197	ILE	2.2
1	A	440	GLY	2.2
1	A	169	LYS	2.2
1	B	167	ARG	2.2
2	C	77	ASP	2.1
1	A	23	ARG	2.1
1	A	150	PRO	2.1
3	F	188	HIS	2.1
3	F	183	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLY	2.1
1	B	148	ALA	2.1
1	A	112	ILE	2.1
2	E	201	VAL	2.1
3	D	159	LEU	2.1
2	C	103	TYR	2.1
3	D	70	TYR	2.1
1	B	59	TRP	2.1
1	B	355	GLY	2.1
3	D	64	SER	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.