



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:17 pm BST

PDB ID : 1OTS  
Title : Structure of the Escherichia coli ClC Chloride channel and Fab Complex  
Authors : Dutzler, R.; Campbell, E.B.; MacKinnon, R.  
Deposited on : 2003-03-22  
Resolution : 2.51 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

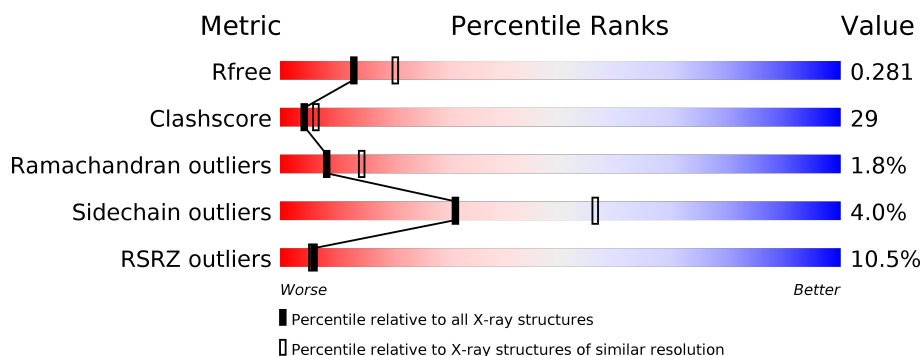
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	465	
1	B	465	
2	C	222	
2	E	222	
3	D	211	
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	CL	B	467	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13654 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 Voltage-gated ClC-type chloride channel eriC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

- 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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		

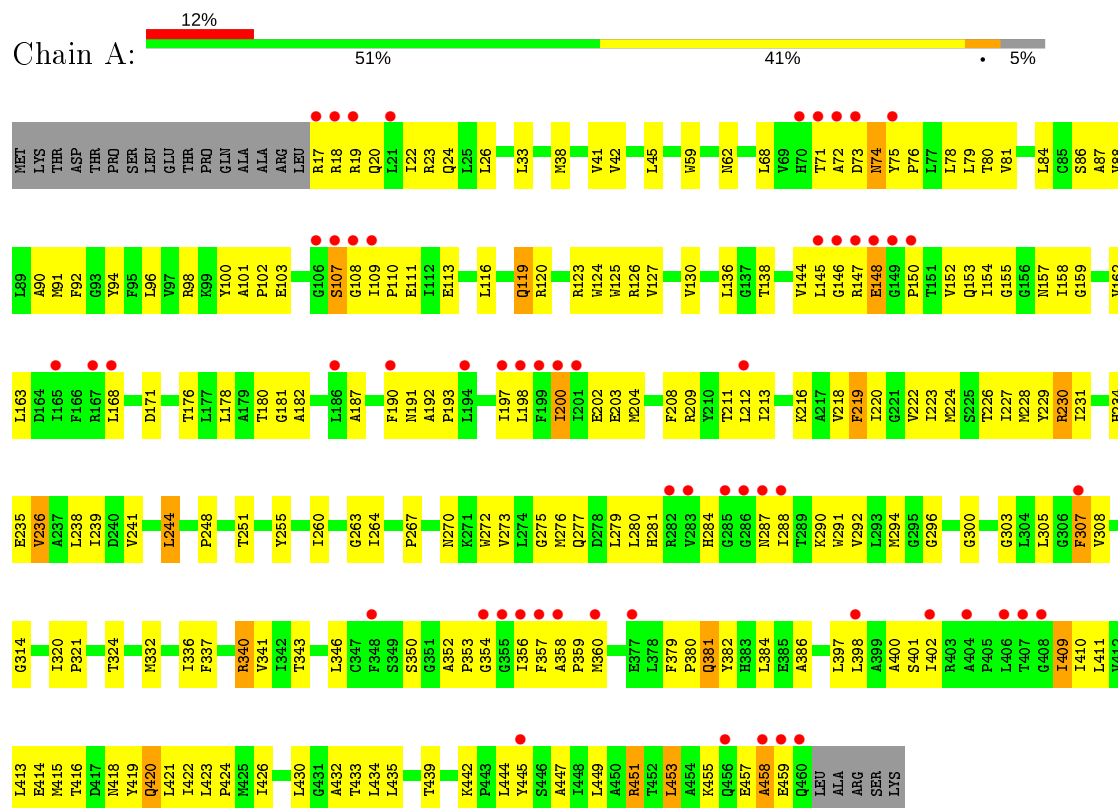
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total 76	O 76	0	0
5	B	91	Total 91	O 91	0	0
5	C	85	Total 85	O 85	0	0
5	D	36	Total 36	O 36	0	0
5	E	69	Total 69	O 69	0	0
5	F	70	Total 70	O 70	0	0

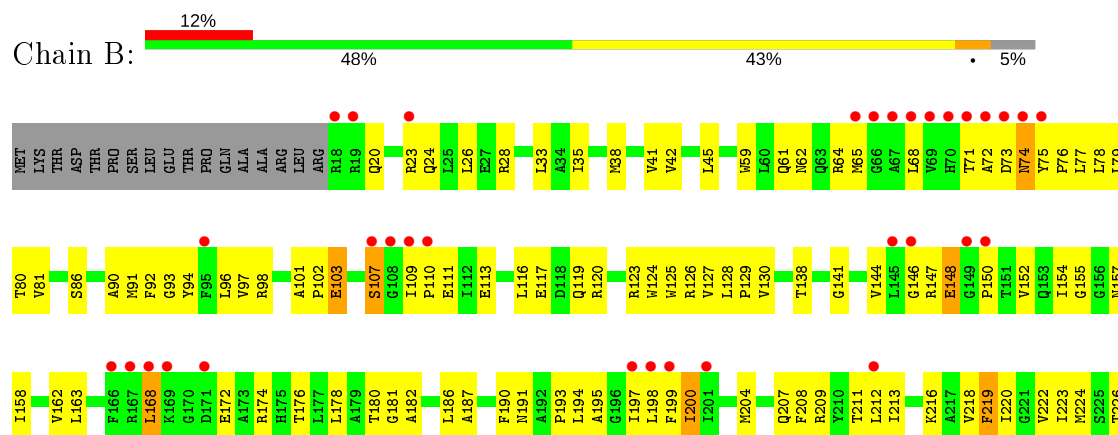
### 3 Residue-property plots [i](#)

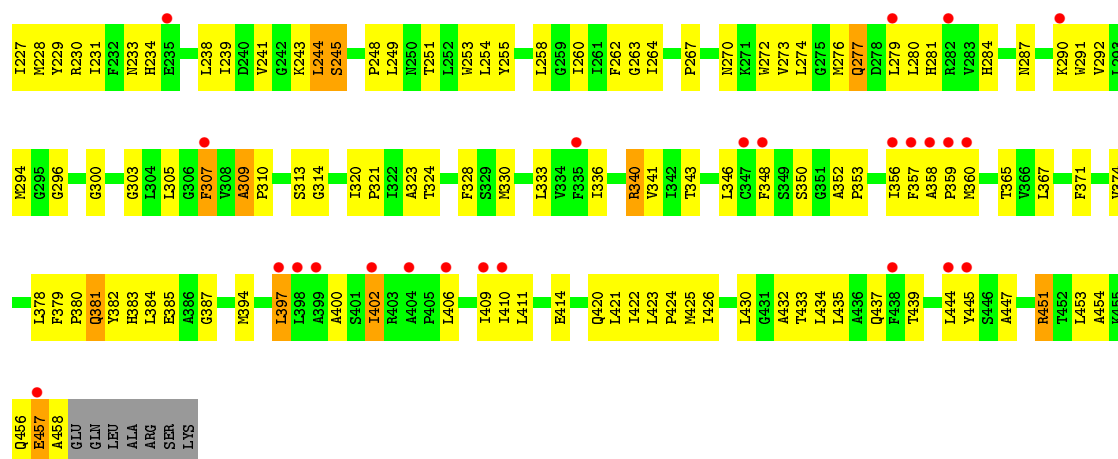
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Voltage-gated ClC-type chloride channel eriC

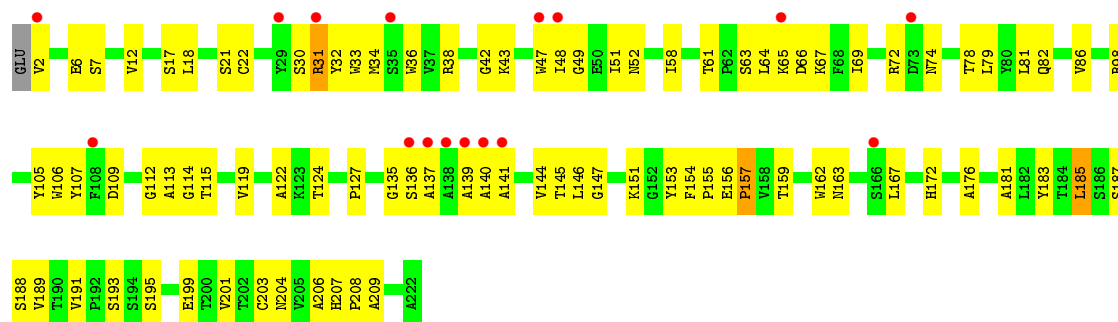


- Molecule 1: Voltage-gated ClC-type chloride channel eriC

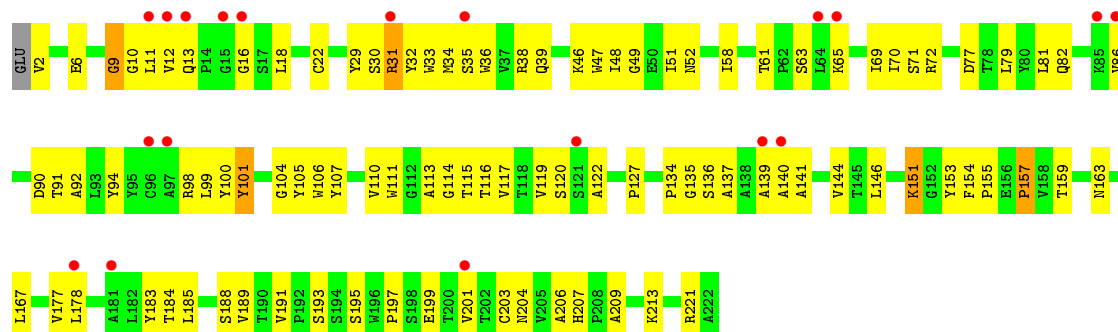




• Molecule 2: Fab fragment (heavy chain)

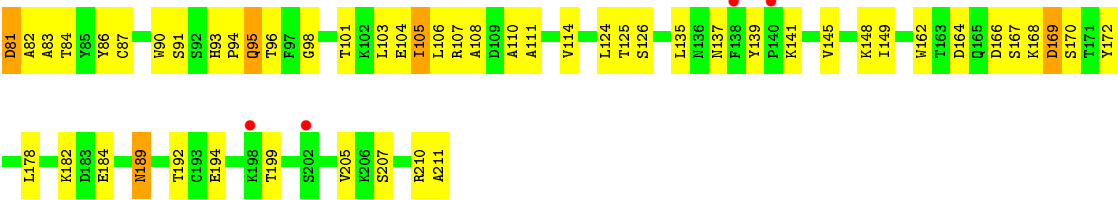


• Molecule 2: Fab fragment (heavy chain)

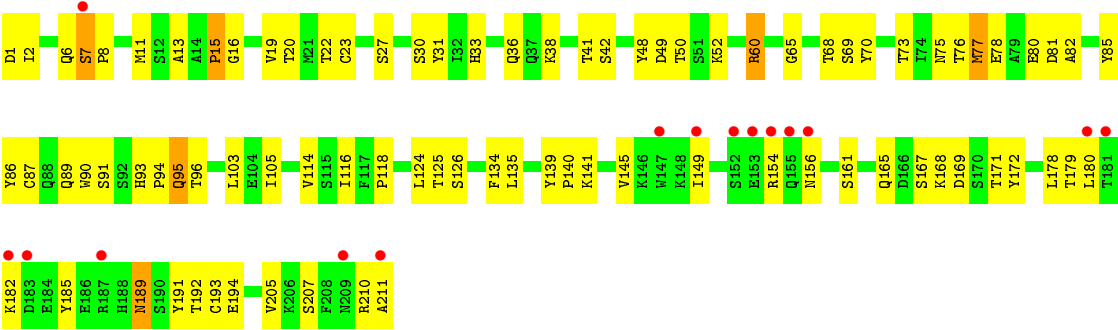


• Molecule 3: Fab fragment (light chain)





● 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, $\alpha$ , $\beta$ , $\gamma$	229.94Å 93.87Å 168.54Å 90.00° 131.72° 90.00°	Depositor
Resolution (Å)	24.58 – 2.51 34.24 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.58-2.51) 95.9 (34.24-2.51)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.264 , 0.299 0.252 , 0.281	Depositor DCC
$R_{free}$ test set	4446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/3405	0.59	0/4621
1	B	0.43	0/3376	0.60	0/4583
2	C	0.44	0/1721	0.68	0/2355
2	E	0.44	0/1721	0.69	0/2355
3	D	0.38	0/1660	0.66	0/2257
3	F	0.47	0/1660	0.70	0/2257
All	All	0.42	0/13543	0.64	0/18428

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	101	TYR	Sidechain

### 5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3484	237	0
1	B	3304	0	3457	241	0
2	C	1672	0	1654	79	0
2	E	1672	0	1654	100	0
3	D	1621	0	1546	89	0
3	F	1621	0	1546	92	0
4	A	2	0	0	1	0
4	B	2	0	0	2	0
5	A	76	0	0	4	0
5	B	91	0	0	11	0
5	C	85	0	0	10	0
5	D	36	0	0	7	0
5	E	69	0	0	10	0
5	F	70	0	0	10	0
All	All	13654	0	13341	776	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 29.

All (776) 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:119:GLN:HA	1:A:119:GLN:HE21	1.07	1.15
2:E:9:GLY:H	2:E:115:THR:HG21	1.11	1.15
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.38	1.06
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.41	1.03
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.40	1.03
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.39	1.01
1:A:381:GLN:N	1:A:381:GLN:HE21	1.58	1.00
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.40	1.00
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.44	0.99
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.43	0.99
3:F:95:GLN:H	3:F:95:GLN:CD	1.66	0.98
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.43	0.98
1:B:251:THR:HG21	5:B:529:HOH:O	1.64	0.98
1:B:381:GLN:N	1:B:381:GLN:HE21	1.61	0.98
1:A:180:THR:HG22	1:A:218:VAL:HA	1.46	0.98
1:A:381:GLN:NE2	1:A:381:GLN:H	1.62	0.97
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.48	0.95
3:D:95:GLN:H	3:D:95:GLN:CD	1.69	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:O	1:A:236:VAL:HG23	1.67	0.95
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.03	0.93
3:D:41:THR:HG23	5:D:222:HOH:O	1.67	0.93
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.47	0.93
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.35	0.91
1:B:381:GLN:NE2	1:B:381:GLN:H	1.66	0.91
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.54	0.89
2:E:9:GLY:N	2:E:115:THR:HG21	1.86	0.88
2:C:113:ALA:HA	3:D:42:SER:OG	1.73	0.88
1:A:119:GLN:HA	1:A:119:GLN:NE2	1.88	0.87
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.56	0.87
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.57	0.87
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.56	0.86
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.56	0.85
1:A:381:GLN:HE21	1:A:381:GLN:H	0.86	0.85
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.59	0.85
2:E:46:LYS:HG3	5:E:273:HOH:O	1.75	0.84
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.43	0.84
1:A:72:ALA:HA	1:A:78:LEU:HD12	1.59	0.84
2:E:9:GLY:HA3	2:E:115:THR:HG22	1.58	0.84
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.60	0.84
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.60	0.83
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.41	0.83
2:E:13:GLN:HG2	5:E:264:HOH:O	1.77	0.83
1:B:78:LEU:HD12	1:B:79:LEU:N	1.95	0.82
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.43	0.82
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.60	0.81
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.59	0.81
2:E:221:ARG:HH12	3:F:118:PRO:HB2	1.43	0.81
3:D:17:ASP:H	3:D:76:THR:HA	1.46	0.81
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.61	0.81
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.46	0.81
3:F:95:GLN:N	3:F:95:GLN:CD	2.30	0.81
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.44	0.80
3:D:95:GLN:N	3:D:95:GLN:CD	2.29	0.80
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.63	0.80
1:B:180:THR:HG22	1:B:218:VAL:HA	1.62	0.79
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.65	0.79
1:A:144:VAL:HG21	1:A:343:THR:HB	1.65	0.78
1:B:409:ILE:HD13	1:B:426:ILE:HA	1.66	0.78
3:F:141:LYS:HG2	5:F:254:HOH:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.66	0.76
1:B:33:LEU:HD23	1:B:33:LEU:O	1.86	0.75
1:B:148:GLU:OE1	1:B:357:PHE:HB3	1.87	0.75
2:E:134:PRO:O	2:E:221:ARG:HG3	1.86	0.75
3:F:189:ASN:HD21	3:F:211:ALA:H	1.34	0.75
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.21	0.74
1:B:144:VAL:HG21	1:B:343:THR:HB	1.69	0.74
3:D:106:LEU:HD23	3:D:107:ARG:N	2.03	0.74
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.69	0.73
3:D:189:ASN:HD21	3:D:211:ALA:H	1.37	0.73
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.23	0.73
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.18	0.73
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.70	0.73
1:B:381:GLN:HE21	1:B:381:GLN:H	0.82	0.73
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.71	0.72
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.70	0.72
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.70	0.72
1:B:176:THR:O	1:B:180:THR:HG23	1.90	0.72
1:A:19:ARG:HB2	1:A:19:ARG:NH1	2.05	0.71
1:A:150:PRO:O	1:A:154:ILE:HG13	1.90	0.71
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.04	0.71
3:F:27:SER:O	3:F:68:THR:HG22	1.90	0.71
1:A:216:LYS:HE2	1:B:433:THR:HG22	1.72	0.71
2:C:7:SER:HA	2:C:115:THR:HG21	1.73	0.71
3:F:38:LYS:O	3:F:41:THR:HG22	1.91	0.71
1:B:346:LEU:O	1:B:350:SER:HB3	1.92	0.70
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.07	0.70
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.56	0.69
2:E:9:GLY:HA3	2:E:115:THR:CG2	2.23	0.69
2:C:195:SER:O	2:C:199:GLU:HB3	1.93	0.69
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.74	0.69
1:A:148:GLU:OE1	1:A:357:PHE:HB3	1.93	0.69
1:A:433:THR:HG22	1:B:216:LYS:HZ3	1.58	0.69
3:F:95:GLN:H	3:F:95:GLN:NE2	1.90	0.68
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.73	0.68
1:B:92:PHE:O	1:B:96:LEU:HD23	1.93	0.68
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.26	0.68
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.75	0.68
2:E:221:ARG:NH1	3:F:118:PRO:HB2	2.09	0.68
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.74	0.68
1:A:33:LEU:HD23	1:A:33:LEU:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:38:LYS:NZ	3:F:80:GLU:O	2.27	0.68
1:A:223:ILE:CD1	1:B:426:ILE:HG22	2.21	0.68
1:B:154:ILE:O	1:B:158:ILE:HG12	1.93	0.68
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.09	0.68
2:C:6:GLU:O	2:C:115:THR:HG23	1.93	0.67
3:D:95:GLN:N	3:D:95:GLN:OE1	2.27	0.67
1:B:422:ILE:HA	1:B:425:MET:HE3	1.77	0.67
3:D:7:SER:HB2	3:D:22:THR:HB	1.76	0.67
2:E:2:VAL:N	5:E:271:HOH:O	2.27	0.67
1:A:180:THR:HG22	1:A:218:VAL:CA	2.24	0.67
1:B:270:ASN:O	1:B:273:VAL:HG12	1.94	0.67
1:B:75:TYR:CE2	1:B:79:LEU:HD11	2.30	0.66
1:B:211:THR:HG22	1:B:213:ILE:HG13	1.78	0.66
1:B:356:ILE:HG23	1:B:360:MET:CE	2.26	0.66
3:D:137:ASN:ND2	5:D:243:HOH:O	2.29	0.66
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.78	0.66
1:A:398:LEU:HD22	1:A:402:ILE:HD12	1.77	0.66
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.31	0.66
1:A:220:ILE:CG1	1:B:430:LEU:HD21	2.24	0.65
2:E:195:SER:O	2:E:199:GLU:HB3	1.96	0.65
1:A:226:THR:O	1:A:230:ARG:HG2	1.95	0.65
3:D:192:THR:HG22	3:D:207:SER:CB	2.26	0.65
2:E:30:SER:C	2:E:32:TYR:H	1.98	0.65
1:A:38:MET:HG3	1:A:168:LEU:CD1	2.24	0.65
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.26	0.65
1:A:74:ASN:HD22	1:A:76:PRO:HD2	1.59	0.65
1:A:176:THR:O	1:A:180:THR:HG23	1.97	0.65
3:D:192:THR:HG23	5:D:212:HOH:O	1.96	0.65
1:B:109:ILE:O	1:B:113:GLU:HG3	1.96	0.65
1:A:241:VAL:CG1	1:A:244:LEU:HD21	2.27	0.65
1:B:211:THR:CG2	1:B:213:ILE:HG13	2.27	0.65
1:A:86:SER:OG	1:A:303:GLY:HA3	1.97	0.64
3:D:30:SER:HA	3:D:70:TYR:OH	1.98	0.64
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.78	0.64
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.61	0.64
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.32	0.64
2:C:145:THR:HB	5:C:249:HOH:O	1.96	0.64
3:F:141:LYS:HB3	3:F:172:TYR:CD1	2.33	0.64
1:B:421:LEU:O	1:B:424:PRO:HD2	1.97	0.64
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.08	0.64
1:A:382:TYR:HB3	1:A:384:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:THR:HG22	1:B:216:LYS:HE2	1.78	0.64
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.33	0.64
3:F:20:THR:HG23	3:F:73:THR:OG1	1.97	0.64
1:A:92:PHE:O	1:A:96:LEU:HD23	1.98	0.63
3:D:125:THR:HG22	3:D:125:THR:O	1.98	0.63
1:B:340:ARG:NH1	5:B:474:HOH:O	2.30	0.63
3:D:6:GLN:NE2	3:D:87:CYS:H	1.95	0.63
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.34	0.62
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.29	0.62
1:B:91:MET:HG2	1:B:292:VAL:O	1.99	0.62
2:C:185:LEU:C	2:C:185:LEU:HD12	2.20	0.62
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.34	0.62
3:D:7:SER:CB	3:D:22:THR:HB	2.30	0.62
3:F:30:SER:HA	3:F:70:TYR:OH	2.00	0.62
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.81	0.62
1:A:346:LEU:O	1:A:350:SER:HB3	1.99	0.62
1:B:241:VAL:CG1	1:B:244:LEU:HD21	2.30	0.62
1:B:409:ILE:CD1	1:B:426:ILE:HA	2.29	0.62
2:E:163:ASN:ND2	2:E:167:LEU:HD22	2.14	0.62
1:A:84:LEU:O	1:A:88:VAL:HG23	2.00	0.61
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.82	0.61
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.82	0.61
1:A:235:GLU:OE2	2:E:101:TYR:O	2.18	0.61
3:D:189:ASN:HD22	3:D:210:ARG:HB2	1.66	0.61
3:F:31:TYR:HA	3:F:50:THR:OG1	2.01	0.61
2:C:208:PRO:HG2	5:C:251:HOH:O	2.01	0.61
1:A:212:LEU:HD12	1:A:212:LEU:N	2.16	0.61
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.83	0.61
1:B:402:ILE:HD12	1:B:445:TYR:CE1	2.35	0.61
2:C:64:LEU:HD12	2:C:67:LYS:HD3	1.83	0.60
1:A:148:GLU:HG2	1:A:357:PHE:HB3	1.82	0.60
3:F:80:GLU:HA	3:F:167:SER:O	2.01	0.60
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.15	0.60
3:F:7:SER:HB3	3:F:8:PRO:CD	2.31	0.60
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.01	0.60
1:B:150:PRO:O	1:B:154:ILE:HG13	2.01	0.60
1:A:19:ARG:HB2	1:A:19:ARG:HH11	1.66	0.60
1:B:445:TYR:HB2	5:B:489:HOH:O	2.02	0.60
3:F:22:THR:HG22	5:F:232:HOH:O	2.02	0.60
3:F:6:GLN:NE2	3:F:87:CYS:H	1.99	0.60
1:A:356:ILE:HG23	1:A:360:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PRO:HG2	1:B:439:THR:OG1	2.02	0.60
1:A:422:ILE:HD11	1:B:194:LEU:HD11	1.84	0.60
1:B:38:MET:HA	1:B:41:VAL:HG12	1.83	0.60
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.82	0.60
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.66	0.59
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.24	0.59
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.65	0.59
2:C:34:MET:HG2	5:C:239:HOH:O	2.02	0.59
2:E:104:GLY:O	2:E:106:TRP:CD1	2.56	0.59
1:B:243:LYS:HB3	2:E:31:ARG:HH21	1.67	0.59
3:F:125:THR:O	3:F:125:THR:HG22	2.02	0.59
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.37	0.59
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.37	0.59
1:A:426:ILE:HG22	1:B:223:ILE:CD1	2.27	0.59
3:F:82:ALA:HB2	3:F:105:ILE:HG12	1.85	0.59
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.37	0.59
2:C:30:SER:C	2:C:32:TYR:H	2.04	0.59
2:C:63:SER:HB3	5:C:284:HOH:O	2.02	0.59
3:D:31:TYR:HA	3:D:50:THR:OG1	2.03	0.59
2:E:91:THR:OG1	2:E:119:VAL:HG23	2.03	0.59
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.84	0.59
1:A:148:GLU:HG3	1:A:190:PHE:CZ	2.38	0.59
1:A:279:LEU:HD23	1:A:279:LEU:O	2.03	0.59
2:C:7:SER:HA	2:C:115:THR:CG2	2.32	0.59
2:C:163:ASN:HD22	2:C:167:LEU:HD22	1.65	0.59
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.28	0.59
1:B:86:SER:OG	1:B:303:GLY:HA3	2.03	0.59
5:C:232:HOH:O	3:D:52:LYS:HE2	2.03	0.59
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.85	0.59
1:A:235:GLU:HG3	5:A:485:HOH:O	2.03	0.58
3:F:7:SER:CB	3:F:8:PRO:HD3	2.31	0.58
1:A:270:ASN:O	1:A:273:VAL:HG12	2.03	0.58
1:A:42:VAL:CG2	1:A:162:VAL:HG21	2.33	0.58
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.84	0.58
1:A:18:ARG:HB2	1:B:119:GLN:OE1	2.02	0.58
3:D:95:GLN:H	3:D:95:GLN:NE2	2.00	0.58
2:E:11:LEU:HD11	2:E:120:SER:HB3	1.86	0.58
3:D:8:PRO:O	3:D:101:THR:HG23	2.03	0.58
3:D:79:ALA:C	3:D:81:ASP:H	2.06	0.58
3:D:7:SER:CB	3:D:8:PRO:HD3	2.33	0.58
2:E:163:ASN:HD22	2:E:167:LEU:HD22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.32	0.58
1:B:279:LEU:HD23	1:B:279:LEU:O	2.03	0.58
2:E:51:ILE:CD1	2:E:72:ARG:HG2	2.33	0.58
1:B:241:VAL:HG12	1:B:244:LEU:CD2	2.33	0.58
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.85	0.58
3:F:189:ASN:HD21	3:F:211:ALA:N	2.00	0.58
1:B:148:GLU:CD	1:B:148:GLU:H	2.05	0.57
3:D:106:LEU:HD23	3:D:107:ARG:H	1.67	0.57
3:F:6:GLN:HA	5:F:223:HOH:O	2.04	0.57
1:B:224:MET:O	1:B:228:MET:HG2	2.04	0.57
3:D:106:LEU:HA	3:D:139:TYR:OH	2.04	0.57
3:D:7:SER:HB3	3:D:8:PRO:CD	2.29	0.57
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.04	0.57
1:A:248:PRO:O	1:A:251:THR:HB	2.05	0.57
3:D:189:ASN:HD21	3:D:211:ALA:N	2.00	0.57
1:B:42:VAL:CG2	1:B:162:VAL:HG21	2.35	0.57
1:B:212:LEU:HD12	1:B:212:LEU:N	2.19	0.57
1:B:245:SER:HB3	1:B:385:GLU:OE2	2.05	0.57
3:F:2:ILE:HD12	3:F:27:SER:HB2	1.85	0.57
1:A:148:GLU:H	1:A:148:GLU:CD	2.07	0.56
1:A:267:PRO:HG2	1:A:439:THR:OG1	2.05	0.56
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.86	0.56
3:D:60:ARG:HD2	3:D:76:THR:O	2.05	0.56
1:A:216:LYS:CE	1:B:433:THR:HG22	2.35	0.56
2:C:112:GLY:O	3:D:42:SER:OG	2.21	0.56
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.69	0.56
3:D:17:ASP:N	3:D:76:THR:HA	2.17	0.56
1:A:241:VAL:HG12	1:A:244:LEU:CD2	2.35	0.56
1:A:430:LEU:HD21	1:B:220:ILE:CG1	2.34	0.56
1:A:433:THR:HG22	1:B:216:LYS:CE	2.35	0.56
1:B:113:GLU:HB3	5:B:513:HOH:O	2.05	0.56
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.88	0.56
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.88	0.56
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.41	0.56
3:F:95:GLN:N	3:F:95:GLN:OE1	2.39	0.56
1:A:68:LEU:CD2	1:A:81:VAL:HG23	2.36	0.55
1:A:211:THR:CG2	1:A:213:ILE:HG13	2.36	0.55
2:C:72:ARG:NH1	5:C:239:HOH:O	2.39	0.55
3:F:192:THR:HG22	3:F:207:SER:CB	2.37	0.55
1:A:273:VAL:HG11	1:A:444:LEU:HD21	1.88	0.55
1:B:200:ILE:HA	1:B:204:MET:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.17	0.55
1:B:78:LEU:HA	1:B:81:VAL:CG2	2.33	0.55
3:D:110:ALA:C	3:D:199:THR:HG21	2.26	0.55
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.41	0.55
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.89	0.55
1:B:227:ILE:O	1:B:231:ILE:HG13	2.04	0.55
3:F:69:SER:HB2	5:F:268:HOH:O	2.06	0.55
1:A:216:LYS:HZ3	1:B:433:THR:HG22	1.72	0.55
1:A:337:PHE:O	1:A:341:VAL:HG23	2.07	0.55
1:B:90:ALA:O	1:B:94:TYR:HD1	1.89	0.55
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.34	0.55
1:B:320:ILE:HD13	1:B:394:MET:HE3	1.87	0.55
2:E:213:LYS:HD3	5:E:226:HOH:O	2.05	0.55
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.42	0.55
2:E:6:GLU:HA	2:E:22:CYS:HA	1.88	0.55
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.71	0.55
2:C:7:SER:CA	2:C:115:THR:HG21	2.35	0.55
1:A:211:THR:HG22	1:A:213:ILE:HG13	1.89	0.55
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.89	0.55
1:A:455:LYS:O	1:A:459:GLU:HG2	2.07	0.55
1:B:147:ARG:N	1:B:148:GLU:OE2	2.40	0.55
2:C:32:TYR:CD2	2:C:98:ARG:HG3	2.41	0.55
2:E:144:VAL:O	2:E:144:VAL:HG13	2.07	0.55
1:A:382:TYR:HB3	1:A:384:LEU:CD2	2.37	0.54
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.22	0.54
1:B:197:ILE:HD13	1:B:219:PHE:CD1	2.42	0.54
1:B:68:LEU:HD22	1:B:78:LEU:HB2	1.89	0.54
1:A:241:VAL:CG1	1:A:324:THR:HG21	2.37	0.54
1:A:192:ALA:HB1	1:A:414:GLU:OE2	2.07	0.54
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.90	0.54
1:A:154:ILE:O	1:A:158:ILE:HG12	2.06	0.54
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.88	0.54
3:D:192:THR:HG22	3:D:207:SER:HB2	1.88	0.54
1:A:98:ARG:HD2	1:A:291:TRP:CD2	2.42	0.54
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.30	0.54
3:F:19:VAL:HG21	3:F:77:MET:HE2	1.90	0.54
1:B:148:GLU:HG2	1:B:357:PHE:HB3	1.89	0.54
3:D:164:ASP:HB3	5:D:226:HOH:O	2.08	0.54
1:A:433:THR:HG22	1:B:216:LYS:NZ	2.23	0.54
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.90	0.54
3:F:22:THR:HG23	5:F:268:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:O	1:A:402:ILE:HB	2.07	0.54
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.73	0.54
3:D:162:TRP:HE3	5:D:221:HOH:O	1.90	0.54
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.08	0.53
2:E:46:LYS:HB3	5:E:225:HOH:O	2.06	0.53
1:A:197:ILE:HD13	1:A:219:PHE:CD1	2.43	0.53
1:A:227:ILE:O	1:A:231:ILE:HG12	2.07	0.53
1:B:148:GLU:HG3	1:B:190:PHE:CZ	2.43	0.53
2:E:86:VAL:HG12	2:E:119:VAL:CG1	2.38	0.53
1:A:119:GLN:CA	1:A:119:GLN:HE21	1.90	0.53
1:B:191:ASN:HB2	1:B:229:TYR:CE2	2.44	0.53
2:C:17:SER:HB3	5:C:238:HOH:O	2.08	0.53
3:D:21:MET:HB2	5:D:224:HOH:O	2.08	0.53
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.89	0.53
2:C:135:GLY:C	2:C:137:ALA:H	2.11	0.53
3:D:104:GLU:CD	3:D:172:TYR:HH	2.11	0.53
2:E:10:GLY:N	2:E:116:THR:O	2.40	0.53
1:A:148:GLU:CG	1:A:357:PHE:HB3	2.39	0.53
1:B:155:GLY:HA3	1:B:181:GLY:O	2.09	0.53
1:B:226:THR:O	1:B:230:ARG:HG2	2.09	0.53
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.43	0.53
1:B:218:VAL:O	1:B:222:VAL:HG23	2.08	0.53
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.91	0.53
1:A:340:ARG:HA	1:A:343:THR:OG1	2.09	0.53
1:B:280:LEU:HD22	1:B:294:MET:SD	2.49	0.53
2:E:30:SER:O	2:E:32:TYR:N	2.42	0.53
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.44	0.52
2:C:113:ALA:HA	3:D:42:SER:HG	1.71	0.52
1:B:61:GLN:HA	1:B:64:ARG:HE	1.74	0.52
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.90	0.52
2:C:86:VAL:HG12	2:C:119:VAL:CG1	2.38	0.52
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.73	0.52
1:A:275:GLY:HA2	5:A:486:HOH:O	2.08	0.52
3:D:75:ASN:O	3:D:76:THR:HB	2.09	0.52
2:E:9:GLY:CA	2:E:115:THR:CG2	2.86	0.52
1:A:226:THR:CG2	1:B:423:LEU:HD11	2.39	0.52
2:C:6:GLU:HA	2:C:22:CYS:HA	1.92	0.52
1:A:451:ARG:CB	1:A:451:ARG:HH11	2.22	0.52
1:B:379:PHE:HA	1:B:381:GLN:HE22	1.74	0.52
2:E:35:SER:HB3	2:E:99:LEU:HD21	1.91	0.52
2:C:141:ALA:O	2:C:193:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:189:ASN:ND2	3:D:210:ARG:HB2	2.25	0.52
3:D:82:ALA:HB2	3:D:105:ILE:HG13	1.91	0.52
1:A:91:MET:HG2	1:A:292:VAL:O	2.09	0.52
1:B:356:ILE:O	1:B:360:MET:HG3	2.09	0.52
3:F:189:ASN:HD22	3:F:210:ARG:HB2	1.74	0.52
3:F:93:HIS:CG	3:F:94:PRO:HA	2.45	0.52
1:B:421:LEU:C	1:B:424:PRO:HD2	2.30	0.52
1:A:379:PHE:HA	1:A:381:GLN:NE2	2.25	0.51
1:B:248:PRO:O	1:B:251:THR:HB	2.10	0.51
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.44	0.51
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.24	0.51
1:A:18:ARG:O	1:A:22:ILE:HG13	2.09	0.51
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.92	0.51
1:A:423:LEU:HD11	1:B:226:THR:CG2	2.40	0.51
2:E:6:GLU:CD	2:E:114:GLY:H	2.14	0.51
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.45	0.51
2:C:31:ARG:HD2	5:C:289:HOH:O	2.11	0.51
3:D:78:GLU:O	3:D:81:ASP:HB2	2.10	0.51
1:B:93:GLY:O	1:B:97:VAL:HG23	2.11	0.51
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.45	0.51
2:E:2:VAL:HG23	2:E:2:VAL:O	2.11	0.51
1:A:38:MET:HA	1:A:41:VAL:HG12	1.92	0.51
1:B:263:GLY:HA3	1:B:435:LEU:HB2	1.92	0.51
1:A:17:ARG:HG3	1:A:18:ARG:N	2.26	0.51
1:B:20:GLN:O	1:B:23:ARG:HB3	2.10	0.51
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.45	0.51
1:B:103:GLU:OE2	5:B:531:HOH:O	2.18	0.51
1:B:77:LEU:O	1:B:80:THR:HB	2.11	0.51
2:C:185:LEU:O	2:C:185:LEU:HD12	2.09	0.51
1:A:159:GLY:O	1:A:162:VAL:HG22	2.11	0.51
1:A:80:THR:O	1:A:84:LEU:HG	2.11	0.51
1:B:180:THR:HG22	1:B:218:VAL:CA	2.37	0.51
1:A:226:THR:HG21	1:B:423:LEU:HD11	1.93	0.51
1:A:356:ILE:O	1:A:360:MET:HG3	2.10	0.50
1:B:260:ILE:O	1:B:264:ILE:HG23	2.11	0.50
3:D:15:PRO:HA	3:D:77:MET:O	2.11	0.50
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.41	0.50
2:E:30:SER:C	2:E:32:TYR:N	2.64	0.50
2:E:39:GLN:O	2:E:92:ALA:HB1	2.11	0.50
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.93	0.50
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:20:THR:HG23	3:D:73:THR:OG1	2.11	0.50
3:F:23:CYS:HB2	5:F:223:HOH:O	2.10	0.50
1:B:182:ALA:HB1	1:B:204:MET:CE	2.41	0.50
1:B:110:PRO:HG2	4:B:467:CL:CL	2.48	0.50
2:E:197:PRO:HD3	5:E:247:HOH:O	2.12	0.50
1:A:411:LEU:HG	1:A:415:MET:HE2	1.92	0.50
2:E:51:ILE:HG23	2:E:51:ILE:O	2.11	0.50
3:F:31:TYR:HB3	3:F:49:ASP:HA	1.93	0.50
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.14	0.50
2:C:30:SER:O	2:C:32:TYR:N	2.45	0.50
1:A:202:GLU:O	1:A:202:GLU:HG2	2.10	0.50
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.76	0.50
2:E:188:SER:HB3	3:F:134:PHE:CE2	2.46	0.50
1:A:410:ILE:O	1:A:414:GLU:HG3	2.11	0.50
1:A:447:ALA:O	1:A:451:ARG:HG2	2.11	0.50
1:A:91:MET:CG	1:A:296:GLY:HA3	2.42	0.50
1:B:180:THR:CG2	1:B:218:VAL:HA	2.37	0.50
3:F:77:MET:CE	3:F:103:LEU:HD11	2.42	0.50
1:B:243:LYS:HD2	5:B:482:HOH:O	2.10	0.50
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.47	0.50
2:C:167:LEU:HD21	2:C:191:VAL:HG11	1.94	0.49
2:E:32:TYR:HA	5:E:223:HOH:O	2.12	0.49
1:A:235:GLU:O	1:A:236:VAL:CG2	2.51	0.49
1:A:449:LEU:O	1:A:453:LEU:HB2	2.12	0.49
1:B:323:ALA:HA	5:B:503:HOH:O	2.11	0.49
3:D:38:LYS:O	3:D:41:THR:HG22	2.11	0.49
1:A:59:TRP:O	1:A:62:ASN:HB3	2.13	0.49
1:B:382:TYR:HB3	1:B:384:LEU:HD21	1.95	0.49
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.93	0.49
1:B:41:VAL:O	1:B:45:LEU:HG	2.11	0.49
2:C:12:VAL:HG11	2:C:18:LEU:HB3	1.94	0.49
1:A:213:ILE:HB	5:A:498:HOH:O	2.12	0.49
3:D:82:ALA:HA	3:D:103:LEU:O	2.12	0.49
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.48	0.49
1:A:420:GLN:NE2	5:A:516:HOH:O	2.45	0.49
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.37	0.49
3:D:2:ILE:O	3:D:96:THR:HG21	2.13	0.49
1:A:416:THR:O	1:A:418:ASN:ND2	2.41	0.49
2:E:71:SER:O	2:E:79:LEU:HD12	2.13	0.49
1:A:41:VAL:O	1:A:45:LEU:HG	2.13	0.48
1:B:200:ILE:CD1	1:B:204:MET:HG3	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:O	1:B:340:ARG:HG3	2.13	0.48
2:E:159:THR:OG1	2:E:206:ALA:HB3	2.13	0.48
3:F:15:PRO:HD3	3:F:105:ILE:HG23	1.95	0.48
1:A:68:LEU:HD23	1:A:81:VAL:HG23	1.95	0.48
1:B:109:ILE:HD12	1:B:445:TYR:OH	2.12	0.48
1:B:387:GLY:N	5:B:502:HOH:O	2.36	0.48
2:C:12:VAL:HG11	2:C:18:LEU:HD13	1.94	0.48
2:C:6:GLU:CG	2:C:114:GLY:HA2	2.43	0.48
2:E:9:GLY:N	2:E:115:THR:CG2	2.68	0.48
2:E:221:ARG:HH11	3:F:118:PRO:HD2	1.79	0.48
3:F:7:SER:CB	3:F:22:THR:HB	2.43	0.48
1:A:423:LEU:HD11	1:B:226:THR:HG21	1.94	0.48
2:E:18:LEU:HD11	2:E:117:VAL:CG2	2.43	0.48
2:E:61:THR:O	2:E:63:SER:N	2.46	0.48
2:E:86:VAL:HG13	2:E:90:ASP:HB2	1.95	0.48
1:A:109:ILE:HD12	1:A:445:TYR:OH	2.13	0.48
1:A:224:MET:O	1:A:228:MET:HG2	2.14	0.48
1:A:336:ILE:O	1:A:340:ARG:HG3	2.11	0.48
1:A:409:ILE:HD12	1:A:426:ILE:HA	1.94	0.48
3:D:93:HIS:CG	3:D:94:PRO:HA	2.49	0.48
1:B:144:VAL:HG21	1:B:343:THR:CB	2.40	0.48
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.49	0.48
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.96	0.48
1:B:163:LEU:HD22	1:B:174:ARG:HA	1.95	0.48
1:B:182:ALA:HB1	1:B:204:MET:HE2	1.95	0.48
2:E:29:TYR:HB2	2:E:77:ASP:OD2	2.14	0.48
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.45	0.48
3:F:2:ILE:CD1	3:F:27:SER:HB2	2.43	0.48
1:B:71:THR:O	1:B:78:LEU:HB3	2.13	0.48
2:C:51:ILE:CD1	2:C:72:ARG:HG2	2.44	0.48
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.96	0.47
2:E:141:ALA:O	2:E:193:SER:HB2	2.15	0.47
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.96	0.47
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.97	0.47
1:B:186:LEU:HD22	1:B:199:PHE:CD2	2.49	0.47
2:E:104:GLY:O	2:E:106:TRP:HD1	1.97	0.47
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.95	0.47
2:E:12:VAL:HG11	2:E:18:LEU:HD13	1.96	0.47
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.29	0.47
1:A:457:GLU:O	1:A:459:GLU:N	2.46	0.47
1:B:270:ASN:O	1:B:273:VAL:CG1	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:O	1:A:23:ARG:HB3	2.14	0.47
1:B:241:VAL:O	1:B:241:VAL:HG12	2.14	0.47
1:B:245:SER:HB2	5:B:550:HOH:O	2.13	0.47
2:C:189:VAL:O	2:C:189:VAL:HG13	2.14	0.47
3:D:12:SER:HA	3:D:104:GLU:O	2.13	0.47
2:E:151:LYS:HB2	2:E:184:THR:OG1	2.15	0.47
3:F:60:ARG:NH2	3:F:81:ASP:CG	2.68	0.47
1:A:123:ARG:HA	1:A:125:TRP:CH2	2.50	0.47
1:B:190:PHE:HA	1:B:238:LEU:CD1	2.45	0.47
1:B:91:MET:CG	1:B:296:GLY:HA3	2.44	0.47
1:A:144:VAL:O	1:A:144:VAL:HG12	2.15	0.47
1:A:239:ILE:HG22	1:A:241:VAL:HG23	1.97	0.47
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.35	0.47
1:A:78:LEU:HD23	1:A:78:LEU:C	2.36	0.47
1:B:109:ILE:N	1:B:110:PRO:CD	2.78	0.47
2:E:94:TYR:O	2:E:114:GLY:HA2	2.14	0.47
2:E:16:GLY:O	2:E:86:VAL:HG23	2.15	0.47
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.30	0.47
1:B:148:GLU:CG	1:B:357:PHE:HB3	2.45	0.47
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.97	0.47
1:A:109:ILE:O	1:A:113:GLU:HG3	2.15	0.47
1:B:374:VAL:O	1:B:378:LEU:HG	2.14	0.47
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.13	0.47
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.97	0.47
1:A:75:TYR:CZ	1:A:79:LEU:HD11	2.50	0.46
1:A:413:LEU:HD11	1:A:419:TYR:HA	1.98	0.46
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.46
2:C:2:VAL:O	2:C:2:VAL:HG23	2.15	0.46
1:A:260:ILE:O	1:A:264:ILE:HG23	2.15	0.46
3:F:192:THR:HG22	3:F:207:SER:HB2	1.97	0.46
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.16	0.46
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.98	0.46
1:B:107:SER:HB3	4:B:467:CL:CL	2.53	0.46
1:B:273:VAL:HG11	1:B:444:LEU:HD21	1.98	0.46
2:E:185:LEU:HD12	2:E:185:LEU:C	2.36	0.46
1:A:144:VAL:HG21	1:A:343:THR:CB	2.41	0.46
1:A:144:VAL:CG2	1:A:343:THR:HB	2.41	0.46
2:E:105:TYR:N	2:E:105:TYR:CD1	2.83	0.46
3:F:6:GLN:HG2	5:F:223:HOH:O	2.14	0.46
1:B:253:TRP:CZ2	1:B:254:LEU:HD21	2.51	0.46
1:B:274:LEU:O	1:B:277:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:ALA:HB1	2:C:181:ALA:HB1	1.98	0.46
2:E:135:GLY:C	2:E:137:ALA:H	2.19	0.46
3:F:90:TRP:CE3	3:F:95:GLN:HG3	2.51	0.46
1:A:209:ARG:HH11	1:A:209:ARG:HG2	1.81	0.46
3:F:169:ASP:HA	5:F:227:HOH:O	2.16	0.46
3:F:75:ASN:O	3:F:76:THR:HB	2.16	0.46
3:D:149:ILE:HD11	3:D:178:LEU:HD21	1.97	0.45
3:D:210:ARG:HH11	3:D:210:ARG:HG2	1.80	0.45
2:E:167:LEU:HD21	2:E:191:VAL:HG11	1.98	0.45
2:E:70:ILE:HG12	2:E:81:LEU:HD13	1.98	0.45
3:D:17:ASP:OD1	3:D:18:LYS:N	2.50	0.45
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.51	0.45
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.50	0.45
3:F:78:GLU:O	3:F:81:ASP:HB2	2.15	0.45
1:A:147:ARG:N	1:A:148:GLU:OE2	2.50	0.45
1:A:155:GLY:HA3	1:A:181:GLY:O	2.16	0.45
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.16	0.45
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.51	0.45
1:B:209:ARG:HH11	1:B:209:ARG:HG2	1.82	0.45
1:B:379:PHE:HA	1:B:381:GLN:NE2	2.32	0.45
2:C:86:VAL:CG1	2:C:119:VAL:CG2	2.95	0.45
3:D:111:ALA:HA	3:D:199:THR:OG1	2.16	0.45
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.51	0.45
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.81	0.45
1:A:26:LEU:HD21	5:B:545:HOH:O	2.17	0.45
1:A:33:LEU:HD23	1:A:33:LEU:C	2.36	0.45
3:D:145:VAL:HA	3:D:194:GLU:O	2.17	0.45
2:E:113:ALA:HA	3:F:42:SER:OG	2.15	0.45
1:A:216:LYS:HZ2	1:B:437:GLN:NE2	2.14	0.45
1:A:78:LEU:C	1:A:80:THR:N	2.70	0.45
1:A:216:LYS:NZ	1:B:433:THR:HG22	2.31	0.45
2:C:86:VAL:HG11	2:C:119:VAL:HG22	1.99	0.45
2:E:9:GLY:CA	2:E:115:THR:HG21	2.45	0.45
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.99	0.45
3:F:7:SER:HB2	3:F:22:THR:HB	1.99	0.45
1:A:270:ASN:HD21	1:A:401:SER:HB3	1.81	0.45
1:A:255:TYR:CE2	1:A:424:PRO:HB3	2.51	0.45
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.32	0.45
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.99	0.45
3:D:192:THR:HG22	3:D:207:SER:HB3	1.98	0.45
1:A:332:MET:O	1:A:336:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ALA:HA	1:B:78:LEU:HD23	1.98	0.45
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.99	0.45
1:A:148:GLU:CG	1:A:190:PHE:CZ	3.00	0.45
1:B:126:ARG:O	1:B:130:VAL:HG23	2.17	0.45
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.99	0.45
1:B:239:ILE:HG22	1:B:241:VAL:HG23	1.99	0.45
1:B:251:THR:HG22	1:B:255:TYR:HE1	1.81	0.45
1:B:33:LEU:HD23	1:B:33:LEU:C	2.37	0.45
2:E:110:VAL:HA	5:E:281:HOH:O	2.16	0.45
1:A:90:ALA:O	1:A:94:TYR:HD1	2.01	0.44
1:B:229:TYR:CE1	1:B:233:ASN:ND2	2.86	0.44
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.87	0.44
1:A:434:LEU:HD23	1:B:216:LYS:HD3	2.00	0.44
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.99	0.44
2:C:86:VAL:HG12	2:C:119:VAL:HG11	1.99	0.44
3:F:7:SER:CB	3:F:8:PRO:CD	2.94	0.44
1:A:218:VAL:O	1:A:222:VAL:HG23	2.17	0.44
1:A:241:VAL:HG12	1:A:241:VAL:O	2.17	0.44
2:E:177:VAL:HG13	5:E:254:HOH:O	2.16	0.44
1:A:187:ALA:HB2	1:A:222:VAL:HG13	1.99	0.44
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.83	0.44
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.98	0.44
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.99	0.44
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.50	0.44
3:F:179:THR:O	3:F:180:LEU:HD23	2.18	0.44
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.86	0.44
1:A:109:ILE:N	1:A:110:PRO:CD	2.80	0.44
1:A:402:ILE:HD13	1:A:445:TYR:CE1	2.53	0.44
1:A:198:LEU:HG	1:A:410:ILE:CD1	2.48	0.44
1:B:148:GLU:O	1:B:152:VAL:HG23	2.18	0.44
1:A:24:GLN:HB3	1:B:208:PHE:CE2	2.53	0.44
1:B:402:ILE:HD12	1:B:445:TYR:HE1	1.82	0.44
1:B:451:ARG:HH11	1:B:451:ARG:CG	2.30	0.44
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.85	0.44
2:C:42:GLY:N	5:C:276:HOH:O	2.51	0.44
2:C:43:LYS:NZ	2:C:43:LYS:HB3	2.32	0.44
1:B:148:GLU:CG	1:B:190:PHE:CZ	3.00	0.44
1:B:280:LEU:HD13	1:B:350:SER:HA	2.00	0.44
3:D:184:GLU:HG2	5:D:239:HOH:O	2.18	0.44
3:D:6:GLN:HA	3:D:22:THR:O	2.17	0.44
2:E:51:ILE:HG13	2:E:58:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:11:MET:CE	3:F:19:VAL:HG13	2.48	0.44
3:F:6:GLN:CG	5:F:223:HOH:O	2.65	0.44
1:A:100:TYR:O	1:A:126:ARG:NH1	2.48	0.43
1:A:162:VAL:HG23	1:A:163:LEU:N	2.33	0.43
1:A:75:TYR:CZ	1:A:79:LEU:HD21	2.53	0.43
1:B:187:ALA:HB2	1:B:222:VAL:HG13	1.99	0.43
1:B:382:TYR:HB3	1:B:384:LEU:CD2	2.48	0.43
1:B:38:MET:O	1:B:41:VAL:HG12	2.18	0.43
1:B:255:TYR:CE2	1:B:424:PRO:HB3	2.53	0.43
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.53	0.43
2:E:188:SER:HB3	3:F:134:PHE:CZ	2.53	0.43
3:F:189:ASN:ND2	3:F:210:ARG:HB2	2.33	0.43
3:F:2:ILE:O	3:F:96:THR:HG21	2.18	0.43
1:B:309:ALA:N	1:B:310:PRO:HD3	2.33	0.43
1:B:330:MET:O	1:B:330:MET:HE2	2.18	0.43
2:C:159:THR:OG1	2:C:206:ALA:HB3	2.18	0.43
2:E:86:VAL:HG12	2:E:119:VAL:HG13	1.98	0.43
1:B:74:ASN:HD22	1:B:76:PRO:HD2	1.83	0.43
3:D:7:SER:CB	3:D:8:PRO:CD	2.95	0.43
3:F:210:ARG:HH11	3:F:210:ARG:HG2	1.82	0.43
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.32	0.43
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.44	0.43
1:A:180:THR:CG2	1:A:218:VAL:HA	2.32	0.43
1:A:305:LEU:C	1:A:307:PHE:H	2.21	0.43
1:A:78:LEU:C	1:A:80:THR:H	2.21	0.43
1:B:194:LEU:O	1:B:198:LEU:HD23	2.19	0.43
1:B:231:ILE:O	1:B:231:ILE:HG22	2.17	0.43
1:B:305:LEU:C	1:B:307:PHE:H	2.22	0.43
1:B:422:ILE:CG2	1:B:423:LEU:N	2.81	0.43
1:B:447:ALA:O	1:B:451:ARG:HG2	2.18	0.43
3:F:149:ILE:HD11	3:F:178:LEU:HD21	2.01	0.43
1:A:200:ILE:CD1	1:A:204:MET:HG3	2.29	0.43
1:A:193:PRO:HA	1:A:222:VAL:CG1	2.49	0.43
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.19	0.43
2:E:139:ALA:O	2:E:141:ALA:N	2.52	0.43
1:A:91:MET:HG3	1:A:296:GLY:CA	2.48	0.43
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.19	0.43
1:B:148:GLU:CD	1:B:357:PHE:HB3	2.38	0.43
1:B:73:ASP:O	1:B:74:ASN:HB3	2.19	0.43
1:B:123:ARG:HA	1:B:125:TRP:CH2	2.54	0.43
1:B:198:LEU:HG	1:B:410:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:LEU:HB2	2:E:183:TYR:CE2	2.54	0.43
3:F:141:LYS:HB3	3:F:172:TYR:CE1	2.53	0.43
1:A:263:GLY:HA3	1:A:435:LEU:CB	2.48	0.43
1:B:124:TRP:CA	1:B:157:ASN:HD22	2.23	0.43
2:C:139:ALA:O	2:C:141:ALA:N	2.52	0.43
2:C:33:TRP:CZ2	2:C:52:ASN:HB3	2.53	0.43
2:E:35:SER:CB	2:E:99:LEU:HD21	2.49	0.43
3:F:124:LEU:O	3:F:182:LYS:HD2	2.19	0.43
3:F:90:TRP:CD2	3:F:95:GLN:HG3	2.54	0.43
1:A:74:ASN:C	1:A:74:ASN:HD22	2.21	0.43
1:B:241:VAL:CG1	1:B:324:THR:HG21	2.49	0.43
1:B:144:VAL:CG2	1:B:343:THR:HB	2.44	0.43
2:C:30:SER:C	2:C:32:TYR:N	2.70	0.43
1:A:314:GLY:O	1:A:340:ARG:NH2	2.52	0.42
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.86	0.42
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.54	0.42
3:D:2:ILE:CD1	3:D:27:SER:HB2	2.48	0.42
1:A:73:ASP:CG	1:A:74:ASN:N	2.72	0.42
1:B:313:SER:OG	1:B:314:GLY:N	2.52	0.42
1:B:78:LEU:C	1:B:78:LEU:HD12	2.38	0.42
1:B:91:MET:HG3	1:B:296:GLY:CA	2.50	0.42
2:C:86:VAL:CG1	2:C:119:VAL:HG22	2.48	0.42
3:D:166:ASP:O	3:D:170:SER:HA	2.18	0.42
3:D:82:ALA:O	3:D:83:ALA:HB2	2.19	0.42
1:B:248:PRO:HB3	2:E:104:GLY:HA2	1.99	0.42
1:A:190:PHE:HA	1:A:238:LEU:CD1	2.49	0.42
1:A:288:ILE:O	1:A:292:VAL:HG23	2.19	0.42
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.84	0.42
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.54	0.42
2:E:106:TRP:CD1	2:E:106:TRP:N	2.86	0.42
3:F:185:TYR:HA	3:F:191:TYR:OH	2.19	0.42
1:B:200:ILE:HD12	1:B:204:MET:CG	2.35	0.42
2:C:6:GLU:O	2:C:115:THR:CG2	2.66	0.42
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.01	0.42
1:B:123:ARG:NH1	5:B:491:HOH:O	2.52	0.42
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.00	0.42
1:B:59:TRP:O	1:B:62:ASN:HB3	2.19	0.42
1:B:74:ASN:HD22	1:B:74:ASN:C	2.22	0.42
3:D:107:ARG:NE	3:D:108:ALA:O	2.44	0.42
2:E:105:TYR:HD2	3:F:91:SER:HA	1.85	0.42
3:F:168:LYS:HD3	3:F:168:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:CE1	1:A:79:LEU:HD21	2.55	0.42
1:B:267:PRO:O	1:B:270:ASN:HB2	2.19	0.42
1:B:348:PHE:CD1	1:B:356:ILE:HB	2.54	0.42
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.55	0.42
2:E:29:TYR:HB3	5:E:265:HOH:O	2.19	0.42
1:B:272:TRP:O	1:B:276:MET:HB2	2.19	0.42
1:A:216:LYS:NZ	1:B:437:GLN:NE2	2.67	0.42
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.84	0.42
3:D:78:GLU:OE2	3:D:78:GLU:HA	2.20	0.42
2:C:105:TYR:HD2	3:D:91:SER:HA	1.85	0.42
2:E:111:TRP:N	2:E:111:TRP:CD1	2.87	0.42
2:E:38:ARG:HD3	2:E:48:ILE:HD11	2.02	0.42
3:D:11:MET:CE	3:D:19:VAL:HG13	2.49	0.42
1:B:123:ARG:HH21	1:B:126:ARG:HD3	1.85	0.41
1:B:272:TRP:HZ3	1:B:341:VAL:HG11	1.85	0.41
2:C:6:GLU:CD	2:C:114:GLY:H	2.24	0.41
2:C:47:TRP:O	2:C:61:THR:HB	2.19	0.41
2:E:106:TRP:H	2:E:106:TRP:HD1	1.67	0.41
2:E:189:VAL:O	2:E:189:VAL:HG13	2.20	0.41
1:A:107:SER:HB3	4:A:467:CL:CL	2.57	0.41
1:B:38:MET:O	1:B:42:VAL:HG23	2.21	0.41
3:F:114:VAL:HA	3:F:134:PHE:O	2.19	0.41
1:A:357:PHE:HE2	1:A:411:LEU:HD22	1.85	0.41
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.55	0.41
1:B:64:ARG:NH1	1:B:141:GLY:O	2.53	0.41
2:C:147:GLY:HA2	2:C:162:TRP:CH2	2.55	0.41
2:C:172:HIS:O	2:C:187:SER:HA	2.21	0.41
1:A:422:ILE:CG2	1:A:423:LEU:N	2.84	0.41
1:A:457:GLU:O	1:A:458:ALA:C	2.59	0.41
1:B:383:HIS:HB3	2:E:33:TRP:CZ2	2.55	0.41
2:C:106:TRP:H	2:C:106:TRP:HD1	1.68	0.41
2:E:185:LEU:O	2:E:185:LEU:HD12	2.21	0.41
1:A:200:ILE:HA	1:A:204:MET:HB2	2.01	0.41
1:A:272:TRP:O	1:A:276:MET:HB2	2.19	0.41
1:A:91:MET:HG3	1:A:296:GLY:HA3	2.01	0.41
1:A:71:THR:O	1:A:78:LEU:HB2	2.20	0.41
1:B:119:GLN:NE2	1:B:119:GLN:HA	2.36	0.41
1:B:195:ALA:N	1:B:414:GLU:OE2	2.53	0.41
2:C:185:LEU:C	2:C:185:LEU:CD1	2.87	0.41
3:D:79:ALA:O	3:D:81:ASP:N	2.49	0.41
2:E:154:PHE:HA	2:E:155:PRO:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.35	0.41
1:A:270:ASN:O	1:A:273:VAL:CG1	2.69	0.41
1:A:280:LEU:HD22	1:A:294:MET:SD	2.60	0.41
1:A:305:LEU:HA	1:A:308:VAL:HG22	2.03	0.41
1:A:421:LEU:O	1:A:424:PRO:HD2	2.21	0.41
1:B:456:GLN:C	1:B:458:ALA:H	2.24	0.41
3:D:84:THR:HA	3:D:101:THR:O	2.19	0.41
3:D:168:LYS:O	3:D:169:ASP:HB3	2.19	0.41
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.50	0.41
3:F:95:GLN:OE1	3:F:95:GLN:O	2.38	0.41
3:F:161:SER:HA	5:F:237:HOH:O	2.20	0.41
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.36	0.41
2:C:2:VAL:N	5:C:252:HOH:O	2.54	0.41
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.56	0.41
3:F:105:ILE:O	3:F:165:GLN:NE2	2.45	0.41
3:F:139:TYR:HA	3:F:140:PRO:C	2.40	0.41
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.56	0.41
1:A:145:LEU:HB3	1:A:354:GLY:HA3	2.03	0.41
1:B:193:PRO:HA	1:B:222:VAL:CG1	2.51	0.41
2:C:6:GLU:HA	2:C:21:SER:O	2.20	0.41
2:E:33:TRP:CZ2	2:E:52:ASN:HB3	2.56	0.41
1:B:207:GLN:HB3	1:B:208:PHE:CE1	2.56	0.41
2:C:124:THR:HA	2:C:154:PHE:O	2.21	0.41
2:E:30:SER:O	2:E:31:ARG:HB2	2.21	0.41
3:F:22:THR:CG2	3:F:23:CYS:N	2.84	0.41
1:A:198:LEU:HG	1:A:410:ILE:HD13	2.03	0.41
1:B:35:ILE:HD13	1:B:172:GLU:HG2	2.03	0.41
1:B:454:ALA:C	1:B:456:GLN:H	2.24	0.41
2:C:106:TRP:CD1	2:C:106:TRP:N	2.89	0.41
2:C:176:ALA:HA	2:C:185:LEU:HB3	2.03	0.41
2:C:172:HIS:HB2	2:C:188:SER:OG	2.21	0.41
3:D:166:ASP:OD1	3:D:167:SER:N	2.54	0.41
1:A:236:VAL:O	1:A:236:VAL:HG12	2.19	0.40
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.51	0.40
1:B:328:PHE:HB2	1:B:333:LEU:HD21	2.02	0.40
1:B:86:SER:HB2	1:B:300:GLY:HA2	2.02	0.40
1:B:98:ARG:NE	1:B:98:ARG:HA	2.37	0.40
2:C:105:TYR:N	2:C:105:TYR:CD1	2.88	0.40
2:C:144:VAL:HG13	2:C:144:VAL:O	2.20	0.40
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.21	0.40
2:E:18:LEU:HD23	2:E:18:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TRP:CA	1:A:157:ASN:HD22	2.22	0.40
1:A:73:ASP:CG	1:A:74:ASN:H	2.23	0.40
1:B:211:THR:HG22	1:B:212:LEU:N	2.36	0.40
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.56	0.40
1:A:22:ILE:HD13	1:B:454:ALA:HB2	2.03	0.40
3:D:124:LEU:O	3:D:182:LYS:HD2	2.22	0.40
3:D:90:TRP:CD2	3:D:95:GLN:HB3	2.56	0.40
1:A:287:ASN:ND2	1:A:290:LYS:H	2.19	0.40
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.51	0.40
1:A:87:ALA:O	1:A:91:MET:HG3	2.21	0.40
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.56	0.40
1:A:148:GLU:O	1:A:152:VAL:HG23	2.20	0.40
1:A:442:LYS:NZ	1:B:26:LEU:HB3	2.36	0.40
2:C:38:ARG:CD	2:C:48:ILE:HD11	2.42	0.40
2:C:22:CYS:O	2:C:78:THR:HG23	2.22	0.40
3:D:79:ALA:C	3:D:81:ASP:N	2.73	0.40
2:E:11:LEU:CD1	2:E:120:SER:HB3	2.51	0.40
2:E:32:TYR:CD2	2:E:98:ARG:HG3	2.56	0.40
3:F:139:TYR:HA	3:F:140:PRO:O	2.21	0.40
3:F:145:VAL:HA	3:F:194:GLU:O	2.21	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	442/465 (95%)	404 (91%)	32 (7%)	6 (1%)	11	20
1	B	439/465 (94%)	396 (90%)	39 (9%)	4 (1%)	17	31
2	C	219/222 (99%)	195 (89%)	18 (8%)	6 (3%)	5	7
2	E	219/222 (99%)	194 (89%)	18 (8%)	7 (3%)	4	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	209/211 (99%)	187 (90%)	16 (8%)	6 (3%)	4	6
3	F	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	15	28
All	All	1737/1796 (97%)	1567 (90%)	139 (8%)	31 (2%)	8	14

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL
2	C	140	ALA
3	D	7	SER
3	D	169	ASP
2	E	140	ALA
3	F	7	SER
1	A	458	ALA
2	C	65	LYS
3	D	67	GLY
3	D	80	GLU
2	E	122	ALA
1	A	171	ASP
2	C	136	SER
3	D	126	SER
2	E	65	LYS
1	A	107	SER
1	A	386	ALA
1	B	107	SER
3	F	126	SER
1	A	307	PHE
1	B	307	PHE
1	B	309	ALA
1	B	365	THR
2	C	31	ARG
2	C	109	ASP
2	E	136	SER
2	E	9	GLY
2	E	31	ARG
3	D	105	ILE
2	C	157	PRO
2	E	157	PRO

### 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	335/353 (95%)	318 (95%)	17 (5%)	24	45
1	B	332/353 (94%)	313 (94%)	19 (6%)	20	39
2	C	181/182 (100%)	174 (96%)	7 (4%)	32	57
2	E	181/182 (100%)	177 (98%)	4 (2%)	52	77
3	D	185/185 (100%)	181 (98%)	4 (2%)	52	77
3	F	185/185 (100%)	180 (97%)	5 (3%)	44	71
All	All	1399/1440 (97%)	1343 (96%)	56 (4%)	31	56

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	103	GLU
1	A	119	GLN
1	A	148	GLU
1	A	200	ILE
1	A	219	PHE
1	A	230	ARG
1	A	234	HIS
1	A	244	LEU
1	A	277	GLN
1	A	340	ARG
1	A	381	GLN
1	A	397	LEU
1	A	409	ILE
1	A	420	GLN
1	A	451	ARG
1	A	453	LEU
1	B	65	MET
1	B	74	ASN
1	B	103	GLU
1	B	148	GLU
1	B	168	LEU

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Mol	Chain	Res	Type
1	B	200	ILE
1	B	219	PHE
1	B	234	HIS
1	B	244	LEU
1	B	245	SER
1	B	277	GLN
1	B	340	ARG
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	451	ARG
1	B	453	LEU
1	B	457	GLU
2	C	66	ASP
2	C	151	LYS
2	C	155	PRO
2	C	157	PRO
2	C	185	LEU
2	C	203	CYS
2	C	204	ASN
3	D	46	TRP
3	D	81	ASP
3	D	95	GLN
3	D	189	ASN
2	E	151	LYS
2	E	157	PRO
2	E	203	CYS
2	E	204	ASN
3	F	15	PRO
3	F	60	ARG
3	F	77	MET
3	F	95	GLN
3	F	189	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	74	ASN
1	A	119	GLN
1	A	153	GLN

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Mol	Chain	Res	Type
1	A	157	ASN
1	A	207	GLN
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
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
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	172	HIS
3	D	6	GLN
3	D	36	GLN
3	D	136	ASN
3	D	137	ASN
3	D	189	ASN
2	E	39	GLN
2	E	172	HIS
3	F	6	GLN
3	F	36	GLN
3	F	37	GLN
3	F	89	GLN
3	F	136	ASN
3	F	189	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	444/465 (95%)	0.68	57 (12%) <b>3</b> <b>3</b>	44, 67, 95, 113	0
1	B	441/465 (94%)	0.68	58 (13%) <b>3</b> <b>3</b>	44, 66, 95, 112	0
2	C	221/222 (99%)	0.50	16 (7%) <b>15</b> <b>16</b>	40, 67, 92, 112	0
2	E	221/222 (99%)	0.54	19 (8%) <b>10</b> <b>10</b>	42, 67, 93, 112	0
3	D	211/211 (100%)	0.69	19 (9%) <b>9</b> <b>9</b>	46, 76, 95, 103	0
3	F	211/211 (100%)	0.38	15 (7%) <b>16</b> <b>16</b>	31, 62, 94, 104	0
All	All	1749/1796 (97%)	0.61	184 (10%) <b>6</b> <b>6</b>	31, 68, 95, 113	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	10.3
1	B	69	VAL	7.8
1	A	168	LEU	6.8
1	A	72	ALA	5.9
1	B	73	ASP	5.8
1	A	71	THR	5.5
2	C	139	ALA	5.3
1	B	70	HIS	5.3
1	B	75	TYR	5.3
2	E	65	LYS	5.0
1	A	146	GLY	5.0
1	B	307	PHE	5.0
1	B	71	THR	4.8
1	A	283	VAL	4.6
1	B	212	LEU	4.6
1	A	357	PHE	4.4
2	C	140	ALA	4.3
3	D	7	SER	4.2
3	F	152	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	137	ALA	4.1
1	B	68	LEU	4.0
3	F	149	ILE	4.0
1	B	356	ILE	4.0
1	B	357	PHE	3.9
1	B	18	ARG	3.9
1	A	458	ALA	3.9
2	E	181	ALA	3.9
1	A	282	ARG	3.9
1	A	145	LEU	3.8
1	A	19	ARG	3.8
1	A	165	ILE	3.8
1	A	445	TYR	3.7
1	A	354	GLY	3.7
3	D	22	THR	3.6
1	B	67	ALA	3.6
3	F	187	ARG	3.6
1	B	406	LEU	3.6
1	A	107	SER	3.5
1	B	445	TYR	3.5
1	B	359	PRO	3.4
2	C	108	PHE	3.4
3	D	58	PRO	3.3
1	B	167	ARG	3.3
3	D	68	THR	3.3
1	B	360	MET	3.3
1	A	407	THR	3.2
3	F	183	ASP	3.2
1	B	107	SER	3.2
3	D	70	TYR	3.2
1	A	398	LEU	3.2
3	F	156	ASN	3.2
1	A	356	ILE	3.1
1	A	17	ARG	3.1
1	B	168	LEU	3.1
1	B	358	ALA	3.1
1	B	19	ARG	3.1
1	A	288	ILE	3.1
2	E	139	ALA	3.1
1	A	70	HIS	3.1
2	E	13	GLN	3.1
1	B	65	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	75	TYR	3.0
2	C	31	ARG	3.0
1	B	74	ASN	3.0
2	E	15	GLY	3.0
1	A	358	ALA	3.0
1	A	212	LEU	2.9
2	E	86	VAL	2.9
2	E	85	LYS	2.9
1	B	457	GLU	2.9
1	A	285	GLY	2.9
1	A	355	GLY	2.9
3	F	155	GLN	2.9
1	B	279	LEU	2.8
1	B	166	PHE	2.8
2	E	64	LEU	2.8
3	D	202	SER	2.8
1	A	406	LEU	2.7
2	E	96	CYS	2.7
1	A	73	ASP	2.7
1	B	235	GLU	2.7
1	A	348	PHE	2.7
1	B	398	LEU	2.7
1	B	108	GLY	2.7
1	B	169	LYS	2.7
1	A	402	ILE	2.6
2	E	178	LEU	2.6
3	D	59	VAL	2.6
1	A	198	LEU	2.6
1	A	18	ARG	2.6
1	A	197	ILE	2.6
1	A	404	ALA	2.6
2	C	136	SER	2.6
3	D	1	ASP	2.6
3	F	211	ALA	2.6
1	A	201	ILE	2.6
2	C	166	SER	2.6
3	D	61	PHE	2.5
2	E	35	SER	2.5
1	B	146	GLY	2.5
1	B	402	ILE	2.5
3	F	153	GLU	2.5
2	C	35	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	199	PHE	2.5
1	B	348	PHE	2.5
1	B	399	ALA	2.5
1	A	149	GLY	2.4
3	F	181	THR	2.4
1	B	290	LYS	2.4
1	A	456	GLN	2.4
1	B	444	LEU	2.4
3	F	180	LEU	2.4
1	A	148	GLU	2.4
3	D	15	PRO	2.4
1	A	459	GLU	2.4
1	B	110	PRO	2.3
1	A	460	GLN	2.3
1	B	198	LEU	2.3
1	B	66	GLY	2.3
1	A	167	ARG	2.3
3	D	69	SER	2.3
3	D	138	PHE	2.3
1	B	410	ILE	2.3
1	B	404	ALA	2.3
2	C	141	ALA	2.3
1	A	360	MET	2.3
2	C	138	ALA	2.3
1	B	149	GLY	2.2
3	D	16	GLY	2.2
1	A	109	ILE	2.2
2	C	48	ILE	2.2
1	B	199	PHE	2.2
1	A	147	ARG	2.2
1	B	282	ARG	2.2
3	D	67	GLY	2.2
3	D	27	SER	2.2
3	F	147	TRP	2.2
3	D	140	PRO	2.2
2	C	2	VAL	2.2
1	B	145	LEU	2.2
1	B	171	ASP	2.2
2	C	47	TRP	2.2
1	A	106	GLY	2.2
1	A	286	GLY	2.2
1	A	408	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	31	ARG	2.2
3	F	154	ARG	2.2
1	B	335	PHE	2.2
1	A	150	PRO	2.2
2	E	16	GLY	2.2
2	C	29	TYR	2.2
2	E	201	VAL	2.2
1	B	397	LEU	2.2
2	C	65	LYS	2.1
3	F	7	SER	2.2
2	E	97	ALA	2.1
3	D	13	ALA	2.1
1	B	109	ILE	2.1
1	B	201	ILE	2.1
1	A	190	PHE	2.1
1	A	287	ASN	2.1
1	A	108	GLY	2.1
3	D	77	MET	2.1
1	B	409	ILE	2.1
1	B	150	PRO	2.1
2	E	12	VAL	2.1
1	B	197	ILE	2.1
2	E	121	SER	2.1
1	A	307	PHE	2.1
1	B	95	PHE	2.1
1	B	438	PHE	2.1
1	B	23	ARG	2.1
3	F	182	LYS	2.0
1	B	347	CYS	2.0
2	E	140	ALA	2.0
1	A	377	GLU	2.0
3	F	209	ASN	2.0
1	A	21	LEU	2.0
1	A	186	LEU	2.0
1	A	194	LEU	2.0
1	A	200	ILE	2.0
2	E	11	LEU	2.0
2	C	73	ASP	2.0
3	D	198	LYS	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	466	1/1	0.83	0.24	52,52,52,52	0
4	CL	B	467	1/1	0.89	0.20	60,60,60,60	0
4	CL	A	466	1/1	0.97	0.24	61,61,61,61	0
4	CL	A	467	1/1	0.98	0.10	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.