



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:58 am GMT

PDB ID : 3EJY
Title : Structure of E203H mutant of E.coli Cl⁻/H⁺ antiporter, CLC-ec1
Authors : Lim, H.-H.; Miller, C.
Deposited on : 2008-09-18
Resolution : 3.20 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

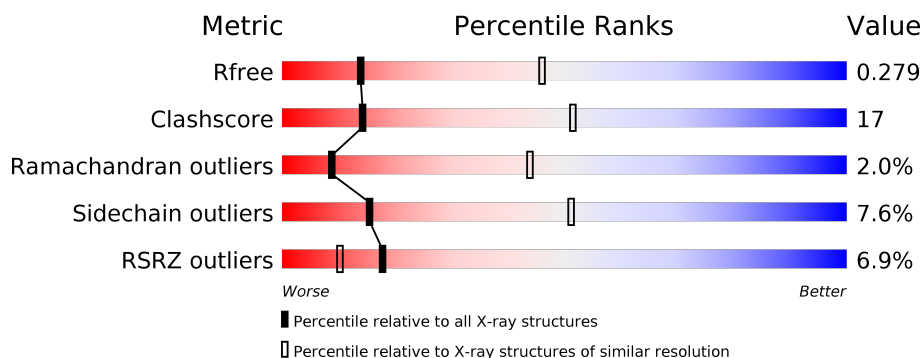
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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

Mol	Chain	Length	Quality of chain
1	A	473	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>6%</div> </div> </div>
1	B	473	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>7%</div> </div> </div>
2	C	221	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>6%</div> </div> </div>
2	E	221	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>5%</div> </div> </div>
3	D	211	<div> <div>8%</div> <div> <div></div> <div>55%</div> <div>43%</div> <div></div> </div> </div>
3	F	211	<div> <div>15%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div></div> </div> </div>

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	501	-	-	-	X
4	BR	B	503	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13218 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
			3334	2191	562	561	20			
1	B	440	Total	C	N	O	S	0	0	0
			3294	2169	551	554	20			

There are 2 discrepancies between the modelled and reference sequences:

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

Continued on next page...

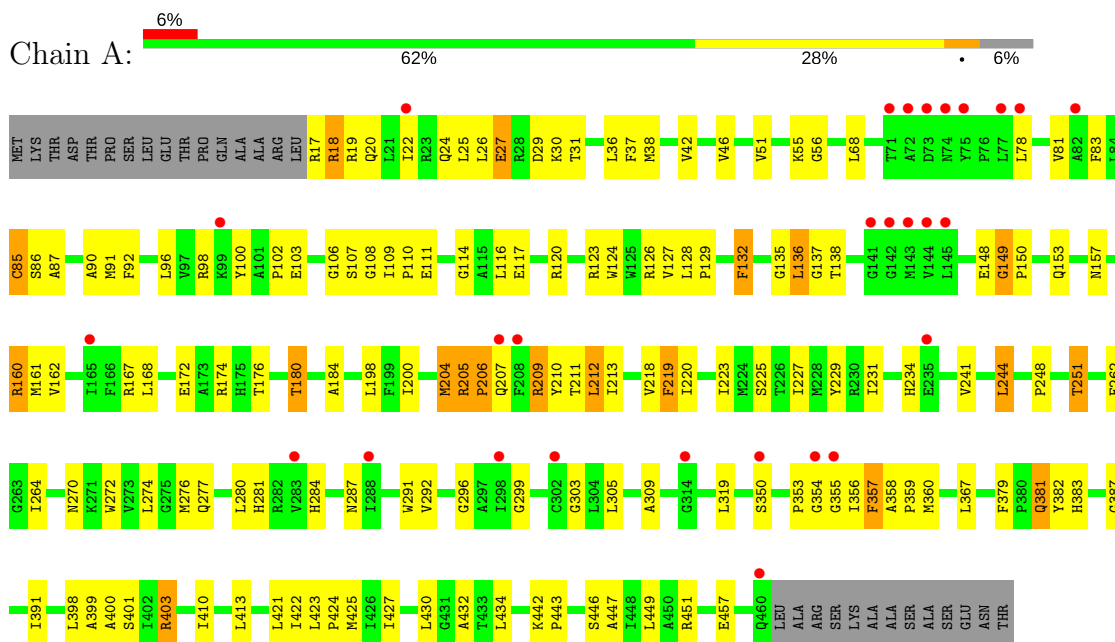
Continued from previous page...

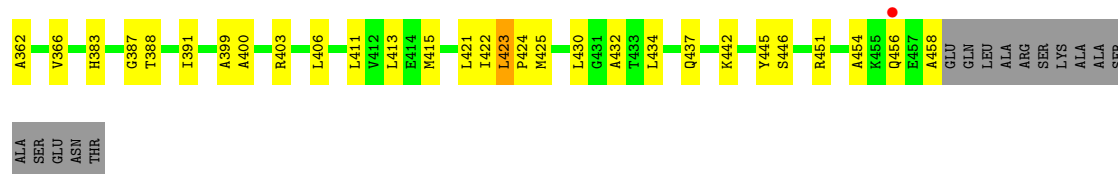
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Br	0	0
			2	2		

3 Residue-property plots [i](#)

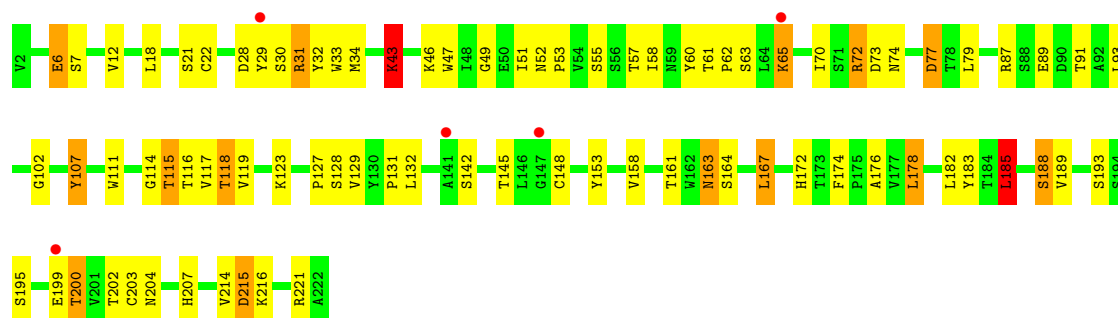
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

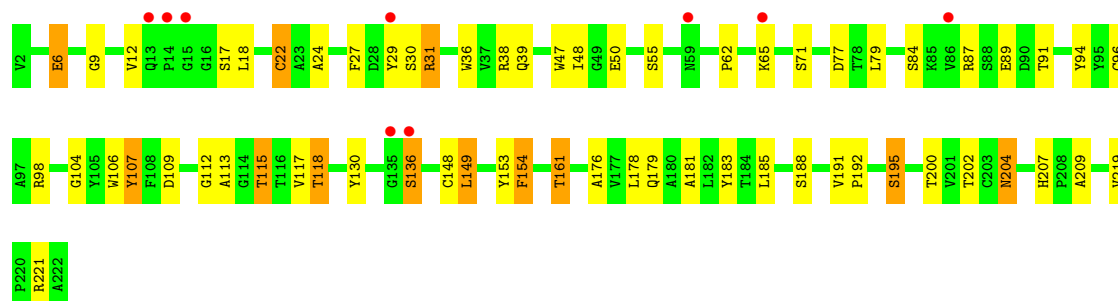




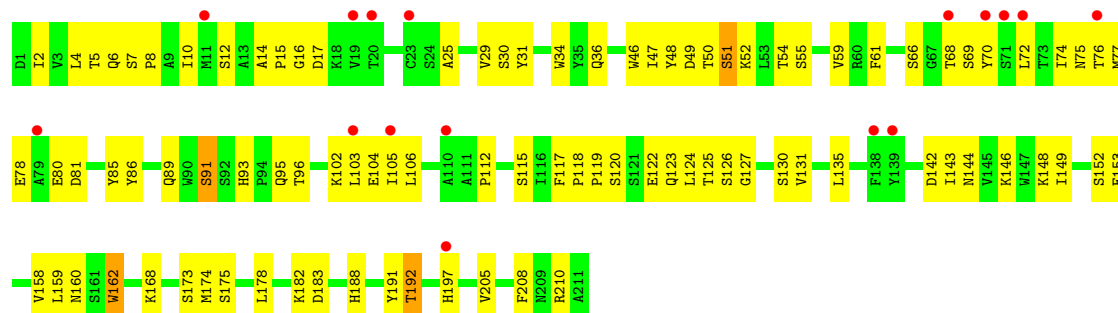
- Molecule 2: Fab fragment, Heavy chain



- Molecule 2: Fab fragment, Heavy chain

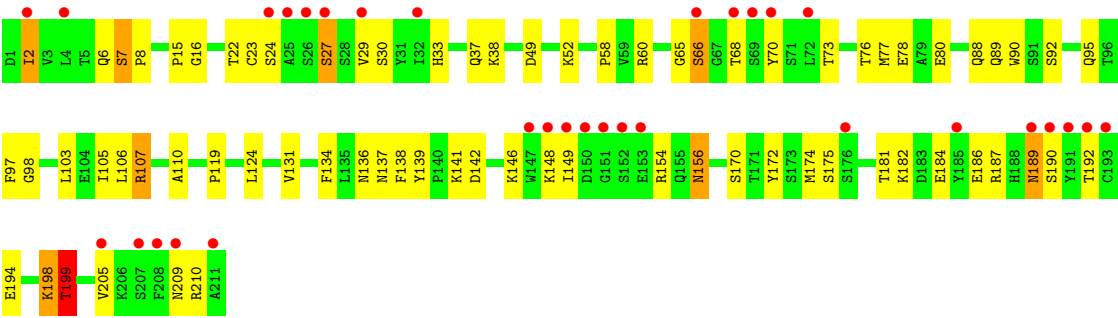


- Molecule 3: Fab fragment, Light chain



- Molecule 3: Fab fragment, Light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.52Å 96.83Å 172.79Å 90.00° 132.81° 90.00°	Depositor
Resolution (Å)	58.52 – 3.20 57.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (58.52-3.20) 99.6 (57.87-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.244 , 0.279 0.237 , 0.279	Depositor DCC
R_{free} test set	2358 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13218	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.48	0/3407	0.59	1/4624 (0.0%)
1	B	0.49	0/3367	0.59	1/4572 (0.0%)
2	C	0.55	0/1721	0.67	1/2355 (0.0%)
2	E	0.51	0/1721	0.67	3/2355 (0.1%)
3	D	0.45	0/1660	0.61	0/2257
3	F	0.48	0/1660	0.63	0/2257
All	All	0.49	0/13536	0.62	6/18420 (0.0%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	GLN	N-CA-C	6.63	128.91	111.00
2	E	154	PHE	C-N-CD	6.48	142.01	128.40
2	E	154	PHE	N-CA-C	6.41	128.32	111.00
2	E	154	PHE	N-CA-CB	5.46	120.44	110.60
1	A	18	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	C	185	LEU	CA-CB-CG	5.07	126.96	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	154	PHE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	23	ARG	Peptide

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	3334	0	3483	137	0
1	B	3294	0	3444	149	0
2	C	1672	0	1654	69	0
2	E	1672	0	1654	41	0
3	D	1621	0	1546	58	0
3	F	1621	0	1546	57	0
4	A	2	0	0	2	0
4	B	2	0	0	6	0
All	All	13218	0	13327	461	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 17.

All (461) 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:F:7:SER:HB3	3:F:8:PRO:HD3	1.26	1.12
1:B:107:SER:OG	4:B:503:BR:BR	2.21	1.10
3:F:7:SER:HB2	3:F:22:THR:H	1.15	1.10
3:F:7:SER:HB3	3:F:8:PRO:CD	1.86	1.05
2:E:31:ARG:HH11	2:E:31:ARG:HG2	1.22	1.03
3:F:7:SER:CB	3:F:8:PRO:HD3	1.89	1.02
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.22	1.01
3:D:95:GLN:N	3:D:95:GLN:OE1	2.04	0.91
2:E:39:GLN:HE22	3:F:37:GLN:HE22	1.07	0.91
1:A:205:ARG:HG2	1:A:205:ARG:HH11	1.36	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:GLN:N	3:F:95:GLN:OE1	2.05	0.89
1:A:206:PRO:HD2	1:A:211:THR:HG21	1.55	0.88
2:E:31:ARG:HH11	2:E:31:ARG:CG	1.85	0.88
1:B:81:VAL:O	1:B:85:CYS:HB2	1.76	0.85
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.61	0.82
2:C:30:SER:O	2:C:31:ARG:HB2	1.78	0.81
1:B:38:MET:O	1:B:42:VAL:HG23	1.81	0.81
1:B:200:ILE:HA	1:B:204:MET:HB3	1.64	0.80
1:B:206:PRO:HD2	1:B:211:THR:HG21	1.63	0.79
2:E:39:GLN:NE2	3:F:37:GLN:HE22	1.80	0.79
3:F:7:SER:HB2	3:F:22:THR:N	1.97	0.78
2:C:158:VAL:HG12	2:C:207:HIS:HB2	1.66	0.78
1:A:81:VAL:O	1:A:85:CYS:HB2	1.84	0.77
1:A:26:LEU:O	1:A:27:GLU:HB2	1.85	0.77
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.67	0.77
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.85	0.76
1:A:430:LEU:HD13	1:B:219:PHE:HB3	1.64	0.76
1:A:449:LEU:CD2	1:B:25:LEU:HD11	2.16	0.75
3:F:7:SER:CB	3:F:22:THR:H	1.97	0.75
1:A:205:ARG:NH1	1:A:205:ARG:HG2	2.01	0.75
1:B:205:ARG:HB3	1:B:207:GLN:NE2	2.00	0.75
2:C:72:ARG:HD3	2:C:74:ASN:HD21	1.51	0.74
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.51	0.74
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.69	0.74
2:C:204:ASN:HD22	2:C:215:ASP:HB3	1.52	0.74
1:A:449:LEU:HD23	1:B:25:LEU:HD11	1.69	0.73
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.70	0.73
2:C:72:ARG:CD	2:C:74:ASN:HD21	2.02	0.72
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.24	0.72
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.72	0.72
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.70	0.72
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.53	0.72
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.24	0.72
2:E:39:GLN:HE22	3:F:37:GLN:NE2	1.86	0.71
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.05	0.71
1:A:42:VAL:HG22	1:A:162:VAL:HG21	1.72	0.71
1:B:288:ILE:O	1:B:288:ILE:HG13	1.91	0.71
2:C:163:ASN:ND2	2:C:167:LEU:HD23	2.06	0.71
3:F:107:ARG:HH21	3:F:110:ALA:HB2	1.55	0.70
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.57	0.70
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:SER:HA	2:C:115:THR:HG21	1.74	0.69
2:C:61:THR:C	2:C:63:SER:H	1.95	0.69
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.27	0.69
3:F:89:GLN:O	3:F:95:GLN:HB2	1.93	0.69
1:A:86:SER:OG	1:A:303:GLY:HA3	1.93	0.69
1:A:422:ILE:HA	1:A:425:MET:HE3	1.74	0.69
2:C:163:ASN:HD22	2:C:167:LEU:HD23	1.57	0.68
2:E:31:ARG:NH1	2:E:31:ARG:HG2	2.01	0.68
1:A:274:LEU:HA	1:A:277:GLN:HE21	1.56	0.68
1:B:26:LEU:O	1:B:27:GLU:HB2	1.93	0.68
2:C:87:ARG:HB3	2:C:89:GLU:OE1	1.94	0.68
2:C:32:TYR:O	2:C:72:ARG:NH2	2.22	0.67
1:A:447:ALA:O	1:A:451:ARG:HG3	1.95	0.67
1:B:357:PHE:HE2	1:B:445:TYR:HE2	1.43	0.67
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.75	0.66
2:C:61:THR:HG23	2:C:63:SER:HB3	1.77	0.66
1:B:24:GLN:HG2	1:B:25:LEU:HG	1.77	0.66
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.78	0.66
3:D:4:LEU:HD23	3:D:25:ALA:HB2	1.77	0.66
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.76	0.65
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.26	0.65
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.78	0.65
1:A:200:ILE:HA	1:A:204:MET:HB3	1.78	0.65
2:C:43:LYS:HE3	2:C:46:LYS:HE3	1.77	0.65
3:D:146:LYS:HD2	3:D:153:GLU:OE2	1.96	0.65
1:B:280:LEU:HD13	1:B:350:SER:HB3	1.78	0.65
2:C:61:THR:O	2:C:63:SER:N	2.30	0.65
1:B:132:PHE:O	1:B:136:LEU:HB2	1.97	0.64
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.79	0.64
1:A:205:ARG:CG	1:A:205:ARG:HH11	2.10	0.64
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.80	0.64
3:F:49:ASP:HB2	3:F:52:LYS:HE3	1.79	0.64
2:C:72:ARG:HD3	2:C:74:ASN:ND2	2.12	0.64
1:B:176:THR:O	1:B:180:THR:HG23	1.97	0.63
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.80	0.63
1:B:272:TRP:O	1:B:276:MET:HB2	1.99	0.63
2:E:31:ARG:NH1	2:E:31:ARG:CG	2.52	0.63
1:B:27:GLU:HG3	1:B:30:LYS:HD3	1.79	0.62
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.63	0.62
3:F:27:SER:O	3:F:68:THR:HG22	1.99	0.62
3:F:6:GLN:HE21	3:F:98:GLY:CA	2.07	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD13	1:A:350:SER:HB3	1.82	0.61
1:A:176:THR:O	1:A:180:THR:HG23	2.01	0.60
1:A:20:GLN:O	1:A:24:GLN:HG2	2.01	0.60
2:C:204:ASN:ND2	2:C:215:ASP:HB3	2.16	0.60
3:F:2:ILE:HG21	3:F:29:VAL:HG13	1.83	0.60
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.84	0.60
1:A:42:VAL:CG2	1:A:162:VAL:HG21	2.31	0.60
1:B:205:ARG:NH2	1:B:210:TYR:HA	2.17	0.60
1:B:22:ILE:HA	1:B:24:GLN:NE2	2.17	0.59
3:F:6:GLN:NE2	3:F:98:GLY:HA3	2.06	0.59
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.84	0.59
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.68	0.59
3:D:188:HIS:O	3:D:210:ARG:NH1	2.35	0.59
2:E:188:SER:HB2	3:F:134:PHE:CE2	2.38	0.59
1:A:184:ALA:HB1	1:A:225:SER:CB	2.32	0.59
2:E:38:ARG:HD3	2:E:48:ILE:HD11	1.84	0.58
3:D:48:TYR:CE1	3:D:52:LYS:HE3	2.38	0.58
1:B:86:SER:HB3	1:B:299:GLY:O	2.04	0.58
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.85	0.58
3:F:149:ILE:HD12	3:F:154:ARG:HD3	1.84	0.58
1:B:90:ALA:HB3	1:B:296:GLY:HA2	1.84	0.58
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.84	0.58
1:A:86:SER:HB3	1:A:299:GLY:O	2.03	0.58
1:A:209:ARG:HA	1:B:210:TYR:HB2	1.86	0.58
3:D:160:ASN:HA	3:D:175:SER:O	2.04	0.57
3:D:149:ILE:HG23	3:D:191:TYR:CE2	2.39	0.57
3:D:31:TYR:HA	3:D:50:THR:OG1	2.03	0.57
1:A:272:TRP:O	1:A:276:MET:HB2	2.03	0.57
1:A:280:LEU:CD1	1:A:350:SER:HB3	2.33	0.57
1:A:207:GLN:HG3	1:B:28:ARG:HH12	1.69	0.57
2:C:172:HIS:CD2	3:D:173:SER:OG	2.57	0.57
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.40	0.57
3:F:136:ASN:HB3	3:F:137:ASN:HD22	1.68	0.57
1:A:18:ARG:HH22	1:B:456:GLN:HB3	1.69	0.57
1:A:91:MET:CG	1:A:296:GLY:HA3	2.34	0.57
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.87	0.57
3:F:124:LEU:HB3	3:F:182:LYS:HE3	1.86	0.57
1:B:100:TYR:O	1:B:126:ARG:NH1	2.35	0.57
1:A:205:ARG:O	1:A:207:GLN:HG2	2.03	0.57
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.86	0.57
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.87	0.57
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.85	0.57
1:B:205:ARG:HB3	1:B:207:GLN:HE22	1.68	0.56
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.39	0.56
1:B:355:GLY:CA	4:B:503:BR:BR	3.09	0.56
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.88	0.56
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.87	0.56
3:D:162:TRP:HE3	3:D:162:TRP:H	1.54	0.56
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.35	0.56
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.88	0.56
1:A:17:ARG:HH22	1:B:118:ASP:HB2	1.70	0.56
2:C:172:HIS:HB2	2:C:188:SER:HB3	1.87	0.56
1:A:379:PHE:HA	1:A:381:GLN:NE2	2.20	0.56
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.40	0.56
2:C:93:LEU:HD13	2:C:116:THR:HG23	1.86	0.56
3:F:107:ARG:NH2	3:F:110:ALA:HB2	2.20	0.56
1:A:132:PHE:O	1:A:136:LEU:HB2	2.06	0.55
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.88	0.55
1:A:205:ARG:HB3	1:A:207:GLN:NE2	2.22	0.55
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.89	0.55
3:D:89:GLN:NE2	3:D:95:GLN:HA	2.22	0.55
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.39	0.55
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.75	0.54
3:F:7:SER:OG	3:F:8:PRO:HD3	2.07	0.54
1:B:148:GLU:O	1:B:152:VAL:HG23	2.07	0.54
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.88	0.54
1:A:25:LEU:HB3	1:B:446:SER:HB3	1.89	0.54
1:A:305:LEU:O	1:A:309:ALA:O	2.25	0.54
2:C:131:PRO:HD3	2:C:216:LYS:HG2	1.90	0.54
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.89	0.54
2:E:6:GLU:OE2	2:E:112:GLY:HA3	2.07	0.54
1:B:184:ALA:HB1	1:B:225:SER:CB	2.37	0.54
1:B:42:VAL:O	1:B:46:VAL:HG23	2.08	0.54
3:D:16:GLY:HA2	3:D:76:THR:HA	1.89	0.54
3:D:2:ILE:O	3:D:96:THR:HG21	2.09	0.53
1:A:124:TRP:CZ3	1:A:161:MET:HG3	2.44	0.53
2:C:72:ARG:CD	2:C:74:ASN:ND2	2.70	0.53
1:A:284:HIS:O	1:A:287:ASN:HB3	2.08	0.53
1:B:421:LEU:O	1:B:425:MET:HG3	2.07	0.53
1:B:60:LEU:O	1:B:64:ARG:HG3	2.09	0.53
3:F:77:MET:SD	3:F:103:LEU:HD21	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD13	1:B:434:LEU:HD21	1.90	0.53
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.24	0.53
1:A:210:TYR:HB2	1:B:209:ARG:HA	1.91	0.53
1:B:356:ILE:N	4:B:503:BR:BR	2.90	0.53
1:B:25:LEU:O	1:B:28:ARG:HB2	2.09	0.53
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.91	0.53
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.44	0.53
2:E:30:SER:O	2:E:31:ARG:HB2	2.09	0.53
1:A:274:LEU:HA	1:A:277:GLN:NE2	2.24	0.53
1:A:381:GLN:NE2	1:A:381:GLN:H	2.07	0.52
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.74	0.52
1:B:116:LEU:HB3	1:B:206:PRO:HG3	1.92	0.52
2:C:28:ASP:O	2:C:30:SER:O	2.26	0.52
2:C:7:SER:CA	2:C:115:THR:HG21	2.40	0.52
3:D:4:LEU:CD2	3:D:25:ALA:HB2	2.39	0.52
1:A:356:ILE:HG23	1:A:360:MET:CE	2.40	0.52
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.90	0.52
3:D:66:SER:HA	3:D:70:TYR:CZ	2.44	0.52
2:C:52:ASN:ND2	2:C:57:THR:HB	2.25	0.52
2:E:38:ARG:HD2	2:E:94:TYR:CE1	2.45	0.52
1:B:305:LEU:O	1:B:309:ALA:O	2.28	0.52
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.92	0.52
1:A:100:TYR:O	1:A:126:ARG:HD3	2.11	0.51
1:A:106:GLY:HA3	4:A:502:BR:BR	2.65	0.51
1:B:399:ALA:O	1:B:403:ARG:HA	2.09	0.51
1:A:124:TRP:CE3	1:A:161:MET:HG3	2.45	0.51
1:A:205:ARG:HG3	1:A:213:ILE:HD12	1.92	0.51
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.25	0.51
3:D:120:SER:HB2	3:D:123:GLN:H	1.74	0.51
2:C:91:THR:HG23	2:C:118:THR:HA	1.91	0.51
2:C:60:TYR:CE2	2:C:70:ILE:HG13	2.38	0.51
3:F:189:ASN:HA	3:F:210:ARG:HD3	1.92	0.51
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.92	0.51
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.93	0.51
3:F:29:VAL:HG11	3:F:89:GLN:HG2	1.93	0.51
1:B:109:ILE:HD12	4:B:503:BR:BR	2.66	0.51
1:B:148:GLU:CD	1:B:148:GLU:H	2.14	0.50
2:E:6:GLU:HA	2:E:22:CYS:HA	1.91	0.50
2:C:29:TYR:HB3	2:C:77:ASP:OD2	2.11	0.50
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.46	0.50
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:O	1:A:251:THR:HG22	2.10	0.50
3:F:107:ARG:O	3:F:139:TYR:CE2	2.65	0.50
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.93	0.50
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.93	0.50
2:C:61:THR:C	2:C:63:SER:N	2.64	0.50
1:A:210:TYR:N	1:B:210:TYR:HB2	2.27	0.50
1:B:274:LEU:HA	1:B:277:GLN:NE2	2.27	0.50
3:F:198:LYS:O	3:F:199:THR:HG23	2.10	0.50
1:A:274:LEU:HD23	1:A:277:GLN:HE22	1.77	0.49
1:B:288:ILE:O	1:B:288:ILE:CG1	2.58	0.49
2:E:91:THR:HG23	2:E:118:THR:HA	1.94	0.49
1:B:108:GLY:HA3	1:B:153:GLN:NE2	2.27	0.49
3:D:14:ALA:O	3:D:17:ASP:HB2	2.12	0.49
1:B:119:GLN:O	1:B:120:ARG:HD2	2.13	0.49
1:B:138:THR:HG22	1:B:143:MET:SD	2.53	0.49
1:A:449:LEU:HD22	1:B:25:LEU:HD11	1.92	0.49
3:D:120:SER:HB3	3:D:122:GLU:OE1	2.12	0.49
3:F:2:ILE:HG21	3:F:29:VAL:CG1	2.41	0.49
1:A:160:ARG:HH21	1:A:174:ARG:HD2	1.78	0.49
1:A:116:LEU:HB3	1:A:206:PRO:HG3	1.95	0.49
1:A:244:LEU:HD11	1:A:387:GLY:HA3	1.94	0.49
1:A:37:PHE:HD2	1:A:38:MET:CE	2.26	0.49
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.43	0.49
1:A:90:ALA:HB2	1:A:299:GLY:HA3	1.94	0.49
2:C:174:PHE:CD1	3:D:175:SER:HB2	2.47	0.49
1:A:109:ILE:N	1:A:110:PRO:CD	2.75	0.48
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.77	0.48
1:B:356:ILE:HG23	1:B:360:MET:CE	2.42	0.48
1:B:454:ALA:O	1:B:458:ALA:HB3	2.12	0.48
1:A:42:VAL:O	1:A:46:VAL:HG23	2.13	0.48
2:E:179:GLN:HG3	2:E:179:GLN:O	2.13	0.48
2:C:91:THR:HA	2:C:117:VAL:O	2.13	0.48
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.95	0.48
3:F:38:LYS:NZ	3:F:80:GLU:O	2.41	0.48
3:F:24:SER:HA	3:F:68:THR:O	2.13	0.48
1:B:244:LEU:HD11	1:B:387:GLY:HA3	1.94	0.48
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.49	0.48
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.39	0.48
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.39	0.48
3:F:189:ASN:ND2	3:F:209:ASN:HB2	2.29	0.48
3:D:143:ILE:C	3:D:144:ASN:HD22	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HA	1:A:212:LEU:HB2	1.96	0.47
1:A:51:VAL:O	1:A:55:LYS:HG2	2.13	0.47
1:B:205:ARG:HH11	1:B:207:GLN:NE2	2.12	0.47
2:C:7:SER:HA	2:C:115:THR:CG2	2.43	0.47
1:B:264:ILE:O	1:B:267:PRO:HD2	2.14	0.47
1:A:24:GLN:HB3	1:B:208:PHE:HZ	1.79	0.47
1:A:68:LEU:HD22	1:A:78:LEU:HG	1.96	0.47
1:B:287:ASN:ND2	1:B:290:LYS:H	2.12	0.47
2:C:195:SER:O	2:C:199:GLU:HB3	2.15	0.47
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.96	0.47
1:B:202:GLU:HG3	1:B:406:LEU:HB3	1.96	0.47
3:D:54:THR:HG22	3:D:55:SER:H	1.80	0.47
3:D:54:THR:HG22	3:D:55:SER:N	2.30	0.47
2:E:6:GLU:OE2	2:E:113:ALA:N	2.48	0.47
1:A:135:GLY:C	1:A:137:GLY:N	2.68	0.47
1:A:274:LEU:HD23	1:A:277:GLN:NE2	2.30	0.47
1:B:206:PRO:HB2	1:B:209:ARG:HH12	1.80	0.47
1:B:274:LEU:HD22	1:B:451:ARG:HD3	1.97	0.47
1:A:399:ALA:O	1:A:403:ARG:HA	2.15	0.47
1:A:403:ARG:NH1	1:B:29:ASP:OD2	2.48	0.47
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.15	0.47
1:B:77:LEU:O	1:B:81:VAL:HG23	2.15	0.47
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.50	0.47
2:C:6:GLU:HA	2:C:22:CYS:HA	1.97	0.47
1:A:90:ALA:HB3	1:A:296:GLY:HA2	1.98	0.46
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.96	0.46
1:B:355:GLY:HA3	4:B:503:BR:BR	2.71	0.46
1:A:381:GLN:HG3	3:D:93:HIS:HB2	1.96	0.46
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.97	0.46
1:A:27:GLU:HG3	1:A:30:LYS:HD3	1.98	0.46
2:C:200:THR:HG22	2:C:200:THR:O	2.16	0.46
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.97	0.46
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.97	0.46
3:F:15:PRO:HD3	3:F:105:ILE:HG23	1.98	0.46
3:D:95:GLN:CD	3:D:95:GLN:H	2.10	0.46
1:B:197:ILE:HG21	1:B:219:PHE:CE1	2.51	0.46
2:E:104:GLY:O	2:E:106:TRP:CD1	2.68	0.46
3:F:23:CYS:N	3:F:70:TYR:O	2.30	0.46
1:B:72:ALA:HA	1:B:78:LEU:HD12	1.98	0.46
2:C:107:TYR:CD1	2:C:107:TYR:C	2.90	0.46
2:E:130:TYR:HD2	2:E:149:LEU:HD23	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HB	1:A:218:VAL:HA	1.98	0.45
1:B:83:PHE:CD2	1:B:83:PHE:C	2.90	0.45
3:D:77:MET:SD	3:D:103:LEU:HD21	2.56	0.45
2:E:6:GLU:OE1	2:E:96:CYS:N	2.42	0.45
2:E:38:ARG:HD2	2:E:94:TYR:CZ	2.51	0.45
3:F:58:PRO:HB2	3:F:60:ARG:HG3	1.98	0.45
1:A:205:ARG:HH21	1:B:205:ARG:NH2	2.14	0.45
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.30	0.45
2:C:111:TRP:N	2:C:111:TRP:CD1	2.84	0.45
2:E:153:TYR:CE1	2:E:183:TYR:HB2	2.52	0.45
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.45	0.45
1:B:91:MET:HG2	1:B:292:VAL:O	2.16	0.45
3:D:112:PRO:HD3	3:D:197:HIS:CD2	2.51	0.45
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.98	0.45
2:C:132:LEU:O	3:D:117:PHE:CE2	2.69	0.45
2:E:36:TRP:HE1	2:E:79:LEU:HG	1.81	0.45
1:A:227:ILE:O	1:A:231:ILE:HG12	2.16	0.45
1:A:29:ASP:OD2	1:B:403:ARG:NH1	2.49	0.45
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.51	0.45
2:C:87:ARG:CB	2:C:89:GLU:OE1	2.64	0.45
3:D:124:LEU:O	3:D:127:GLY:N	2.48	0.45
2:E:178:LEU:HD11	2:E:181:ALA:HA	1.98	0.45
1:A:262:PHE:CE2	1:A:367:LEU:HD23	2.52	0.45
1:A:434:LEU:HD21	1:B:36:LEU:HD13	1.99	0.45
1:B:357:PHE:HE2	1:B:445:TYR:CE2	2.28	0.45
3:D:77:MET:HG2	3:D:78:GLU:N	2.32	0.45
1:A:205:ARG:HB3	1:A:207:GLN:CD	2.37	0.45
1:A:22:ILE:C	1:A:24:GLN:H	2.20	0.45
1:A:87:ALA:O	1:A:91:MET:HG3	2.17	0.45
2:C:29:TYR:HE2	2:C:74:ASN:HD22	1.65	0.45
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.52	0.45
2:E:87:ARG:CZ	2:E:89:GLU:HB2	2.47	0.45
3:F:174:MET:HG2	3:F:175:SER:N	2.31	0.45
1:A:117:GLU:OE1	1:A:206:PRO:HB3	2.17	0.45
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.99	0.45
1:B:403:ARG:NH2	1:B:437:GLN:HA	2.31	0.45
2:C:129:VAL:O	2:C:216:LYS:HE3	2.17	0.45
1:A:421:LEU:O	1:A:425:MET:HG3	2.16	0.44
1:B:160:ARG:NH2	1:B:174:ARG:HD2	2.32	0.44
3:D:127:GLY:HA2	3:D:182:LYS:HB2	1.99	0.44
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ILE:N	1:B:110:PRO:CD	2.80	0.44
2:C:72:ARG:HH11	2:C:74:ASN:HD21	1.65	0.44
3:D:31:TYR:HD2	3:D:49:ASP:HB3	1.81	0.44
1:A:211:THR:HB	1:A:213:ILE:HG13	1.99	0.44
1:A:356:ILE:HG23	1:A:360:MET:HE1	1.99	0.44
1:B:144:VAL:O	1:B:144:VAL:HG12	2.18	0.44
3:D:10:ILE:HG23	3:D:102:LYS:HB3	1.99	0.44
3:F:186:GLU:HG2	3:F:210:ARG:HH22	1.82	0.44
1:A:135:GLY:O	1:A:137:GLY:N	2.50	0.44
1:A:92:PHE:C	1:A:92:PHE:CD2	2.91	0.44
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.18	0.44
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.53	0.44
1:B:38:MET:O	1:B:41:VAL:HG22	2.18	0.44
3:F:106:LEU:HA	3:F:139:TYR:OH	2.18	0.44
2:C:161:THR:O	2:C:204:ASN:HB2	2.17	0.44
2:C:6:GLU:HA	2:C:21:SER:O	2.18	0.44
3:D:130:SER:HA	3:D:178:LEU:O	2.16	0.44
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.52	0.44
1:A:212:LEU:HD12	1:A:212:LEU:N	2.33	0.44
1:A:355:GLY:CA	4:A:501:BR:BR	3.21	0.44
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.18	0.44
2:C:12:VAL:CG2	2:C:119:VAL:HG22	2.46	0.44
1:A:210:TYR:HB2	1:B:210:TYR:N	2.33	0.44
1:A:209:ARG:C	1:B:210:TYR:HB2	2.38	0.43
1:B:355:GLY:HA2	4:B:503:BR:BR	2.73	0.43
1:B:51:VAL:O	1:B:55:LYS:HG2	2.18	0.43
1:B:83:PHE:HB2	1:B:304:LEU:HD12	2.00	0.43
2:C:93:LEU:HD11	2:C:114:GLY:HA3	2.00	0.43
1:A:19:ARG:HA	1:A:22:ILE:HD12	1.99	0.43
1:B:235:GLU:OE2	2:C:102:GLY:HA2	2.17	0.43
1:B:413:LEU:HD22	1:B:422:ILE:HD13	2.00	0.43
1:A:135:GLY:C	1:A:137:GLY:H	2.22	0.43
1:A:91:MET:HG2	1:A:292:VAL:O	2.18	0.43
1:B:148:GLU:CG	1:B:190:PHE:CZ	3.00	0.43
2:C:29:TYR:HE2	2:C:74:ASN:ND2	2.16	0.43
2:C:221:ARG:HH22	3:D:120:SER:HA	1.84	0.43
3:D:125:THR:O	3:D:126:SER:CB	2.66	0.43
3:D:158:VAL:O	3:D:159:LEU:HD23	2.19	0.43
1:A:148:GLU:OE1	1:A:357:PHE:HB2	2.18	0.43
1:B:205:ARG:HH21	1:B:210:TYR:HA	1.82	0.43
1:B:172:GLU:HA	1:B:212:LEU:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLY:CA	1:A:449:LEU:HD11	2.49	0.43
3:F:141:LYS:HB3	3:F:172:TYR:CE1	2.54	0.43
3:D:30:SER:H	3:D:91:SER:CB	2.32	0.43
3:D:61:PHE:HD2	3:D:72:LEU:HD21	1.84	0.43
3:F:194:GLU:HG2	3:F:205:VAL:HG12	2.01	0.43
1:A:56:GLY:HA3	1:A:136:LEU:HD11	2.01	0.43
1:A:148:GLU:O	1:A:149:GLY:C	2.57	0.43
1:B:68:LEU:HD21	1:B:82:ALA:HB2	2.00	0.43
1:B:411:LEU:O	1:B:415:MET:HG3	2.19	0.43
1:B:75:TYR:HB3	1:B:76:PRO:HD3	2.01	0.43
2:C:142:SER:O	2:C:193:SER:HB2	2.18	0.42
3:D:36:GLN:HB2	3:D:85:TYR:HE2	1.80	0.42
1:A:22:ILE:O	1:A:24:GLN:N	2.45	0.42
1:B:138:THR:O	1:B:143:MET:HB2	2.19	0.42
1:B:317:PHE:HA	1:B:320:ILE:HD12	2.00	0.42
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.87	0.42
3:D:30:SER:HB3	3:D:31:TYR:HD1	1.85	0.42
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.83	0.42
3:D:50:THR:O	3:D:51:SER:HB3	2.19	0.42
1:A:209:ARG:HA	1:B:210:TYR:CB	2.49	0.42
1:A:270:ASN:HD21	1:A:401:SER:HB3	1.84	0.42
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.19	0.42
1:B:362:ALA:O	1:B:366:VAL:HG23	2.20	0.42
2:C:145:THR:HG22	3:D:117:PHE:HZ	1.85	0.42
3:F:107:ARG:O	3:F:139:TYR:HE2	2.03	0.42
1:A:446:SER:HB3	1:B:25:LEU:HB3	2.00	0.42
2:E:9:GLY:H	2:E:115:THR:HG21	1.84	0.42
1:B:128:LEU:CB	1:B:129:PRO:CD	2.96	0.42
1:B:148:GLU:HG2	1:B:190:PHE:CZ	2.55	0.42
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.55	0.42
2:E:161:THR:HG23	2:E:204:ASN:HB2	2.01	0.42
1:A:31:THR:H	1:B:437:GLN:NE2	2.17	0.41
1:A:38:MET:O	1:A:42:VAL:HG23	2.20	0.41
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.88	0.41
2:C:202:THR:HG22	2:C:203:CYS:N	2.35	0.41
3:F:30:SER:HA	3:F:70:TYR:OH	2.20	0.41
1:A:400:ALA:HB2	1:A:432:ALA:HB1	2.01	0.41
1:A:413:LEU:HD22	1:A:422:ILE:HD13	2.03	0.41
1:B:287:ASN:HD22	1:B:290:LYS:H	1.68	0.41
2:E:207:HIS:HE2	2:E:209:ALA:HB3	1.85	0.41
1:B:356:ILE:HG23	1:B:360:MET:HE1	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:PRO:O	2:E:195:SER:HB3	2.20	0.41
1:A:379:PHE:HB3	1:A:382:TYR:CD2	2.55	0.41
1:A:209:ARG:CA	1:B:210:TYR:HB2	2.50	0.41
1:B:84:LEU:O	1:B:88:VAL:HG23	2.21	0.41
2:C:12:VAL:O	2:C:119:VAL:HA	2.21	0.41
2:C:215:ASP:OD1	2:C:215:ASP:N	2.53	0.41
2:E:17:SER:HB3	2:E:84:SER:HA	2.01	0.41
1:B:143:MET:HA	1:B:302:CYS:SG	2.60	0.41
3:F:110:ALA:O	3:F:138:PHE:HA	2.21	0.41
1:A:51:VAL:CG2	1:A:229:TYR:HA	2.50	0.41
1:B:56:GLY:HA3	1:B:136:LEU:HD11	2.03	0.41
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.50	0.41
1:B:123:ARG:O	1:B:127:VAL:HG23	2.19	0.41
3:D:12:SER:HA	3:D:104:GLU:O	2.21	0.41
3:D:148:LYS:HA	3:D:152:SER:O	2.20	0.41
1:A:423:LEU:O	1:A:427:ILE:HG13	2.20	0.41
1:B:122:VAL:HB	1:B:160:ARG:HH11	1.86	0.41
1:B:148:GLU:OE1	1:B:357:PHE:HB2	2.21	0.41
2:E:24:ALA:HB1	2:E:27:PHE:CZ	2.55	0.41
2:E:30:SER:O	2:E:31:ARG:CB	2.69	0.41
1:B:383:HIS:NE2	2:E:50:GLU:OE1	2.54	0.41
1:A:24:GLN:HA	1:A:24:GLN:OE1	2.21	0.41
1:B:388:THR:HG22	1:B:421:LEU:HD11	2.03	0.41
3:F:156:ASN:OD1	3:F:156:ASN:N	2.34	0.41
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.39	0.40
2:C:47:TRP:CD2	3:D:95:GLN:NE2	2.89	0.40
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.21	0.40
1:B:88:VAL:HA	1:B:91:MET:CE	2.51	0.40
2:E:12:VAL:HG11	2:E:18:LEU:HB3	2.04	0.40
2:E:98:ARG:O	2:E:109:ASP:HB3	2.21	0.40
3:F:77:MET:HG2	3:F:78:GLU:N	2.36	0.40
1:B:135:GLY:C	1:B:137:GLY:N	2.75	0.40
1:B:53:PHE:O	1:B:57:VAL:HG23	2.22	0.40
2:C:221:ARG:NH1	3:D:118:PRO:HG2	2.35	0.40
3:D:34:TRP:HB2	3:D:47:ILE:HB	2.03	0.40
2:E:176:ALA:HB2	2:E:185:LEU:HD23	2.02	0.40
3:F:184:GLU:O	3:F:187:ARG:HG2	2.21	0.40
1:A:443:PRO:HB2	1:A:446:SER:HB2	2.04	0.40
1:A:83:PHE:CD2	1:A:83:PHE:C	2.94	0.40
3:D:30:SER:H	3:D:91:SER:HB2	1.86	0.40
2:C:33:TRP:CE2	2:C:52:ASN:HB3	2.57	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%)	381 (86%)	55 (12%)	6 (1%)	13	53
1	B	438/473 (93%)	380 (87%)	51 (12%)	7 (2%)	11	50
2	C	219/221 (99%)	192 (88%)	18 (8%)	9 (4%)	3	24
2	E	219/221 (99%)	188 (86%)	25 (11%)	6 (3%)	6	35
3	D	209/211 (99%)	179 (86%)	27 (13%)	3 (1%)	13	53
3	F	209/211 (99%)	181 (87%)	24 (12%)	4 (2%)	9	46
All	All	1736/1810 (96%)	1501 (86%)	200 (12%)	35 (2%)	9	44

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	65	LYS
2	C	164	SER
3	D	51	SER
3	F	7	SER
3	F	199	THR
1	A	136	LEU
1	B	136	LEU
2	C	55	SER
2	E	65	LYS
2	E	136	SER
2	E	195	SER
2	E	221	ARG
3	F	198	LYS
1	A	132	PHE
1	B	21	LEU
1	B	132	PHE
2	C	43	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	62	PRO
2	E	62	PRO
2	E	154	PHE
3	F	66	SER
1	A	96	LEU
1	A	206	PRO
1	B	96	LEU
2	C	163	ASN
2	C	167	LEU
3	D	15	PRO
1	A	167	ARG
1	B	22	ILE
1	B	206	PRO
3	D	105	ILE
1	A	149	GLY
2	C	31	ARG
2	C	189	VAL
1	B	149	GLY

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	335/358 (94%)	314 (94%)	21 (6%)	21	59
1	B	331/358 (92%)	314 (95%)	17 (5%)	28	66
2	C	181/181 (100%)	161 (89%)	20 (11%)	7	30
2	E	181/181 (100%)	164 (91%)	17 (9%)	10	38
3	D	185/185 (100%)	167 (90%)	18 (10%)	9	36
3	F	185/185 (100%)	172 (93%)	13 (7%)	18	54
All	All	1398/1448 (96%)	1292 (92%)	106 (8%)	15	51

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	85	CYS
1	A	103	GLU
1	A	107	SER
1	A	160	ARG
1	A	180	THR
1	A	204	MET
1	A	205	ARG
1	A	209	ARG
1	A	212	LEU
1	A	219	PHE
1	A	234	HIS
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	319	LEU
1	A	357	PHE
1	A	381	GLN
1	A	403	ARG
1	A	442	LYS
1	A	457	GLU
1	B	20	GLN
1	B	24	GLN
1	B	28	ARG
1	B	85	CYS
1	B	160	ARG
1	B	186	LEU
1	B	205	ARG
1	B	208	PHE
1	B	209	ARG
1	B	234	HIS
1	B	244	LEU
1	B	251	THR
1	B	270	ASN
1	B	288	ILE
1	B	319	LEU
1	B	423	LEU
1	B	442	LYS
2	C	6	GLU
2	C	18	LEU
2	C	43	LYS
2	C	65	LYS
2	C	72	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	73	ASP
2	C	77	ASP
2	C	107	TYR
2	C	115	THR
2	C	118	THR
2	C	123	LYS
2	C	128	SER
2	C	148	CYS
2	C	178	LEU
2	C	182	LEU
2	C	185	LEU
2	C	188	SER
2	C	200	THR
2	C	214	VAL
2	C	215	ASP
3	D	5	THR
3	D	29	VAL
3	D	46	TRP
3	D	59	VAL
3	D	68	THR
3	D	69	SER
3	D	75	ASN
3	D	80	GLU
3	D	91	SER
3	D	115	SER
3	D	135	LEU
3	D	142	ASP
3	D	162	TRP
3	D	168	LYS
3	D	174	MET
3	D	183	ASP
3	D	192	THR
3	D	205	VAL
2	E	6	GLU
2	E	22	CYS
2	E	31	ARG
2	E	55	SER
2	E	71	SER
2	E	107	TYR
2	E	115	THR
2	E	118	THR
2	E	136	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	148	CYS
2	E	149	LEU
2	E	161	THR
2	E	191	VAL
2	E	200	THR
2	E	202	THR
2	E	204	ASN
2	E	219	VAL
3	F	2	ILE
3	F	27	SER
3	F	66	SER
3	F	73	THR
3	F	92	SER
3	F	107	ARG
3	F	142	ASP
3	F	156	ASN
3	F	170	SER
3	F	181	THR
3	F	189	ASN
3	F	190	SER
3	F	199	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	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	24	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	74	ASN
2	C	163	ASN
2	C	204	ASN
3	D	6	GLN
3	D	136	ASN
3	D	137	ASN
3	D	144	ASN
3	D	197	HIS
2	E	172	HIS
3	F	6	GLN
3	F	36	GLN
3	F	37	GLN
3	F	136	ASN
3	F	137	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 ⓘ

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/473 (93%)	0.49	28 (6%) 21 12	72, 93, 123, 139	0
1	B	440/473 (93%)	0.59	30 (6%) 18 10	73, 92, 122, 133	0
2	C	221/221 (100%)	0.25	5 (2%) 61 46	66, 85, 102, 114	0
2	E	221/221 (100%)	0.22	9 (4%) 38 25	63, 85, 106, 119	0
3	D	211/211 (100%)	0.61	16 (7%) 15 8	74, 95, 109, 113	0
3	F	211/211 (100%)	0.81	32 (15%) 2 1	59, 79, 113, 115	0
All	All	1748/1810 (96%)	0.50	120 (6%) 18 10	59, 89, 114, 139	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	6.4
1	B	71	THR	5.8
1	A	72	ALA	5.6
1	B	20	GLN	5.5
1	B	72	ALA	5.4
3	D	79	ALA	5.4
1	B	289	THR	5.1
3	F	211	ALA	5.1
1	A	73	ASP	5.0
1	B	74	ASN	4.7
2	C	147	GLY	4.5
2	E	59	ASN	4.3
3	D	110	ALA	4.2
3	F	189	ASN	4.1
1	B	280	LEU	3.9
1	A	74	ASN	3.9
1	B	119	GLN	3.9
1	B	70	HIS	3.8
1	B	177	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	353	PRO	3.7
1	A	71	THR	3.7
3	F	191	TYR	3.5
3	F	151	GLY	3.5
3	F	2	ILE	3.5
3	F	147	TRP	3.3
2	C	199	GLU	3.3
1	B	291	TRP	3.3
1	B	104	ALA	3.2
2	E	14	PRO	3.2
3	D	105	ILE	3.2
3	F	4	LEU	3.1
1	B	94	TYR	3.1
1	B	290	LYS	3.1
1	B	284	HIS	3.0
3	F	149	ILE	3.0
3	F	150	ASP	2.9
2	E	15	GLY	2.9
1	B	307	PHE	2.8
1	A	314	GLY	2.8
3	F	176	SER	2.8
3	F	208	PHE	2.8
1	A	283	VAL	2.8
3	F	192	THR	2.8
3	D	19	VAL	2.8
1	B	287	ASN	2.8
1	B	293	LEU	2.8
3	D	103	LEU	2.8
3	D	20	THR	2.8
1	A	141	GLY	2.7
3	F	193	CYS	2.7
1	B	283	VAL	2.7
1	A	77	LEU	2.7
3	D	70	TYR	2.7
1	B	75	TYR	2.7
3	F	190	SER	2.7
3	D	23	CYS	2.7
1	A	144	VAL	2.6
3	F	209	ASN	2.6
3	F	148	LYS	2.6
3	D	71	SER	2.6
3	D	72	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	197	HIS	2.5
1	B	69	VAL	2.5
1	B	138	THR	2.5
3	F	32	ILE	2.5
1	B	168	LEU	2.5
3	F	27	SER	2.5
1	B	27	GLU	2.5
3	D	11	MET	2.5
1	A	288	ILE	2.5
1	B	29	ASP	2.5
3	F	69	SER	2.4
1	A	207	GLN	2.4
3	D	76	THR	2.4
1	B	309	ALA	2.4
1	A	143	MET	2.4
1	B	25	LEU	2.4
2	C	65	LYS	2.4
3	D	68	THR	2.4
1	B	77	LEU	2.4
1	A	208	PHE	2.3
3	F	153	GLU	2.3
3	F	29	VAL	2.3
1	A	145	LEU	2.3
2	E	13	GLN	2.3
3	F	66	SER	2.3
1	B	456	GLN	2.3
2	C	29	TYR	2.3
2	E	86	VAL	2.3
1	A	75	TYR	2.3
2	E	65	LYS	2.3
1	A	302	CYS	2.2
1	A	235	GLU	2.2
2	E	135	GLY	2.2
3	F	26	SER	2.2
3	F	207	SER	2.2
1	A	142	GLY	2.2
3	F	70	TYR	2.2
2	E	136	SER	2.1
3	F	152	SER	2.1
1	A	99	LYS	2.1
1	A	460	GLN	2.1
3	F	68	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	205	VAL	2.1
1	A	82	ALA	2.1
2	C	141	ALA	2.1
3	F	25	ALA	2.1
3	F	24	SER	2.1
1	A	22	ILE	2.1
1	A	355	GLY	2.1
3	F	185	TYR	2.1
1	A	165	ILE	2.1
3	D	138	PHE	2.0
3	F	72	LEU	2.0
1	A	78	LEU	2.0
3	D	139	TYR	2.0
1	A	350	SER	2.0
2	E	29	TYR	2.0
1	A	298	ILE	2.0
1	A	354	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	BR	B	504	1/1	0.94	0.35	1.98	100,100,100,100	0
4	BR	B	503	1/1	0.94	0.33	1.58	100,100,100,100	0
4	BR	A	501	1/1	0.95	0.42	1.57	100,100,100,100	0
4	BR	A	502	1/1	0.78	0.40	1.00	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.