



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:30 PM UTC

PDB ID : 4KK9 / pdb_00004kk9
Title : Structure of the E148A mutant of CLC-ec1 deltaNC construct in 100mM fluoride and 2mM Bromide
Authors : Lim, H.-H.; Miller, C.
Deposited on : 2013-05-05
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

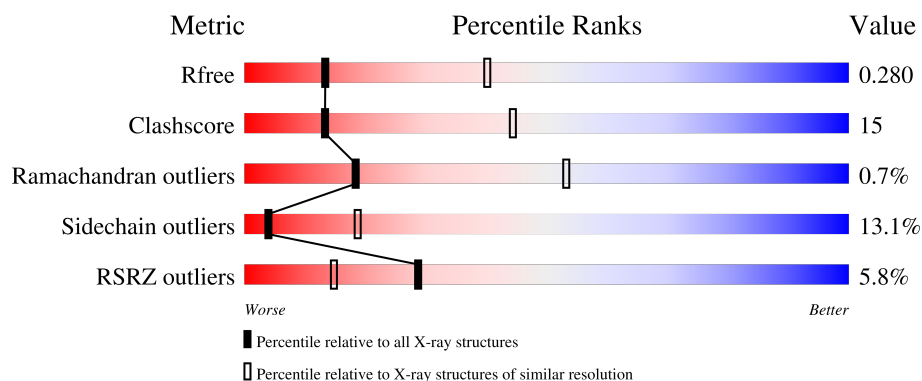
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	446	 6% 62% 31% 6%
1	B	446	 5% 59% 33% 7%
2	C	222	 9% 66% 29%
2	E	222	 4% 70% 24% 5%
3	D	211	 9% 57% 36% 6%

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Mol	Chain	Length	Quality of chain
3	F	211	3% 66% 31%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13206 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3320	2183	558	559	20			
1	B	441	Total	C	N	O	S	0	0	0
			3300	2172	553	555	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P37019
A	148	ALA	GLU	engineered mutation	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	expression tag	UNP P37019
B	148	ALA	GLU	engineered mutation	UNP P37019
B	461	LYS	-	expression tag	UNP P37019

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

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

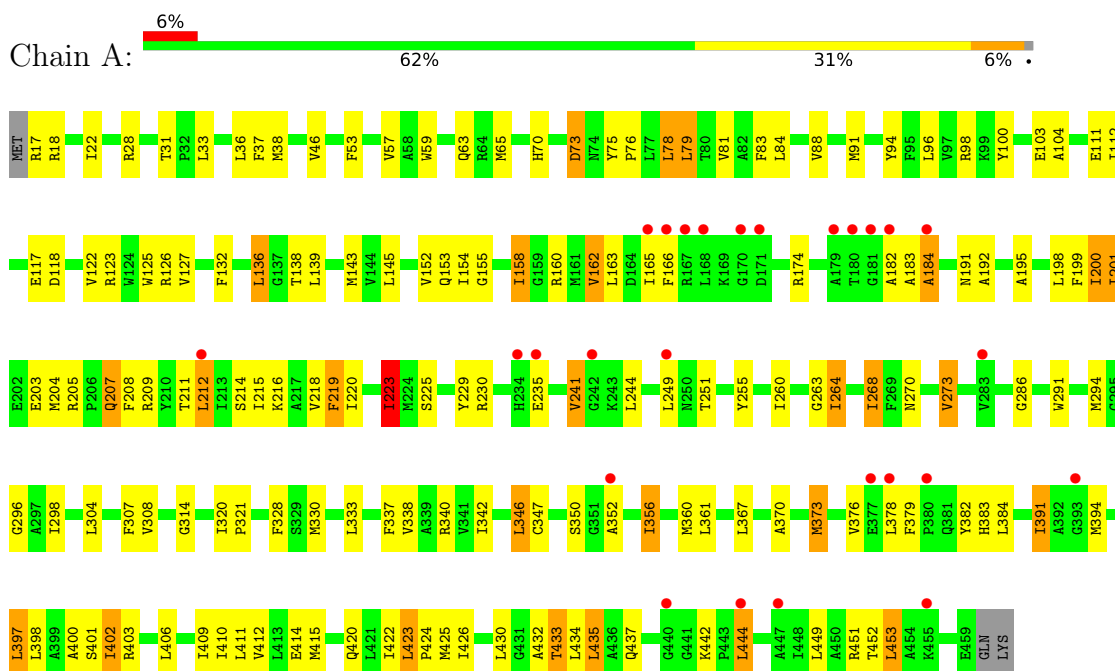
- Molecule 3 is a protein called Fab, light chain.

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

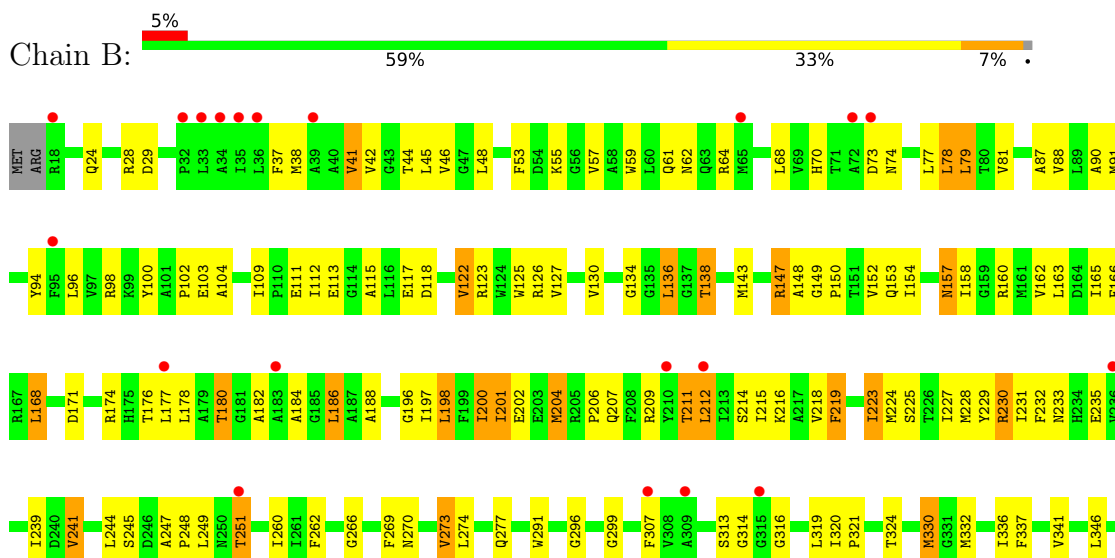
3 Residue-property plots

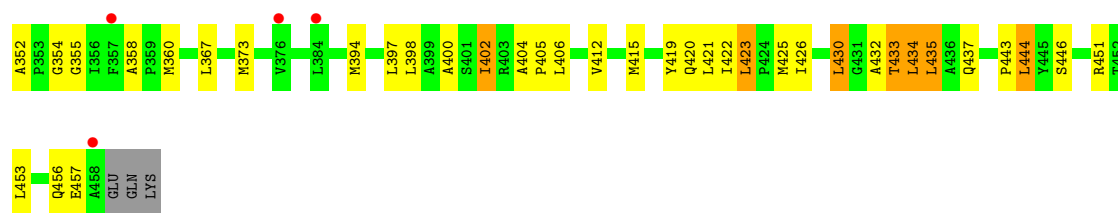
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

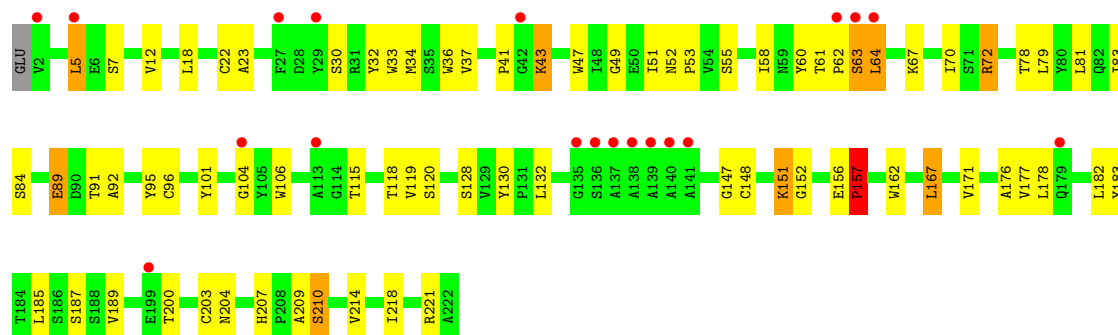


- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

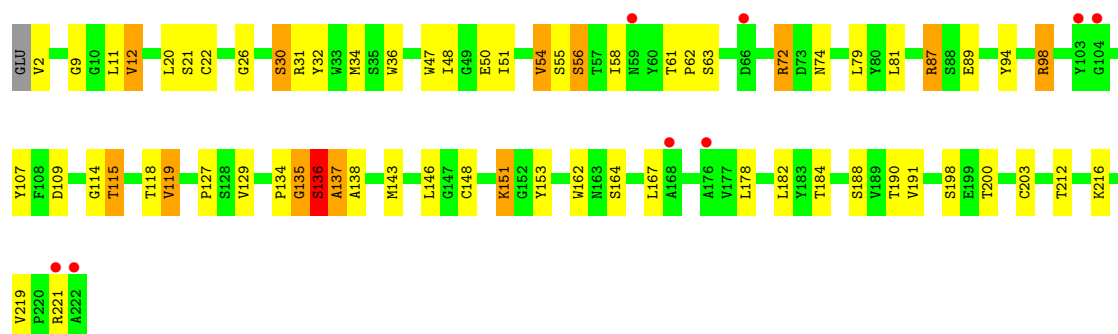




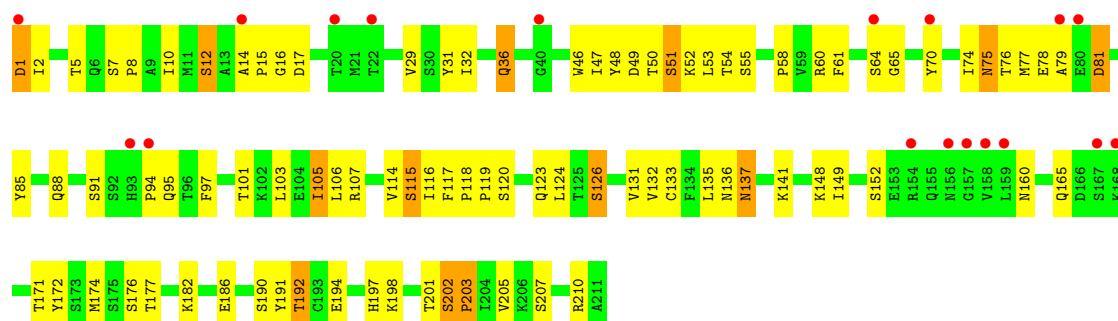
• Molecule 2: Fab, heavy chain



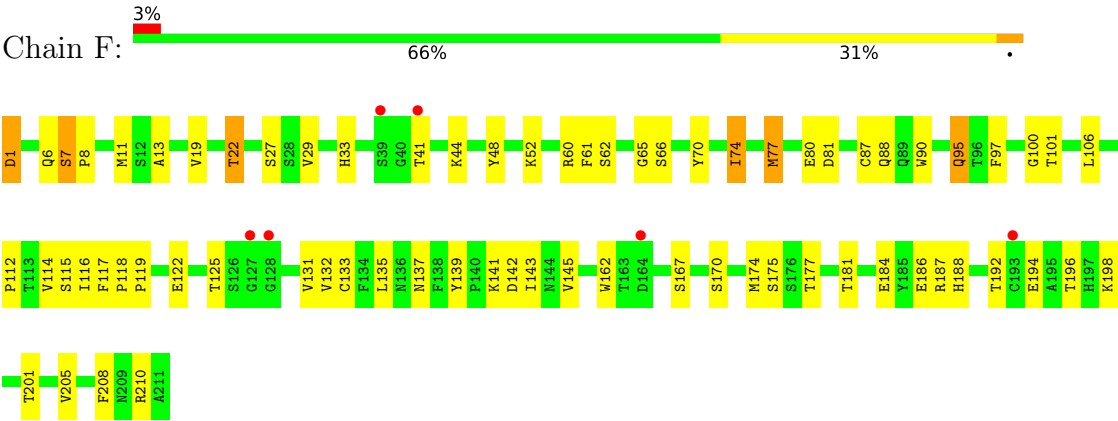
• Molecule 2: Fab, heavy chain



• Molecule 3: Fab, light chain



● Molecule 3: Fab, 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	231.62Å 98.86Å 170.39Å 90.00° 131.88° 90.00°	Depositor
Resolution (Å)	39.93 – 3.00 39.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.93-3.00) 99.8 (39.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.217 , 0.270 0.229 , 0.280	Depositor DCC
R_{free} test set	2925 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13206	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.59	0/3392	0.95	8/4604 (0.2%)
1	B	0.56	0/3372	0.99	10/4578 (0.2%)
2	C	0.65	0/1721	0.93	1/2355 (0.0%)
2	E	0.58	0/1721	0.91	2/2355 (0.1%)
3	D	0.55	0/1660	0.97	5/2257 (0.2%)
3	F	0.55	0/1660	0.99	5/2257 (0.2%)
All	All	0.58	0/13526	0.96	31/18406 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	CA-C-N	-11.06	106.01	119.84
3	F	7	SER	C-N-CA	-11.06	106.01	119.84
1	B	148	ALA	N-CA-C	8.66	120.41	110.97
3	D	137	ASN	N-CA-C	7.36	120.22	111.02
1	B	247	ALA	CA-C-N	6.94	126.98	119.90
1	B	247	ALA	C-N-CA	6.94	126.98	119.90
3	D	202	SER	CA-C-N	6.37	127.80	119.84
3	D	202	SER	C-N-CA	6.37	127.80	119.84
3	D	171	THR	CB-CA-C	-5.81	104.02	113.37
1	A	158	ILE	N-CA-C	-5.81	104.69	110.62
1	A	192	ALA	N-CA-C	5.67	119.29	108.97
3	F	117	PHE	CA-C-N	5.67	126.22	120.38
3	F	117	PHE	C-N-CA	5.67	126.22	120.38
3	D	105	ILE	CB-CA-C	-5.47	105.39	111.35
3	F	137	ASN	N-CA-C	5.40	119.16	111.92
1	A	184	ALA	N-CA-C	-5.37	105.99	112.54
1	A	223	ILE	CB-CA-C	-5.36	104.84	111.70
2	E	138	ALA	CB-CA-C	5.28	118.44	109.53
1	A	342	ILE	N-CA-C	5.23	115.85	110.36
1	A	442	LYS	CA-C-N	5.21	125.51	119.93
1	A	442	LYS	C-N-CA	5.21	125.51	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	GLY	N-CA-C	-5.20	108.29	114.48
1	B	223	ILE	CB-CA-C	-5.19	105.33	111.81
1	B	355	GLY	N-CA-C	5.17	121.03	112.66
1	B	358	ALA	CA-C-N	-5.16	114.51	119.87
1	B	358	ALA	C-N-CA	-5.16	114.51	119.87
1	B	266	GLY	CA-C-N	5.14	124.75	119.05
1	B	266	GLY	C-N-CA	5.14	124.75	119.05
1	B	148	ALA	CB-CA-C	-5.14	103.05	110.96
2	C	119	VAL	N-CA-C	5.14	114.14	106.85
2	E	119	VAL	CB-CA-C	-5.13	107.47	113.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3320	0	3475	118	0
1	B	3300	0	3456	133	0
2	C	1672	0	1654	39	0
2	E	1672	0	1654	35	0
3	D	1621	0	1546	57	0
3	F	1621	0	1546	46	0
All	All	13206	0	13331	391	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 15.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:95:GLN:OE1	3:D:95:GLN:N	2.03	0.90
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.43	0.81
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.63	0.80
3:F:1:ASP:OD2	3:F:1:ASP:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.65	0.79
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.18	0.78
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.48	0.77
2:E:136:SER:O	2:E:137:ALA:CB	2.35	0.74
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.53	0.74
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.68	0.73
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.71	0.72
2:E:136:SER:O	2:E:137:ALA:HB2	1.88	0.72
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.55	0.70
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.73	0.70
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.73	0.69
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.75	0.69
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.73	0.68
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.75	0.68
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.76	0.68
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.09	0.68
1:A:73:ASP:OD1	1:A:73:ASP:N	2.27	0.67
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.26	0.67
3:D:76:THR:HG22	3:D:76:THR:O	1.93	0.67
3:F:95:GLN:N	3:F:95:GLN:OE1	2.27	0.67
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.76	0.67
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.75	0.67
1:A:200:ILE:HA	1:A:204:MET:HB2	1.76	0.67
2:E:32:TYR:O	2:E:72:ARG:NH2	2.27	0.67
2:E:30:SER:O	2:E:31:ARG:HB2	1.95	0.67
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.76	0.66
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.77	0.66
3:F:95:GLN:H	3:F:95:GLN:CD	2.03	0.66
3:F:95:GLN:N	3:F:95:GLN:CD	2.54	0.65
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.79	0.65
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.78	0.65
1:B:150:PRO:HG3	1:B:354:GLY:HA2	1.79	0.65
1:B:157:ASN:N	1:B:157:ASN:HD22	1.94	0.64
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.33	0.64
1:B:157:ASN:HD22	1:B:157:ASN:H	1.44	0.64
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.34	0.63
1:A:422:ILE:HA	1:A:425:MET:HE3	1.80	0.63
2:E:87:ARG:HE	2:E:89:GLU:HB2	1.63	0.62
1:A:403:ARG:HE	1:A:433:THR:HG22	1.64	0.62
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.80	0.62
1:B:360:MET:HE1	1:B:402:ILE:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.82	0.61
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.36	0.60
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.67	0.60
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.84	0.60
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.84	0.60
1:A:403:ARG:NH2	1:B:29:ASP:OD1	2.35	0.60
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.17	0.60
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.83	0.59
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.38	0.59
1:B:422:ILE:HA	1:B:425:MET:HE3	1.83	0.59
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.37	0.59
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.84	0.59
1:A:314:GLY:O	1:A:340:ARG:NH2	2.35	0.59
1:B:38:MET:O	1:B:42:VAL:HG23	2.03	0.59
1:B:212:LEU:HD12	1:B:212:LEU:H	1.66	0.59
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.85	0.59
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.37	0.59
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.18	0.59
2:C:207:HIS:ND1	2:C:210:SER:OG	2.28	0.58
1:A:361:LEU:HD13	1:A:415:MET:HE1	1.85	0.58
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.34	0.58
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.39	0.58
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.38	0.58
1:B:337:PHE:O	1:B:341:VAL:HG23	2.04	0.57
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.86	0.57
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.87	0.57
1:A:337:PHE:CE1	1:A:367:LEU:HB2	2.40	0.57
1:A:414:GLU:OE1	1:B:419:TYR:OH	2.19	0.57
2:C:5:LEU:HB3	2:C:23:ALA:HB3	1.85	0.57
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.18	0.57
1:A:394:MET:HE2	1:A:412:VAL:HG13	1.87	0.56
3:D:78:GLU:O	3:D:81:ASP:HB2	2.05	0.56
2:E:9:GLY:H	2:E:115:THR:HG21	1.68	0.56
3:F:6:GLN:HG3	3:F:100:GLY:N	2.20	0.56
1:A:406:LEU:HB2	1:B:219:PHE:HE1	1.70	0.56
3:D:1:ASP:OD2	3:D:1:ASP:N	2.20	0.56
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.87	0.56
3:F:19:VAL:HB	3:F:74:ILE:HG13	1.88	0.56
1:B:78:LEU:HD13	1:B:79:LEU:HD23	1.88	0.56
2:C:101:TYR:HB2	2:C:104:GLY:HA2	1.88	0.55
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:MET:HE3	2:E:190:THR:HG22	1.89	0.55
1:A:214:SER:O	1:A:218:VAL:HG23	2.07	0.55
1:B:88:VAL:HA	1:B:91:MET:HE2	1.88	0.55
3:F:66:SER:HA	3:F:70:TYR:CZ	2.41	0.55
1:B:42:VAL:O	1:B:46:VAL:HG23	2.07	0.54
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.42	0.54
1:B:180:THR:HA	1:B:218:VAL:HG13	1.89	0.54
3:F:188:HIS:O	3:F:210:ARG:HD3	2.06	0.54
1:A:88:VAL:HA	1:A:91:MET:HE2	1.89	0.54
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.23	0.54
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.90	0.54
1:A:152:VAL:HG13	1:A:182:ALA:HB1	1.89	0.54
1:B:53:PHE:O	1:B:57:VAL:HG23	2.07	0.54
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.43	0.54
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.90	0.54
3:F:6:GLN:NE2	3:F:100:GLY:H	2.06	0.54
1:A:212:LEU:HD12	1:A:212:LEU:H	1.73	0.53
1:B:109:ILE:HG23	1:B:204:MET:SD	2.48	0.53
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.89	0.53
3:D:160:ASN:OD1	3:D:176:SER:OG	2.10	0.53
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.89	0.53
1:B:64:ARG:O	1:B:68:LEU:HG	2.09	0.53
1:B:176:THR:O	1:B:180:THR:HG23	2.08	0.53
1:A:37:PHE:CD2	1:A:38:MET:HE2	2.40	0.53
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.23	0.53
1:B:154:ILE:O	1:B:158:ILE:HG12	2.09	0.53
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.74	0.53
3:F:7:SER:HB2	3:F:22:THR:HB	1.91	0.53
1:A:122:VAL:HB	1:A:160:ARG:HD3	1.91	0.53
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.89	0.52
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.77	0.52
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.44	0.52
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.92	0.52
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.44	0.52
1:B:38:MET:HA	1:B:41:VAL:HG13	1.92	0.52
3:D:192:THR:HB	3:D:207:SER:HB3	1.91	0.52
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.18	0.52
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.24	0.52
3:F:184:GLU:O	3:F:187:ARG:HG2	2.10	0.52
3:D:116:ILE:HD13	3:D:207:SER:HA	1.92	0.52
2:E:94:TYR:O	2:E:114:GLY:HA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:151:LYS:HB3	2:E:184:THR:HG23	1.92	0.52
3:F:6:GLN:HG3	3:F:100:GLY:H	1.73	0.52
1:A:383:HIS:HD1	2:C:106:TRP:CD1	2.27	0.51
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.36	0.51
1:B:150:PRO:O	1:B:154:ILE:HG13	2.11	0.51
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.45	0.51
1:B:241:VAL:HG22	1:B:324:THR:HG21	1.93	0.51
1:B:332:MET:O	1:B:336:ILE:HG13	2.10	0.51
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.91	0.51
1:B:394:MET:HE2	1:B:412:VAL:HG22	1.92	0.51
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.45	0.51
3:D:186:GLU:O	3:D:210:ARG:NH2	2.44	0.51
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.92	0.51
3:D:29:VAL:O	3:D:70:TYR:OH	2.15	0.51
1:A:330:MET:HE1	1:A:370:ALA:CB	2.41	0.51
1:B:147:ARG:C	1:B:150:PRO:HD2	2.36	0.51
2:C:37:VAL:O	2:C:95:TYR:HB2	2.11	0.50
2:C:41:PRO:HD3	2:C:92:ALA:HA	1.94	0.50
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.93	0.50
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.93	0.50
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.93	0.50
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.92	0.50
3:D:12:SER:HB3	3:D:106:LEU:HD12	1.93	0.50
3:F:61:PHE:CE2	3:F:74:ILE:HD13	2.47	0.50
1:B:37:PHE:CD2	1:B:38:MET:HE2	2.46	0.50
2:C:132:LEU:HB2	2:C:147:GLY:HA3	1.94	0.50
1:A:154:ILE:O	1:A:158:ILE:HG12	2.11	0.50
1:A:294:MET:O	1:A:298:ILE:HG13	2.12	0.50
2:C:63:SER:O	2:C:64:LEU:O	2.30	0.50
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.94	0.50
1:B:227:ILE:O	1:B:231:ILE:HG12	2.12	0.50
1:A:100:TYR:O	1:A:126:ARG:NH1	2.45	0.49
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.94	0.49
1:A:264:ILE:O	1:A:268:ILE:HG13	2.12	0.49
1:B:37:PHE:HD2	1:B:38:MET:HE2	1.77	0.49
2:C:167:LEU:HD23	2:C:189:VAL:HG21	1.94	0.49
3:D:115:SER:HB3	3:D:117:PHE:CE1	2.48	0.49
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.94	0.49
3:D:106:LEU:HD23	3:D:107:ARG:N	2.28	0.49
1:B:313:SER:OG	1:B:314:GLY:N	2.46	0.49
2:E:12:VAL:HG23	2:E:119:VAL:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.76	0.49
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.94	0.49
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.10	0.49
1:B:44:THR:O	1:B:48:LEU:HG	2.12	0.49
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.47	0.49
1:B:171:ASP:OD2	1:B:174:ARG:NH1	2.34	0.49
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.94	0.49
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.45	0.49
1:A:330:MET:HE1	1:A:370:ALA:HB1	1.93	0.49
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.28	0.49
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.93	0.49
2:E:129:VAL:O	2:E:216:LYS:HE3	2.12	0.49
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.95	0.49
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.48	0.49
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.33	0.49
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.48	0.49
1:A:437:GLN:HE21	1:B:216:LYS:NZ	2.11	0.48
1:B:229:TYR:O	1:B:233:ASN:HB2	2.13	0.48
1:B:330:MET:HE3	1:B:330:MET:HA	1.93	0.48
1:B:316:GLY:O	1:B:319:LEU:HG	2.11	0.48
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.48	0.48
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.13	0.48
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.49	0.48
1:B:165:ILE:HG22	1:B:166:PHE:CD2	2.49	0.48
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.95	0.48
1:A:78:LEU:HD13	1:A:79:LEU:HD23	1.94	0.48
1:B:274:LEU:O	1:B:277:GLN:HB2	2.14	0.48
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.49	0.48
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.49	0.48
2:E:135:GLY:HA2	2:E:221:ARG:CD	2.44	0.48
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.49	0.47
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.82	0.47
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.50	0.47
2:E:47:TRP:HZ2	2:E:50:GLU:HG2	1.78	0.47
3:D:95:GLN:H	3:D:95:GLN:CD	2.05	0.47
1:A:270:ASN:O	1:A:273:VAL:HG13	2.14	0.47
1:A:330:MET:HE3	1:A:333:LEU:HB2	1.97	0.47
1:A:430:LEU:HD11	1:B:219:PHE:CG	2.49	0.47
1:B:214:SER:O	1:B:218:VAL:HG23	2.13	0.47
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.50	0.47
3:F:188:HIS:O	3:F:210:ARG:CD	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.97	0.47
1:A:220:ILE:HD11	1:B:434:LEU:HD21	1.97	0.47
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.50	0.47
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.97	0.47
1:B:197:ILE:O	1:B:201:ILE:HG12	2.15	0.47
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.60	0.47
3:F:7:SER:CB	3:F:22:THR:HB	2.45	0.47
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.97	0.46
1:B:138:THR:HG22	1:B:143:MET:SD	2.55	0.46
3:D:197:HIS:CD2	3:D:198:LYS:H	2.33	0.46
1:B:269:PHE:O	1:B:273:VAL:HG12	2.16	0.46
3:D:46:TRP:O	3:D:47:ILE:HG13	2.15	0.46
2:E:2:VAL:HA	2:E:26:GLY:HA3	1.97	0.46
1:B:130:VAL:O	1:B:134:GLY:N	2.39	0.46
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.80	0.46
3:F:186:GLU:HA	3:F:210:ARG:NH1	2.31	0.46
1:A:199:PHE:CE1	1:A:203:GLU:HG2	2.51	0.46
1:A:449:LEU:HG	1:A:453:LEU:HD22	1.97	0.46
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.98	0.46
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.97	0.46
1:A:360:MET:HE1	1:A:402:ILE:CD1	2.46	0.46
1:B:112:ILE:HG13	1:B:153:GLN:HA	1.97	0.46
1:A:249:LEU:HD13	1:B:231:ILE:HD13	1.97	0.46
1:B:188:ALA:HB2	1:B:225:SER:OG	2.16	0.46
3:D:31:TYR:HA	3:D:50:THR:OG1	2.15	0.46
2:E:143:MET:HB3	2:E:190:THR:HG23	1.98	0.46
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.80	0.45
3:D:14:ALA:O	3:D:17:ASP:HB2	2.16	0.45
3:D:165:GLN:HG3	3:D:172:TYR:CZ	2.51	0.45
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.98	0.45
3:D:1:ASP:HB3	3:D:94:PRO:HD2	1.99	0.45
3:D:124:LEU:O	3:D:126:SER:N	2.50	0.45
3:F:8:PRO:O	3:F:101:THR:HG23	2.16	0.45
1:B:59:TRP:O	1:B:62:ASN:HB3	2.16	0.45
1:A:195:ALA:N	1:A:414:GLU:OE2	2.47	0.45
1:A:394:MET:HE2	1:A:412:VAL:HG22	1.99	0.45
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.99	0.45
1:A:59:TRP:O	1:A:63:GLN:HG2	2.15	0.45
1:A:437:GLN:HE21	1:B:216:LYS:HZ2	1.62	0.45
1:B:41:VAL:O	1:B:45:LEU:HG	2.16	0.45
3:D:141:LYS:HB3	3:D:172:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.98	0.45
1:A:346:LEU:O	1:A:350:SER:HB3	2.16	0.45
2:E:61:THR:O	2:E:63:SER:N	2.50	0.45
3:F:145:VAL:HA	3:F:194:GLU:O	2.17	0.45
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.52	0.45
3:F:6:GLN:HE22	3:F:87:CYS:H	1.63	0.45
3:F:60:ARG:HG3	3:F:74:ILE:HG22	1.99	0.45
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.98	0.44
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.17	0.44
3:D:47:ILE:HG12	3:D:53:LEU:CD2	2.47	0.44
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.99	0.44
3:F:106:LEU:HA	3:F:139:TYR:OH	2.17	0.44
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.67	0.44
3:D:141:LYS:HB3	3:D:172:TYR:CE2	2.52	0.44
1:B:73:ASP:OD1	1:B:73:ASP:N	2.49	0.44
1:B:202:GLU:OE2	1:B:405:PRO:HD2	2.17	0.44
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.99	0.44
1:A:401:SER:O	1:A:444:LEU:HB2	2.17	0.44
2:C:60:TYR:HE2	2:C:70:ILE:H	1.66	0.44
3:D:54:THR:O	3:D:55:SER:C	2.61	0.44
1:A:200:ILE:HG22	1:A:201:ILE:HG23	1.99	0.44
1:B:239:ILE:HD12	1:B:415:MET:HE3	2.00	0.44
2:C:203:CYS:O	2:C:203:CYS:SG	2.76	0.44
1:B:118:ASP:OD1	1:B:174:ARG:NH2	2.34	0.44
1:B:200:ILE:HD12	1:B:204:MET:HG3	2.00	0.44
2:C:151:LYS:HE3	2:C:151:LYS:HB2	1.67	0.44
2:E:48:ILE:HD13	2:E:48:ILE:HA	1.86	0.44
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.53	0.44
1:B:149:GLY:N	1:B:150:PRO:CD	2.80	0.44
1:B:224:MET:O	1:B:228:MET:HG2	2.17	0.44
1:B:319:LEU:HG	1:B:319:LEU:H	1.74	0.44
2:C:30:SER:C	2:C:32:TYR:H	2.26	0.44
3:D:54:THR:HG22	3:D:55:SER:N	2.33	0.44
1:A:53:PHE:O	1:A:57:VAL:HG23	2.18	0.43
1:B:53:PHE:CE2	1:B:147:ARG:HB3	2.53	0.43
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.17	0.43
3:D:76:THR:O	3:D:76:THR:CG2	2.64	0.43
2:E:178:LEU:HD12	2:E:182:LEU:O	2.18	0.43
1:A:433:THR:HB	1:B:216:LYS:HE2	2.00	0.43
1:B:53:PHE:HE2	1:B:147:ARG:HB3	1.83	0.43
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.54	0.43
1:A:158:ILE:O	1:A:162:VAL:HG13	2.19	0.43
2:C:91:THR:HG23	2:C:118:THR:HA	2.00	0.43
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.51	0.43
1:A:411:LEU:HG	1:A:415:MET:HE2	1.99	0.43
1:B:201:ILE:HG12	1:B:201:ILE:H	1.46	0.43
1:B:202:GLU:OE1	1:B:404:ALA:HB1	2.19	0.43
1:A:31:THR:HB	1:A:36:LEU:HD21	2.00	0.43
1:A:409:ILE:HD13	1:A:426:ILE:HA	2.01	0.43
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.00	0.43
1:B:346:LEU:HD12	1:B:346:LEU:HA	1.74	0.43
3:D:77:MET:SD	3:D:103:LEU:HD21	2.59	0.43
1:A:398:LEU:O	1:A:402:ILE:HB	2.19	0.43
1:B:249:LEU:C	1:B:251:THR:H	2.26	0.43
1:B:270:ASN:HD22	1:B:270:ASN:HA	1.55	0.43
2:C:22:CYS:O	2:C:78:THR:HG23	2.19	0.43
2:E:30:SER:C	2:E:32:TYR:H	2.26	0.43
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.54	0.43
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.49	0.42
1:A:183:ALA:HB2	1:A:200:ILE:HG12	2.01	0.42
1:A:328:PHE:O	1:A:373:MET:HE1	2.19	0.42
1:B:87:ALA:O	1:B:91:MET:HG3	2.19	0.42
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.54	0.42
1:B:157:ASN:N	1:B:157:ASN:ND2	2.61	0.42
1:B:200:ILE:HA	1:B:204:MET:HB2	2.00	0.42
3:D:148:LYS:HA	3:D:152:SER:O	2.19	0.42
1:B:260:ILE:HG23	1:B:435:LEU:HG	2.01	0.42
2:C:37:VAL:HG22	2:C:47:TRP:HA	2.00	0.42
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.54	0.42
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.53	0.42
3:D:49:ASP:O	3:D:51:SER:N	2.51	0.42
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.83	0.42
1:B:123:ARG:O	1:B:127:VAL:HG23	2.19	0.42
3:D:79:ALA:O	3:D:105:ILE:HD11	2.20	0.42
2:E:134:PRO:HD3	2:E:146:LEU:HD23	2.00	0.42
3:F:143:ILE:HG13	3:F:196:THR:O	2.19	0.42
1:A:143:MET:HE2	1:A:347:CYS:SG	2.59	0.42
1:B:204:MET:HB3	1:B:204:MET:HE3	1.70	0.42
1:A:216:LYS:HE2	1:B:433:THR:HB	2.02	0.42
1:B:90:ALA:HB3	1:B:296:GLY:HA2	2.02	0.42
1:B:100:TYR:O	1:B:126:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HA	1:B:136:LEU:HD12	1.74	0.42
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.55	0.42
1:B:248:PRO:HB2	1:B:251:THR:HB	2.01	0.42
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.02	0.42
1:A:410:ILE:O	1:A:414:GLU:HG3	2.19	0.42
3:D:75:ASN:O	3:D:76:THR:HB	2.20	0.42
1:A:91:MET:HG3	1:A:296:GLY:CA	2.50	0.42
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.91	0.42
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.55	0.41
1:B:273:VAL:O	1:B:277:GLN:HG3	2.19	0.41
3:F:80:GLU:HA	3:F:167:SER:O	2.20	0.41
3:F:115:SER:O	3:F:133:CYS:HA	2.20	0.41
1:A:160:ARG:O	1:A:163:LEU:HB3	2.20	0.41
1:A:216:LYS:HE3	1:A:216:LYS:HB2	1.78	0.41
2:C:7:SER:HA	2:C:115:THR:HG21	2.03	0.41
1:A:83:PHE:HD1	1:A:84:LEU:HD23	1.85	0.41
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.47	0.41
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.56	0.41
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.55	0.41
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.38	0.41
1:B:74:ASN:HB3	1:B:77:LEU:HB3	2.01	0.41
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.50	0.41
1:A:18:ARG:O	1:A:22:ILE:HG13	2.20	0.41
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.56	0.41
3:D:36:GLN:HB2	3:D:85:TYR:HE2	1.84	0.41
3:D:65:GLY:HA3	3:D:70:TYR:HA	2.01	0.41
3:D:114:VAL:HG22	3:D:135:LEU:HD22	2.01	0.41
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.55	0.41
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.55	0.41
3:D:136:ASN:HB3	3:D:137:ASN:ND2	2.35	0.41
3:D:202:SER:HA	3:D:203:PRO:HD2	1.67	0.41
3:F:112:PRO:HG3	3:F:143:ILE:HD11	2.01	0.41
1:B:104:ALA:HB2	1:B:127:VAL:HG13	2.02	0.41
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.50	0.41
2:E:11:LEU:HD12	2:E:11:LEU:HA	1.88	0.41
1:A:360:MET:HG2	1:A:397:LEU:HD13	2.03	0.41
1:B:160:ARG:O	1:B:163:LEU:HB3	2.21	0.41
1:B:197:ILE:HG22	1:B:201:ILE:HD11	2.03	0.41
3:D:132:VAL:HG22	3:D:177:THR:HG23	2.01	0.41
3:F:119:PRO:HD3	3:F:131:VAL:HG22	2.02	0.41
3:F:141:LYS:HE3	3:F:141:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.56	0.41
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.56	0.41
1:B:231:ILE:HB	1:B:232:PHE:HD1	1.85	0.41
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.91	0.41
1:A:182:ALA:HB1	1:A:204:MET:HE2	2.03	0.40
1:B:102:PRO:C	1:B:104:ALA:H	2.28	0.40
1:B:115:ALA:HB1	1:B:178:LEU:HD21	2.02	0.40
2:C:89:GLU:OE2	2:C:89:GLU:N	2.53	0.40
3:D:149:ILE:HG23	3:D:191:TYR:CE2	2.56	0.40
3:D:182:LYS:HE2	3:D:186:GLU:OE1	2.20	0.40
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.29	0.40
1:A:184:ALA:HB1	1:A:225:SER:CB	2.48	0.40
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.86	0.40
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.22	0.40
1:A:132:PHE:O	1:A:136:LEU:HB2	2.22	0.40
3:F:6:GLN:CG	3:F:100:GLY:H	2.34	0.40
3:F:11:MET:HE2	3:F:19:VAL:HG13	2.04	0.40
3:F:162:TRP:CE2	3:F:174:MET:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	409 (93%)	32 (7%)	0	100	100
1	B	439/446 (98%)	403 (92%)	36 (8%)	0	100	100
2	C	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	9	36
2	E	219/222 (99%)	191 (87%)	22 (10%)	6 (3%)	4	22
3	D	209/211 (99%)	183 (88%)	23 (11%)	3 (1%)	9	36
3	F	209/211 (99%)	187 (90%)	22 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1736/1758 (99%)	1570 (90%)	154 (9%)	12 (1%)	18	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
3	D	126	SER
2	E	137	ALA
2	E	62	PRO
2	E	136	SER
3	D	15	PRO
2	E	55	SER
2	C	62	PRO
3	D	203	PRO
2	E	54	VAL
2	E	135	GLY
2	C	157	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/336 (99%)	285 (86%)	48 (14%)	3	15
1	B	331/336 (98%)	282 (85%)	49 (15%)	3	15
2	C	181/182 (100%)	156 (86%)	25 (14%)	3	17
2	E	181/182 (100%)	161 (89%)	20 (11%)	6	25
3	D	185/185 (100%)	165 (89%)	20 (11%)	6	26
3	F	185/185 (100%)	164 (89%)	21 (11%)	5	24
All	All	1396/1406 (99%)	1213 (87%)	183 (13%)	4	19

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	33	LEU
1	A	65	MET
1	A	70	HIS
1	A	73	ASP
1	A	78	LEU
1	A	79	LEU
1	A	81	VAL
1	A	96	LEU
1	A	103	GLU
1	A	111	GLU
1	A	136	LEU
1	A	162	VAL
1	A	200	ILE
1	A	201	ILE
1	A	205	ARG
1	A	207	GLN
1	A	211	THR
1	A	212	LEU
1	A	215	ILE
1	A	219	PHE
1	A	223	ILE
1	A	235	GLU
1	A	241	VAL
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	268	ILE
1	A	273	VAL
1	A	304	LEU
1	A	308	VAL
1	A	338	VAL
1	A	346	LEU
1	A	356	ILE
1	A	373	MET
1	A	378	LEU
1	A	391	ILE
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	423	LEU
1	A	433	THR
1	A	434	LEU

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Mol	Chain	Res	Type
1	A	435	LEU
1	A	444	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	41	VAL
1	B	55	LYS
1	B	70	HIS
1	B	78	LEU
1	B	79	LEU
1	B	81	VAL
1	B	96	LEU
1	B	103	GLU
1	B	111	GLU
1	B	113	GLU
1	B	122	VAL
1	B	136	LEU
1	B	138	THR
1	B	147	ARG
1	B	157	ASN
1	B	162	VAL
1	B	168	LEU
1	B	177	LEU
1	B	180	THR
1	B	186	LEU
1	B	198	LEU
1	B	200	ILE
1	B	201	ILE
1	B	204	MET
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	230	ARG
1	B	235	GLU
1	B	241	VAL
1	B	244	LEU
1	B	245	SER
1	B	251	THR
1	B	273	VAL
1	B	330	MET
1	B	373	MET

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Mol	Chain	Res	Type
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	423	LEU
1	B	430	LEU
1	B	433	THR
1	B	434	LEU
1	B	435	LEU
1	B	444	LEU
1	B	451	ARG
1	B	453	LEU
1	B	456	GLN
2	C	5	LEU
2	C	12	VAL
2	C	18	LEU
2	C	43	LYS
2	C	55	SER
2	C	61	THR
2	C	63	SER
2	C	72	ARG
2	C	83	ILE
2	C	84	SER
2	C	89	GLU
2	C	96	CYS
2	C	120	SER
2	C	128	SER
2	C	148	CYS
2	C	151	LYS
2	C	157	PRO
2	C	167	LEU
2	C	177	VAL
2	C	187	SER
2	C	200	THR
2	C	204	ASN
2	C	210	SER
2	C	214	VAL
2	C	218	ILE
3	D	1	ASP
3	D	2	ILE
3	D	5	THR
3	D	10	ILE
3	D	12	SER

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Mol	Chain	Res	Type
3	D	32	ILE
3	D	36	GLN
3	D	51	SER
3	D	64	SER
3	D	75	ASN
3	D	81	ASP
3	D	91	SER
3	D	101	THR
3	D	115	SER
3	D	120	SER
3	D	133	CYS
3	D	174	MET
3	D	190	SER
3	D	192	THR
3	D	201	THR
2	E	12	VAL
2	E	21	SER
2	E	30	SER
2	E	56	SER
2	E	72	ARG
2	E	87	ARG
2	E	98	ARG
2	E	115	THR
2	E	118	THR
2	E	136	SER
2	E	148	CYS
2	E	151	LYS
2	E	164	SER
2	E	167	LEU
2	E	188	SER
2	E	191	VAL
2	E	198	SER
2	E	200	THR
2	E	212	THR
2	E	219	VAL
3	F	1	ASP
3	F	22	THR
3	F	27	SER
3	F	29	VAL
3	F	41	THR
3	F	44	LYS
3	F	62	SER

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Mol	Chain	Res	Type
3	F	74	ILE
3	F	77	MET
3	F	95	GLN
3	F	116	ILE
3	F	122	GLU
3	F	125	THR
3	F	142	ASP
3	F	170	SER
3	F	175	SER
3	F	181	THR
3	F	192	THR
3	F	198	LYS
3	F	201	THR
3	F	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	270	ASN
1	A	420	GLN
1	A	437	GLN
1	B	157	ASN
1	B	270	ASN
1	B	284	HIS
1	B	420	GLN
1	B	437	GLN
2	C	39	GLN
2	C	172	HIS
3	D	37	GLN
3	D	136	ASN
3	D	137	ASN
3	F	6	GLN
3	F	36	GLN
3	F	137	ASN
3	F	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.18	26 (5%)	28	14	34, 52, 82, 115	0
1	B	441/446 (98%)	0.19	24 (5%)	31	16	33, 58, 93, 131	0
2	C	221/222 (99%)	0.23	19 (8%)	16	8	24, 51, 87, 125	0
2	E	221/222 (99%)	0.13	8 (3%)	46	26	30, 51, 82, 119	0
3	D	211/211 (100%)	0.48	18 (8%)	16	8	34, 59, 83, 94	0
3	F	211/211 (100%)	-0.09	6 (2%)	55	32	29, 46, 95, 114	0
All	All	1748/1758 (99%)	0.19	101 (5%)	29	15	24, 53, 88, 131	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	20	THR	7.2
1	A	235	GLU	7.1
1	A	168	LEU	5.1
1	A	166	PHE	4.8
2	E	221	ARG	4.6
3	D	40	GLY	4.6
3	D	1	ASP	4.3
2	E	222	ALA	4.0
1	A	212	LEU	3.9
2	C	29	TYR	3.9
1	B	34	ALA	3.9
1	A	447	ALA	3.8
2	C	139	ALA	3.8
1	B	95	PHE	3.8
3	D	158	VAL	3.7
1	A	234	HIS	3.7
1	B	73	ASP	3.6
1	A	378	LEU	3.5
3	F	193	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	380	PRO	3.3
2	C	137	ALA	3.2
1	B	376	VAL	3.2
2	C	2	VAL	3.2
2	C	141	ALA	3.2
1	A	165	ILE	3.2
1	A	182	ALA	3.1
1	A	283	VAL	3.1
2	C	42	GLY	3.1
1	B	384	LEU	3.1
1	B	72	ALA	3.0
1	A	242	GLY	3.0
3	D	156	ASN	3.0
1	B	210	TYR	2.9
2	C	64	LEU	2.9
1	B	307	PHE	2.9
1	A	170	GLY	2.9
1	A	184	ALA	2.9
3	D	22	THR	2.9
2	C	104	GLY	2.8
1	A	180	THR	2.8
1	B	33	LEU	2.8
2	C	140	ALA	2.8
1	B	177	LEU	2.8
2	C	138	ALA	2.8
1	B	35	ILE	2.8
1	B	212	LEU	2.8
1	A	455	LYS	2.8
1	A	444	LEU	2.7
3	F	164	ASP	2.7
1	A	167	ARG	2.7
3	D	80	GLU	2.7
1	A	377	GLU	2.7
3	D	159	LEU	2.7
3	F	41	THR	2.7
3	F	127	GLY	2.6
1	A	352	ALA	2.6
3	D	168	LYS	2.6
1	B	236	VAL	2.6
2	C	27	PHE	2.6
2	C	179	GLN	2.6
3	D	93	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	128	GLY	2.5
2	C	199	GLU	2.5
2	C	136	SER	2.5
1	B	36	LEU	2.5
1	A	440	GLY	2.5
3	D	79	ALA	2.5
1	B	251	THR	2.4
1	B	357	PHE	2.4
2	E	59	ASN	2.4
2	C	63	SER	2.4
1	B	65	MET	2.4
3	F	39	SER	2.3
1	A	181	GLY	2.3
3	D	70	TYR	2.3
1	B	309	ALA	2.3
2	E	104	GLY	2.3
3	D	154	ARG	2.2
1	B	32	PRO	2.2
2	C	62	PRO	2.2
1	A	393	GLY	2.2
1	A	171	ASP	2.2
3	D	157	GLY	2.2
3	D	167	SER	2.2
1	A	249	LEU	2.2
2	C	113	ALA	2.2
3	D	14	ALA	2.1
1	A	179	ALA	2.1
1	B	183	ALA	2.1
2	E	66	ASP	2.1
1	B	315	GLY	2.1
1	B	18	ARG	2.1
1	B	458	ALA	2.1
2	E	103	TYR	2.1
2	C	5	LEU	2.0
1	B	39	ALA	2.0
2	E	176	ALA	2.0
3	D	64	SER	2.0
3	D	94	PRO	2.0
2	C	135	GLY	2.0
2	E	168	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.