



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:14 AM UTC

PDB ID : 4KKA / pdb_00004kka
Title : Structure of the E148A mutant of CLC-ec1 deltaNC construct in 100mM fluoride and 20mM 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

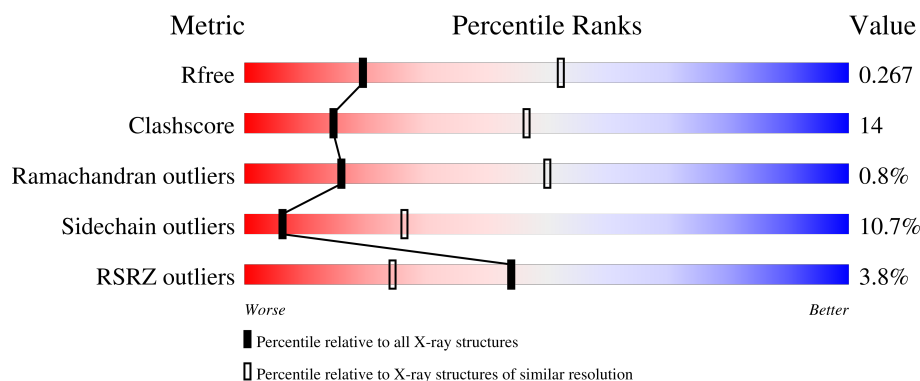
1 Overall quality at a glance

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	5% 64% 30% • •
1	B	446	4% 63% 31% • •
2	C	222	5% 66% 29% 5%
2	E	222	2% 71% 25% •
3	D	211	5% 61% 33% 5%

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Mol	Chain	Length	Quality of chain
3	F	211	2% 70% 27%

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			

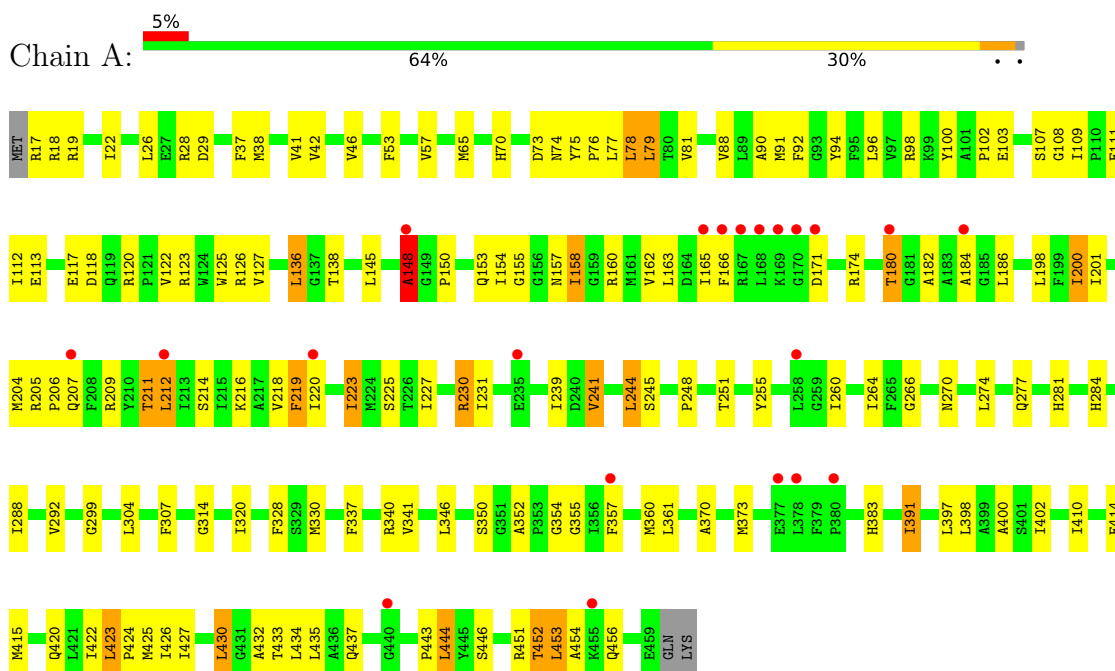
- Molecule 3 is a protein called Fab, light chain.

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			

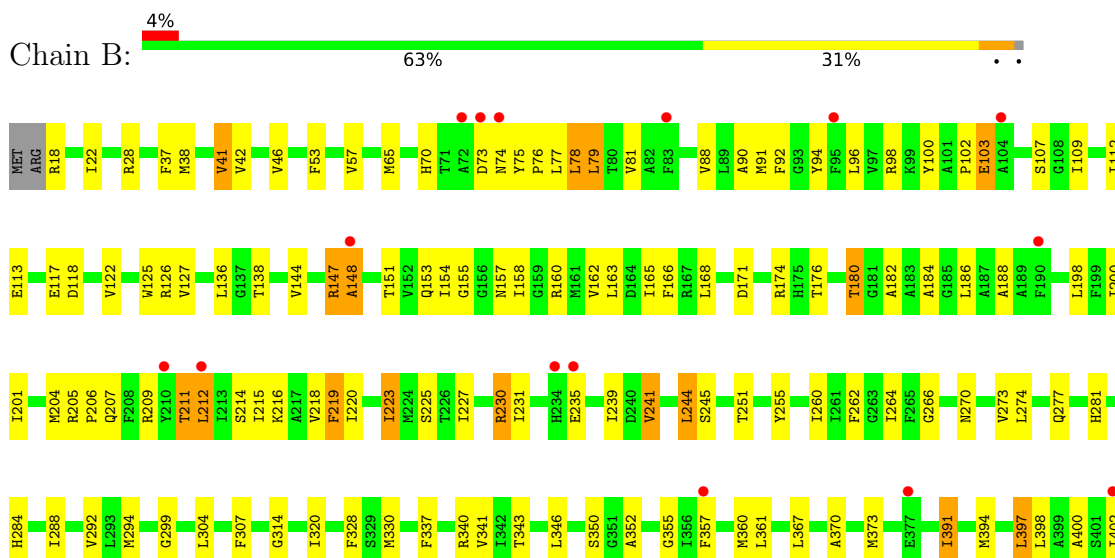
3 Residue-property plots

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

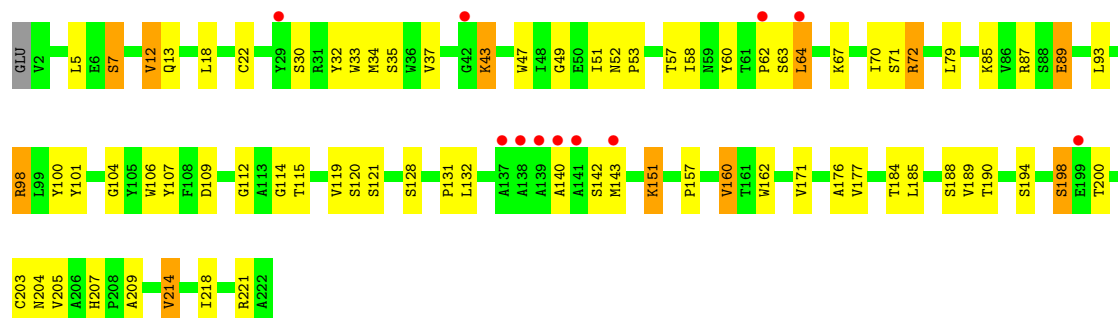


- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

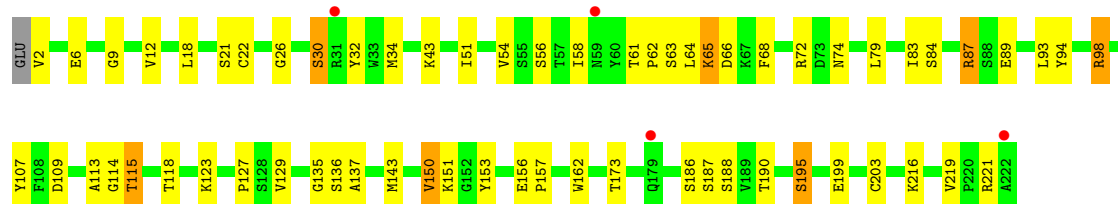




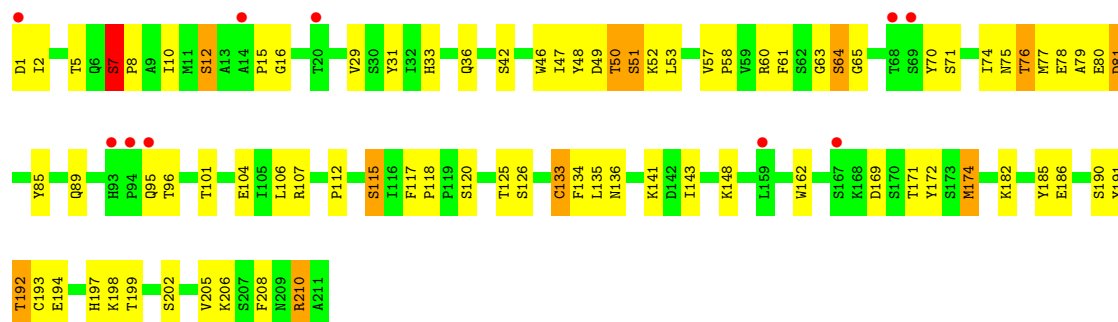
• Molecule 2: Fab, heavy chain



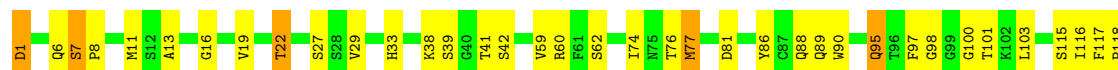
• Molecule 2: Fab, heavy chain

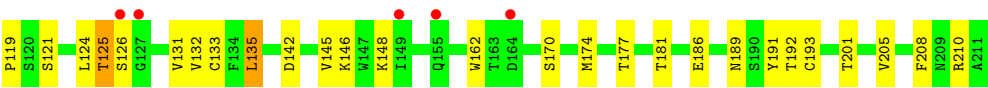


• Molecule 3: Fab, light chain



• 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	231.34Å 99.34Å 170.29Å 90.00° 131.94° 90.00°	Depositor
Resolution (Å)	39.85 – 3.00 39.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.85-3.00) 99.6 (39.85-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.220 , 0.265 0.223 , 0.267	Depositor DCC
R_{free} test set	2818 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.7	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	0.91	EDS
Total number of atoms	13206	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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

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	0.58	1/3392 (0.0%)	0.90	6/4604 (0.1%)
1	B	0.56	0/3372	0.92	5/4578 (0.1%)
2	C	0.67	0/1721	0.96	1/2355 (0.0%)
2	E	0.61	0/1721	0.90	1/2355 (0.0%)
3	D	0.58	0/1660	0.99	5/2257 (0.2%)
3	F	0.61	0/1660	0.95	2/2257 (0.1%)
All	All	0.60	1/13526 (0.0%)	0.93	20/18406 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ALA	CA-CB	5.40	1.62	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	CA-C-N	-10.97	107.73	120.13
3	F	7	SER	C-N-CA	-10.97	107.73	120.13
3	D	7	SER	CA-C-N	-7.28	110.73	119.84
3	D	7	SER	C-N-CA	-7.28	110.73	119.84
2	C	214	VAL	N-CA-C	6.44	117.98	108.45
1	B	355	GLY	N-CA-C	5.82	121.42	112.51
3	D	202	SER	CA-C-N	5.81	127.10	119.84
3	D	202	SER	C-N-CA	5.81	127.10	119.84
1	B	266	GLY	CA-C-N	5.79	125.48	119.05
1	B	266	GLY	C-N-CA	5.79	125.48	119.05
1	A	223	ILE	CB-CA-C	-5.60	104.53	111.70
1	A	108	GLY	N-CA-C	-5.44	107.51	114.85
2	E	30	SER	N-CA-C	-5.40	103.56	110.53
1	B	223	ILE	CB-CA-C	-5.24	105.00	111.70
1	B	147	ARG	N-CA-C	-5.23	106.85	113.18
1	A	266	GLY	CA-C-N	5.21	125.26	119.32
1	A	266	GLY	C-N-CA	5.21	125.26	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	136	ASN	N-CA-C	5.19	118.47	110.42
1	A	158	ILE	N-CA-C	-5.10	105.42	110.62
1	A	355	GLY	N-CA-C	5.08	120.90	112.66

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	116	0
1	B	3300	0	3456	120	0
2	C	1672	0	1654	40	0
2	E	1672	0	1654	38	0
3	D	1621	0	1548	57	0
3	F	1621	0	1546	46	0
All	All	13206	0	13333	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (368) 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:19:ARG:HD3	1:B:457:GLU:OE1	1.50	1.11
3:D:95:GLN:OE1	3:D:95:GLN:N	2.03	0.91
3:D:133:CYS:SG	3:D:193:CYS:CB	2.63	0.85
1:B:457:GLU:O	1:B:457:GLU:HG3	1.78	0.81
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.63	0.80
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.63	0.79
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.15	0.79
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.47	0.79
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.64	0.78
3:D:133:CYS:HG	3:D:193:CYS:CB	1.96	0.77
3:F:95:GLN:H	3:F:95:GLN:CD	1.93	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:133:CYS:CB	3:D:193:CYS:HG	1.99	0.75
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.51	0.74
3:F:1:ASP:OD2	3:F:1:ASP:N	2.19	0.74
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.69	0.74
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.22	0.72
1:A:200:ILE:HA	1:A:204:MET:HB2	1.71	0.71
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.71	0.71
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.22	0.71
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.25	0.71
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.73	0.71
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.74	0.70
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.25	0.69
1:B:200:ILE:HA	1:B:204:MET:HB2	1.75	0.68
1:A:422:ILE:HA	1:A:425:MET:HE3	1.75	0.68
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.76	0.68
1:B:422:ILE:HA	1:B:425:MET:HE3	1.75	0.67
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.07	0.67
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.25	0.67
3:F:189:ASN:HA	3:F:210:ARG:HD3	1.74	0.67
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.75	0.67
3:D:29:VAL:O	3:D:70:TYR:OH	2.11	0.67
3:D:49:ASP:O	3:D:51:SER:N	2.26	0.66
3:F:95:GLN:H	3:F:95:GLN:NE2	1.94	0.65
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.78	0.65
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.29	0.65
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.78	0.65
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.79	0.65
3:D:133:CYS:CB	3:D:193:CYS:SG	2.83	0.65
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.62	0.65
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.12	0.64
1:A:73:ASP:N	1:A:73:ASP:OD1	2.31	0.64
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.62	0.64
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.80	0.64
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.78	0.64
3:D:133:CYS:SG	3:D:193:CYS:HB3	2.38	0.64
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.80	0.64
2:E:129:VAL:HG22	2:E:150:VAL:HG13	1.80	0.64
3:F:38:LYS:O	3:F:41:THR:HG22	1.98	0.63
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.80	0.63
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.63	0.63
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.34	0.63
3:F:95:GLN:CD	3:F:95:GLN:N	2.55	0.62
1:B:330:MET:HE1	1:B:370:ALA:HB1	1.81	0.62
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.81	0.62
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.64	0.62
1:B:154:ILE:O	1:B:158:ILE:HG12	1.98	0.61
1:B:73:ASP:OD1	1:B:73:ASP:N	2.34	0.61
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.82	0.61
2:C:160:VAL:HG13	2:C:205:VAL:HG22	1.82	0.61
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.83	0.61
1:A:330:MET:HE1	1:A:370:ALA:HB1	1.81	0.61
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.82	0.60
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.82	0.60
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.83	0.60
1:A:88:VAL:HA	1:A:91:MET:HE2	1.84	0.60
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.37	0.60
1:B:88:VAL:HA	1:B:91:MET:HE2	1.82	0.59
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.37	0.59
2:E:32:TYR:O	2:E:72:ARG:NH2	2.35	0.59
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.38	0.59
1:B:37:PHE:HD2	1:B:38:MET:HE2	1.66	0.59
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.84	0.59
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.85	0.59
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.38	0.58
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.85	0.58
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.85	0.58
2:E:12:VAL:HG11	2:E:18:LEU:HD22	1.83	0.58
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.86	0.58
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.18	0.58
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.85	0.58
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.39	0.58
2:E:143:MET:HE3	2:E:190:THR:HG22	1.85	0.58
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.39	0.58
3:F:135:LEU:HG	3:F:174:MET:HE2	1.85	0.58
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.20	0.57
1:A:360:MET:HE1	1:A:402:ILE:HG13	1.87	0.57
2:E:9:GLY:H	2:E:115:THR:HG21	1.68	0.57
2:E:61:THR:O	2:E:63:SER:N	2.37	0.57
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.85	0.56
3:D:2:ILE:O	3:D:96:THR:HG21	2.05	0.56
1:B:360:MET:HE1	1:B:402:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HH11	1:B:457:GLU:CB	2.18	0.56
1:A:154:ILE:O	1:A:158:ILE:HG12	2.04	0.56
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.88	0.56
1:A:437:GLN:HE21	1:B:216:LYS:NZ	2.04	0.56
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.41	0.56
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.88	0.56
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.40	0.55
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.38	0.55
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.88	0.55
3:F:7:SER:HB3	3:F:22:THR:HB	1.88	0.55
1:A:314:GLY:O	1:A:340:ARG:NH2	2.40	0.55
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.22	0.55
2:E:94:TYR:O	2:E:114:GLY:HA2	2.06	0.55
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.07	0.54
1:A:148:ALA:HB1	1:A:357:PHE:HB3	1.90	0.54
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.89	0.54
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.07	0.54
1:A:37:PHE:CD2	1:A:38:MET:HE2	2.43	0.54
1:A:248:PRO:HB3	2:C:104:GLY:HA3	1.90	0.53
1:B:314:GLY:O	1:B:340:ARG:NH2	2.41	0.53
2:E:173:THR:HG23	2:E:187:SER:HB2	1.90	0.53
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.91	0.53
1:B:214:SER:O	1:B:218:VAL:HG23	2.08	0.53
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.90	0.53
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.90	0.53
1:B:112:ILE:HG13	1:B:153:GLN:HA	1.90	0.53
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.91	0.52
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.24	0.52
2:C:151:LYS:HB3	2:C:184:THR:HG23	1.92	0.52
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.78	0.52
3:D:169:ASP:OD1	3:D:171:THR:OG1	2.17	0.52
1:A:361:LEU:HD13	1:A:415:MET:HE1	1.91	0.52
1:A:227:ILE:O	1:A:231:ILE:HG12	2.10	0.52
3:F:145:VAL:HG11	3:F:174:MET:HE1	1.90	0.52
1:B:227:ILE:O	1:B:231:ILE:HG12	2.10	0.52
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.91	0.52
1:B:182:ALA:HB1	1:B:204:MET:HE2	1.92	0.52
2:E:129:VAL:O	2:E:216:LYS:HE3	2.09	0.52
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.92	0.51
1:B:239:ILE:HD13	1:B:320:ILE:HG21	1.92	0.51
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.92	0.51
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.93	0.51
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.91	0.51
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.92	0.51
1:B:212:LEU:HD12	1:B:212:LEU:H	1.75	0.51
2:C:143:MET:HE3	2:C:190:THR:HG22	1.91	0.51
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.92	0.51
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.46	0.51
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.46	0.51
3:D:12:SER:HA	3:D:104:GLU:O	2.10	0.51
1:B:361:LEU:HD13	1:B:415:MET:HE1	1.93	0.51
1:A:414:GLU:OE1	1:B:419:TYR:OH	2.21	0.50
1:B:37:PHE:CD2	1:B:38:MET:HE2	2.45	0.50
1:B:42:VAL:O	1:B:46:VAL:HG23	2.12	0.50
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.27	0.50
1:A:26:LEU:O	1:B:442:LYS:NZ	2.38	0.50
3:D:46:TRP:O	3:D:57:VAL:HG21	2.11	0.50
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.41	0.50
1:A:214:SER:O	1:A:218:VAL:HG23	2.11	0.50
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.26	0.50
3:D:112:PRO:HG3	3:D:143:ILE:HD11	1.92	0.50
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.47	0.50
1:A:100:TYR:O	1:A:126:ARG:NH1	2.41	0.50
1:A:383:HIS:HD1	2:C:106:TRP:CD1	2.30	0.50
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.47	0.49
1:A:427:ILE:HD11	1:B:227:ILE:HD11	1.93	0.49
3:F:6:GLN:NE2	3:F:100:GLY:H	2.10	0.49
2:C:89:GLU:OE2	2:C:89:GLU:N	2.45	0.49
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.27	0.49
1:A:239:ILE:HD13	1:A:320:ILE:HG21	1.94	0.49
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.94	0.49
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.27	0.49
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.12	0.49
1:A:330:MET:HE1	1:A:370:ALA:CB	2.42	0.49
3:D:31:TYR:HA	3:D:50:THR:OG1	2.12	0.49
2:E:135:GLY:O	2:E:137:ALA:N	2.39	0.49
1:A:328:PHE:O	1:A:373:MET:HE1	2.12	0.49
1:B:78:LEU:HD13	1:B:79:LEU:HD23	1.95	0.49
1:B:148:ALA:HB1	1:B:357:PHE:HB3	1.94	0.49
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.95	0.49
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.20	0.48
1:A:274:LEU:O	1:A:277:GLN:HB2	2.13	0.48
3:F:186:GLU:HG2	3:F:210:ARG:NH1	2.28	0.48
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.48	0.48
3:D:15:PRO:HA	3:D:77:MET:O	2.13	0.48
3:D:182:LYS:HE2	3:D:186:GLU:OE1	2.13	0.48
1:A:19:ARG:CD	1:B:457:GLU:OE1	2.42	0.48
1:A:78:LEU:HD13	1:A:79:LEU:HD23	1.95	0.48
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.49	0.48
2:C:131:PRO:O	2:C:132:LEU:HD23	2.14	0.48
2:C:151:LYS:HB2	2:C:151:LYS:HE3	1.61	0.48
1:A:410:ILE:O	1:A:414:GLU:HG3	2.14	0.47
2:C:64:LEU:HD11	2:C:87:ARG:HH12	1.79	0.47
3:D:106:LEU:HD23	3:D:107:ARG:N	2.29	0.47
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.96	0.47
3:D:191:TYR:HB2	3:D:208:PHE:CE2	2.49	0.47
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.96	0.47
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.77	0.47
3:D:53:LEU:HD13	3:D:57:VAL:HG12	1.96	0.47
2:E:113:ALA:HA	3:F:42:SER:OG	2.15	0.47
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.29	0.47
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.97	0.47
1:B:330:MET:HE1	1:B:370:ALA:CB	2.44	0.47
2:C:64:LEU:HD12	2:C:67:LYS:HD3	1.96	0.47
3:F:11:MET:CE	3:F:19:VAL:HG13	2.45	0.47
1:B:100:TYR:O	1:B:126:ARG:NH1	2.44	0.47
3:D:115:SER:HB3	3:D:117:PHE:CE1	2.49	0.47
3:F:191:TYR:HB2	3:F:208:PHE:CE2	2.50	0.47
1:B:103:GLU:H	1:B:103:GLU:HG3	1.29	0.47
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.55	0.47
3:F:6:GLN:HE21	3:F:98:GLY:C	2.23	0.47
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.97	0.47
1:B:176:THR:O	1:B:180:THR:HG23	2.15	0.46
3:D:60:ARG:HD2	3:D:76:THR:O	2.15	0.46
2:E:64:LEU:HB3	2:E:65:LYS:H	1.54	0.46
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.97	0.46
3:D:162:TRP:CG	3:D:174:MET:HG3	2.50	0.46
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.79	0.46
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.50	0.46
1:B:274:LEU:O	1:B:277:GLN:HB2	2.15	0.46
2:C:7:SER:HA	2:C:115:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:ASN:ND2	2:C:57:THR:HB	2.31	0.46
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.50	0.46
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.51	0.46
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.98	0.46
1:A:437:GLN:HE21	1:B:216:LYS:HZ1	1.64	0.46
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.97	0.46
3:D:95:GLN:H	3:D:95:GLN:CD	2.05	0.46
3:D:197:HIS:ND1	3:D:199:THR:OG1	2.35	0.46
2:E:68:PHE:HD2	2:E:83:ILE:HG12	1.81	0.46
3:D:78:GLU:O	3:D:81:ASP:HB2	2.16	0.46
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.51	0.46
1:B:53:PHE:O	1:B:57:VAL:HG23	2.16	0.46
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.82	0.46
1:A:22:ILE:HD13	1:B:454:ALA:HB2	1.98	0.45
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.97	0.45
1:B:160:ARG:O	1:B:163:LEU:HB3	2.16	0.45
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.71	0.45
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.99	0.45
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.31	0.45
3:F:11:MET:HE2	3:F:19:VAL:HG13	1.99	0.45
3:F:186:GLU:HA	3:F:210:ARG:NH1	2.31	0.45
1:B:109:ILE:HG23	1:B:204:MET:SD	2.56	0.45
1:A:98:ARG:HB3	1:A:288:ILE:HG13	1.99	0.45
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.81	0.45
2:C:30:SER:C	2:C:32:TYR:H	2.25	0.45
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.98	0.45
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.51	0.45
2:C:107:TYR:HB3	3:D:33:HIS:CE1	2.51	0.45
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.98	0.45
1:B:273:VAL:O	1:B:277:GLN:HG3	2.16	0.45
3:F:124:LEU:C	3:F:126:SER:H	2.25	0.45
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.51	0.45
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.34	0.45
1:B:91:MET:HG2	1:B:292:VAL:O	2.17	0.45
1:B:241:VAL:HG13	1:B:244:LEU:HD21	1.99	0.45
1:A:91:MET:HG2	1:A:292:VAL:O	2.17	0.44
1:B:410:ILE:O	1:B:414:GLU:HG3	2.17	0.44
1:A:18:ARG:O	1:A:22:ILE:HG13	2.16	0.44
3:F:90:TRP:CE3	3:F:95:GLN:HG3	2.52	0.44
1:A:53:PHE:O	1:A:57:VAL:HG23	2.17	0.44
1:A:184:ALA:HB1	1:A:225:SER:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.53	0.44
2:C:188:SER:HB3	3:D:134:PHE:CE2	2.51	0.44
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.47	0.44
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.16	0.44
1:B:78:LEU:HD11	1:B:307:PHE:CZ	2.53	0.44
3:D:64:SER:OG	3:D:65:GLY:N	2.48	0.44
3:D:89:GLN:O	3:D:95:GLN:HB2	2.17	0.44
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.51	0.44
2:E:135:GLY:C	2:E:137:ALA:H	2.23	0.44
3:F:6:GLN:HA	3:F:22:THR:O	2.18	0.44
1:A:90:ALA:HB2	1:A:299:GLY:HA3	2.00	0.44
1:A:180:THR:HB	1:A:218:VAL:HA	1.99	0.44
1:B:75:TYR:HA	1:B:78:LEU:HD12	1.99	0.44
2:E:6:GLU:CD	2:E:114:GLY:H	2.25	0.44
2:E:87:ARG:HH21	2:E:89:GLU:CB	2.31	0.44
3:F:77:MET:HE2	3:F:103:LEU:HD21	2.00	0.44
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.98	0.44
1:B:328:PHE:O	1:B:373:MET:HE1	2.18	0.44
1:A:426:ILE:HG23	1:B:219:PHE:HE2	1.83	0.43
1:B:165:ILE:HG22	1:B:166:PHE:CD2	2.53	0.43
2:E:113:ALA:HA	3:F:42:SER:HG	1.83	0.43
1:A:160:ARG:O	1:A:163:LEU:HB3	2.18	0.43
1:A:426:ILE:HG23	1:B:219:PHE:CE2	2.54	0.43
1:B:98:ARG:CB	1:B:288:ILE:HG13	2.48	0.43
2:C:85:LYS:HA	2:C:85:LYS:HD3	1.85	0.43
2:E:2:VAL:HA	2:E:26:GLY:HA3	2.01	0.43
1:A:220:ILE:HD11	1:B:434:LEU:HD11	2.00	0.43
1:A:337:PHE:O	1:A:341:VAL:HG23	2.19	0.43
1:B:38:MET:HA	1:B:41:VAL:HG13	2.00	0.43
2:E:123:LYS:HE2	2:E:123:LYS:HB3	1.73	0.43
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.18	0.43
1:A:212:LEU:HD12	1:A:212:LEU:H	1.84	0.43
1:A:346:LEU:O	1:A:350:SER:HB3	2.18	0.43
1:A:42:VAL:O	1:A:46:VAL:HG23	2.19	0.43
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.54	0.43
1:B:337:PHE:O	1:B:341:VAL:HG23	2.19	0.43
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.84	0.43
2:E:87:ARG:HH21	2:E:89:GLU:HB2	1.83	0.43
2:E:93:LEU:HD11	2:E:114:GLY:HA3	2.01	0.43
1:A:98:ARG:CB	1:A:288:ILE:HG13	2.49	0.43
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HB3	1:B:22:ILE:HG12	2.01	0.43
2:C:101:TYR:HB2	2:C:104:GLY:HA2	2.01	0.43
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.54	0.43
1:A:109:ILE:HG23	1:A:204:MET:SD	2.59	0.43
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.53	0.43
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.49	0.43
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.83	0.43
1:B:147:ARG:O	1:B:151:THR:HG23	2.19	0.42
1:B:235:GLU:OE1	2:C:100:TYR:HE2	2.01	0.42
2:E:156:GLU:OE1	2:E:157:PRO:HA	2.19	0.42
1:B:394:MET:HE2	1:B:412:VAL:HG22	2.01	0.42
2:C:107:TYR:CD1	2:C:107:TYR:C	2.98	0.42
1:B:92:PHE:O	1:B:96:LEU:HD23	2.19	0.42
3:D:174:MET:HE2	3:D:174:MET:HB3	1.63	0.42
1:B:46:VAL:HG22	1:B:155:GLY:HA2	2.02	0.42
3:D:7:SER:HB3	3:D:8:PRO:HD3	2.00	0.42
3:D:141:LYS:HB3	3:D:172:TYR:CZ	2.55	0.42
1:B:294:MET:HE2	1:B:294:MET:HB3	1.83	0.42
2:C:43:LYS:HE2	2:C:43:LYS:HB3	1.61	0.42
3:D:46:TRP:O	3:D:47:ILE:HG13	2.18	0.42
3:D:133:CYS:HG	3:D:193:CYS:HB3	1.81	0.42
2:E:65:LYS:HB2	2:E:66:ASP:H	1.55	0.42
3:D:133:CYS:HB3	3:D:193:CYS:HG	1.83	0.42
3:D:185:TYR:CZ	3:D:210:ARG:HD2	2.55	0.42
2:C:93:LEU:HD11	2:C:114:GLY:HA3	2.02	0.42
3:D:51:SER:HB3	3:D:63:GLY:O	2.19	0.42
1:A:75:TYR:HA	1:A:78:LEU:HD12	2.01	0.42
1:A:454:ALA:HB2	1:B:22:ILE:HG21	2.01	0.42
1:A:92:PHE:O	1:A:96:LEU:HD23	2.20	0.42
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.54	0.41
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.84	0.41
1:A:434:LEU:HD23	1:B:216:LYS:HD3	2.02	0.41
1:B:160:ARG:HD2	1:B:160:ARG:HA	1.66	0.41
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.55	0.41
2:E:6:GLU:HA	2:E:22:CYS:HA	2.02	0.41
3:F:115:SER:O	3:F:133:CYS:HA	2.20	0.41
1:A:227:ILE:HD11	1:B:427:ILE:HD11	2.02	0.41
1:B:171:ASP:OD2	1:B:174:ARG:NH1	2.42	0.41
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.20	0.41
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.28	0.41
1:A:171:ASP:OD2	1:A:174:ARG:NH1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:MET:HG3	1:B:168:LEU:HD11	2.02	0.41
2:C:194:SER:O	2:C:198:SER:OG	2.38	0.41
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.27	0.41
1:B:420:GLN:H	1:B:420:GLN:HG3	1.32	0.41
2:E:98:ARG:O	2:E:109:ASP:HB3	2.20	0.41
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.71	0.41
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.56	0.41
3:F:16:GLY:HA2	3:F:76:THR:HG23	2.01	0.41
1:A:120:ARG:NH1	1:A:452:THR:HG23	2.35	0.41
1:A:122:VAL:HG11	1:A:160:ARG:HB2	2.02	0.41
1:A:150:PRO:CG	1:A:354:GLY:HA2	2.51	0.41
1:A:241:VAL:HG13	1:A:244:LEU:HD21	2.03	0.41
1:B:160:ARG:HH11	1:B:160:ARG:HD3	1.76	0.41
1:B:421:LEU:C	1:B:424:PRO:HD2	2.45	0.41
2:C:35:SER:OG	2:C:49:GLY:O	2.34	0.41
2:E:195:SER:O	2:E:199:GLU:HB3	2.21	0.41
1:B:144:VAL:HG21	1:B:343:THR:OG1	2.20	0.41
1:B:270:ASN:HD22	1:B:270:ASN:HA	1.65	0.41
3:D:141:LYS:HB3	3:D:172:TYR:CE2	2.56	0.41
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.87	0.40
1:B:346:LEU:O	1:B:350:SER:HB3	2.22	0.40
2:C:112:GLY:O	3:D:42:SER:HB3	2.21	0.40
3:D:79:ALA:C	3:D:81:ASP:H	2.28	0.40
3:F:8:PRO:O	3:F:101:THR:HG23	2.21	0.40
3:D:197:HIS:CD2	3:D:198:LYS:H	2.38	0.40
1:A:160:ARG:HH11	1:A:160:ARG:HD3	1.71	0.40
1:A:29:ASP:OD2	1:A:216:LYS:HE3	2.21	0.40
1:B:188:ALA:HB2	1:B:225:SER:OG	2.21	0.40
3:F:29:VAL:HG11	3:F:89:GLN:HG2	2.02	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%)	415 (94%)	25 (6%)	1 (0%)	43	76
1	B	439/446 (98%)	416 (95%)	22 (5%)	1 (0%)	43	76
2	C	219/222 (99%)	198 (90%)	18 (8%)	3 (1%)	9	36
2	E	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	9	36
3	D	209/211 (99%)	183 (88%)	21 (10%)	5 (2%)	4	24
3	F	209/211 (99%)	188 (90%)	20 (10%)	1 (0%)	24	60
All	All	1736/1758 (99%)	1597 (92%)	125 (7%)	14 (1%)	16	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	B	148	ALA
2	C	140	ALA
3	D	50	THR
2	E	62	PRO
2	E	65	LYS
2	E	136	SER
3	D	76	THR
3	D	126	SER
3	F	125	THR
2	C	62	PRO
3	D	80	GLU
3	D	7	SER
2	C	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	333/336 (99%)	294 (88%)	39 (12%)	5	23
1	B	331/336 (98%)	297 (90%)	34 (10%)	7	28
2	C	181/182 (100%)	157 (87%)	24 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	181/182 (100%)	167 (92%)	14 (8%)	12	40
3	D	185/185 (100%)	165 (89%)	20 (11%)	6	26
3	F	185/185 (100%)	167 (90%)	18 (10%)	8	30
All	All	1396/1406 (99%)	1247 (89%)	149 (11%)	6	26

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	41	VAL
1	A	65	MET
1	A	70	HIS
1	A	78	LEU
1	A	79	LEU
1	A	81	VAL
1	A	103	GLU
1	A	107	SER
1	A	111	GLU
1	A	113	GLU
1	A	136	LEU
1	A	145	LEU
1	A	162	VAL
1	A	180	THR
1	A	186	LEU
1	A	200	ILE
1	A	201	ILE
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	230	ARG
1	A	241	VAL
1	A	244	LEU
1	A	245	SER
1	A	251	THR
1	A	264	ILE
1	A	304	LEU
1	A	391	ILE
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	433	THR
1	A	444	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	41	VAL
1	B	65	MET
1	B	70	HIS
1	B	78	LEU
1	B	79	LEU
1	B	81	VAL
1	B	103	GLU
1	B	107	SER
1	B	113	GLU
1	B	136	LEU
1	B	162	VAL
1	B	180	THR
1	B	186	LEU
1	B	201	ILE
1	B	205	ARG
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	230	ARG
1	B	241	VAL
1	B	244	LEU
1	B	245	SER
1	B	251	THR
1	B	264	ILE
1	B	304	LEU
1	B	391	ILE
1	B	397	LEU
1	B	420	GLN
1	B	423	LEU
1	B	430	LEU
1	B	433	THR
1	B	444	LEU
1	B	453	LEU
2	C	5	LEU
2	C	7	SER

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Mol	Chain	Res	Type
2	C	12	VAL
2	C	13	GLN
2	C	18	LEU
2	C	43	LYS
2	C	63	SER
2	C	64	LEU
2	C	71	SER
2	C	72	ARG
2	C	89	GLU
2	C	98	ARG
2	C	120	SER
2	C	121	SER
2	C	128	SER
2	C	142	SER
2	C	151	LYS
2	C	160	VAL
2	C	177	VAL
2	C	198	SER
2	C	200	THR
2	C	204	ASN
2	C	214	VAL
2	C	218	ILE
3	D	1	ASP
3	D	5	THR
3	D	10	ILE
3	D	12	SER
3	D	51	SER
3	D	64	SER
3	D	71	SER
3	D	75	ASN
3	D	81	ASP
3	D	101	THR
3	D	115	SER
3	D	120	SER
3	D	125	THR
3	D	133	CYS
3	D	135	LEU
3	D	174	MET
3	D	190	SER
3	D	192	THR
3	D	206	LYS
3	D	210	ARG

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Mol	Chain	Res	Type
2	E	21	SER
2	E	30	SER
2	E	43	LYS
2	E	84	SER
2	E	87	ARG
2	E	98	ARG
2	E	115	THR
2	E	118	THR
2	E	150	VAL
2	E	151	LYS
2	E	186	SER
2	E	188	SER
2	E	195	SER
2	E	219	VAL
3	F	1	ASP
3	F	22	THR
3	F	27	SER
3	F	39	SER
3	F	59	VAL
3	F	62	SER
3	F	74	ILE
3	F	77	MET
3	F	95	GLN
3	F	121	SER
3	F	125	THR
3	F	135	LEU
3	F	142	ASP
3	F	146	LYS
3	F	170	SER
3	F	181	THR
3	F	201	THR
3	F	205	VAL

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

Mol	Chain	Res	Type
1	A	153	GLN
1	A	234	HIS
1	A	270	ASN
1	A	437	GLN
1	B	24	GLN
1	B	153	GLN

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Mol	Chain	Res	Type
1	B	175	HIS
1	B	270	ASN
1	B	420	GLN
1	B	437	GLN
3	D	136	ASN
3	D	137	ASN
3	D	209	ASN
3	F	6	GLN
3	F	36	GLN
3	F	136	ASN

5.3.3 RNA [i](#)

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%)	0.21	21 (4%)	36 19	38, 57, 83, 126	0
1	B	441/446 (98%)	0.20	16 (3%)	46 26	37, 63, 101, 133	0
2	C	221/222 (99%)	0.04	11 (4%)	34 18	28, 56, 91, 124	0
2	E	221/222 (99%)	-0.07	4 (1%)	67 44	34, 54, 86, 123	0
3	D	211/211 (100%)	0.23	10 (4%)	36 19	40, 65, 89, 100	0
3	F	211/211 (100%)	-0.17	5 (2%)	59 36	31, 49, 99, 120	0
All	All	1748/1758 (99%)	0.11	67 (3%)	44 24	28, 58, 93, 133	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	6.3
1	B	357	PHE	5.2
1	B	72	ALA	5.2
1	B	73	ASP	5.1
2	C	139	ALA	4.9
1	A	380	PRO	4.9
2	C	141	ALA	4.1
1	A	166	PHE	3.9
1	A	377	GLU	3.7
2	E	59	ASN	3.6
1	A	171	ASP	3.6
1	B	210	TYR	3.5
3	F	164	ASP	3.5
1	A	148	ALA	3.4
1	A	207	GLN	3.4
3	D	93	HIS	3.4
2	C	137	ALA	3.3
1	A	170	GLY	3.3
3	D	20	THR	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	1	ASP	3.1
3	D	94	PRO	3.1
1	A	378	LEU	3.1
1	A	235	GLU	3.1
2	C	140	ALA	2.9
2	C	138	ALA	2.9
1	B	104	ALA	2.9
1	A	357	PHE	2.9
1	B	234	HIS	2.8
3	F	155	GLN	2.8
1	B	148	ALA	2.8
1	A	455	LYS	2.8
2	E	31	ARG	2.8
1	B	212	LEU	2.8
1	A	167	ARG	2.8
1	B	235	GLU	2.7
3	D	95	GLN	2.6
2	C	199	GLU	2.6
2	E	222	ALA	2.6
3	D	69	SER	2.6
3	D	159	LEU	2.5
1	A	212	LEU	2.4
1	B	74	ASN	2.3
2	C	42	GLY	2.3
1	A	180	THR	2.3
1	A	165	ILE	2.3
1	B	402	ILE	2.3
3	F	126	SER	2.3
1	B	458	ALA	2.3
2	C	29	TYR	2.3
1	A	184	ALA	2.2
3	D	167	SER	2.2
1	B	377	GLU	2.2
3	D	14	ALA	2.2
1	B	190	PHE	2.2
3	F	149	ILE	2.2
2	C	143	MET	2.2
3	F	127	GLY	2.2
1	A	440	GLY	2.2
1	B	95	PHE	2.1
3	D	68	THR	2.1
2	C	62	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	83	PHE	2.1
1	A	258	LEU	2.1
1	A	220	ILE	2.0
2	C	64	LEU	2.0
1	A	169	LYS	2.0
2	E	179	GLN	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.