



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:38 AM UTC

PDB ID : 4KJQ / pdb_00004kjq
Title : Structure of the CLC-ec1 deltaNC construct in 100mM fluoride
Authors : Lim, H.-H.; Miller, C.
Deposited on : 2013-05-03
Resolution : 2.88 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

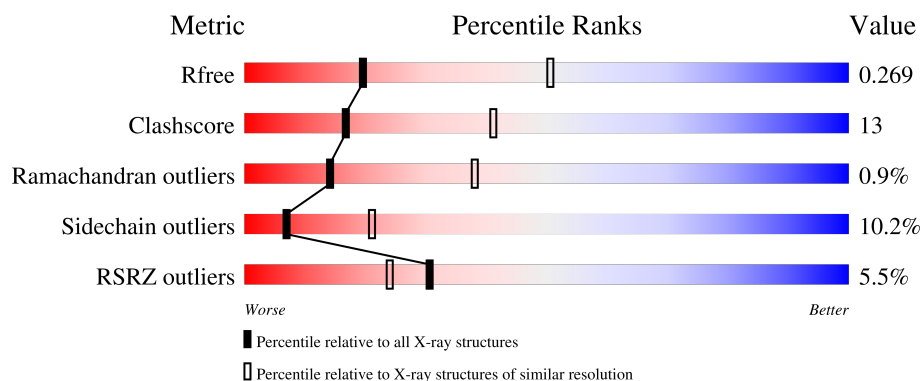
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	7% 67% 28% 5%
1	B	446	7% 66% 28% ..
2	C	222	5% 69% 26% .
2	E	222	2% 68% 27% .
3	D	211	8% 70% 27% ..

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Mol	Chain	Length	Quality of chain
3	F	211	2% 74% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13225 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
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	expression tag	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			

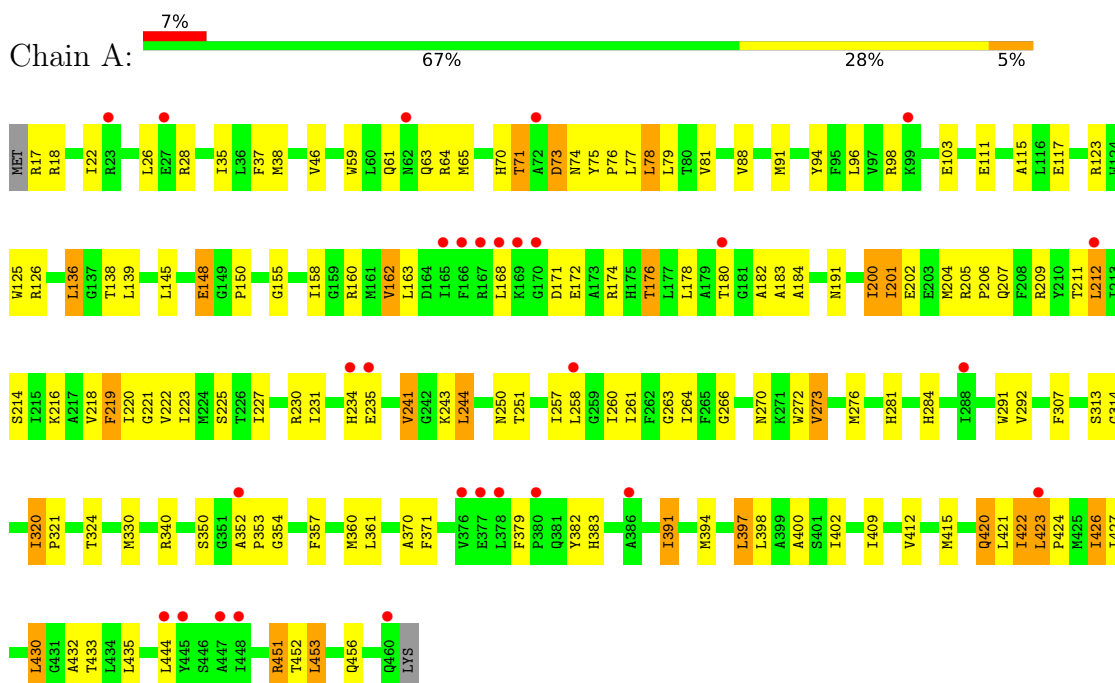
- Molecule 4 is FLUORIDE ION (CCD ID: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	F	0	0
			1	1		
4	B	1	Total	F	0	0
			1	1		

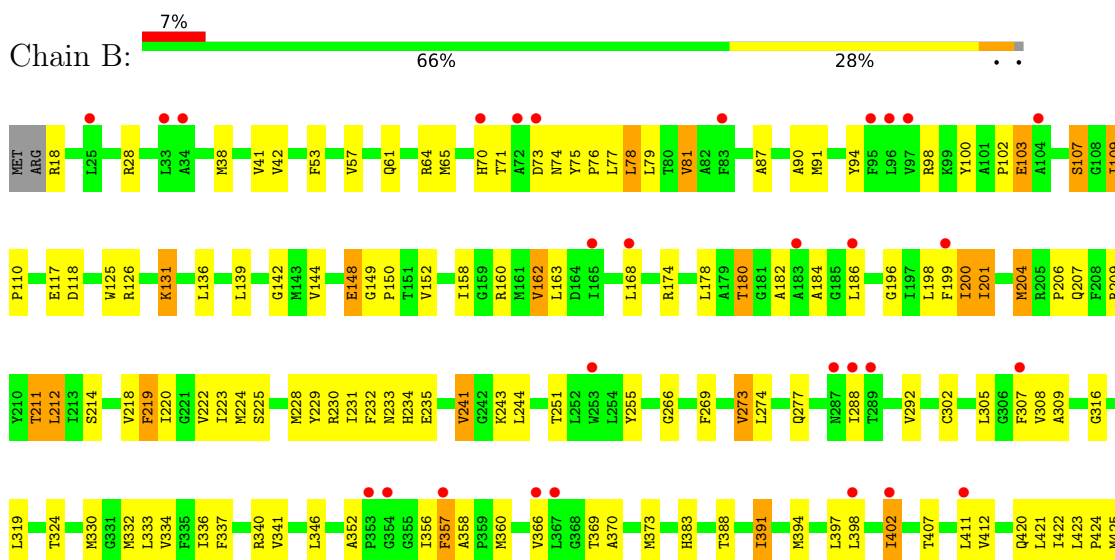
3 Residue-property plots

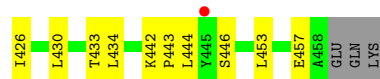
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

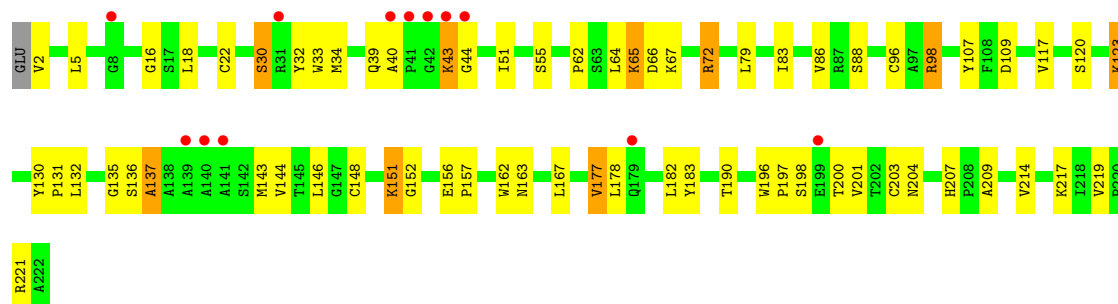


- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

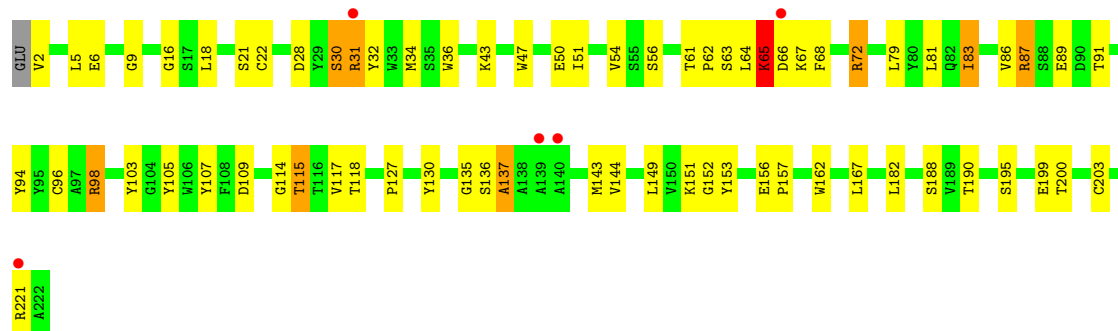




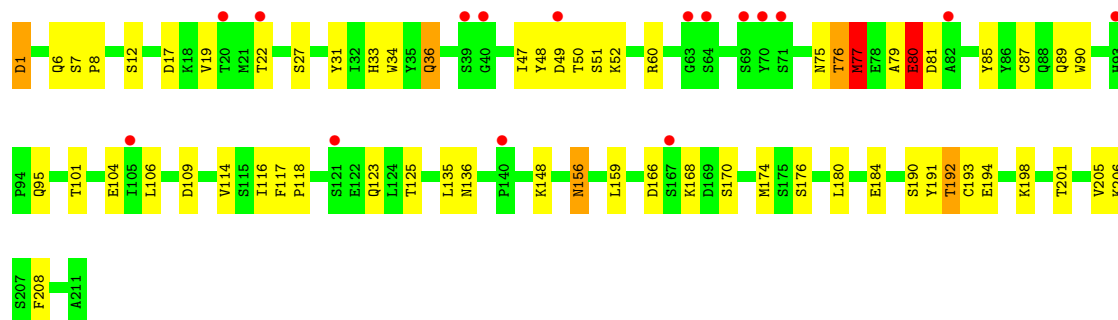
• Molecule 2: Fab, heavy chain



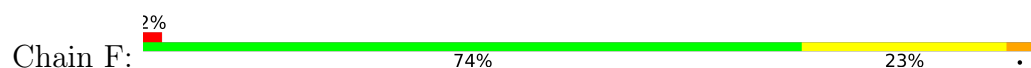
• Molecule 2: Fab, heavy chain

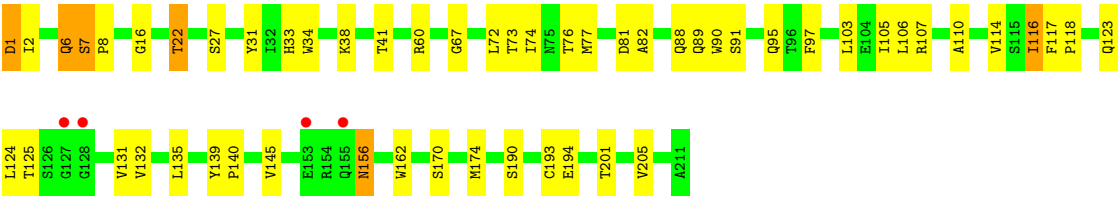


• Molecule 3: Fab, light chain



• 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	231.31Å 100.15Å 169.97Å 90.00° 132.02° 90.00°	Depositor
Resolution (Å)	39.37 – 2.88 39.37 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.37-2.88) 99.4 (39.37-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.220 , 0.263 0.226 , 0.269	Depositor DCC
R_{free} test set	3317 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13225	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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:
F

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	0.60	0/3405	0.98	9/4621 (0.2%)
1	B	0.58	0/3376	0.97	8/4583 (0.2%)
2	C	0.61	0/1721	0.93	1/2355 (0.0%)
2	E	0.58	0/1721	0.89	1/2355 (0.0%)
3	D	0.58	0/1660	0.94	3/2257 (0.1%)
3	F	0.57	0/1660	0.91	4/2257 (0.2%)
All	All	0.59	0/13543	0.95	26/18428 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	PHE	N-CA-C	9.49	121.23	111.07
1	A	427	ILE	N-CA-C	9.16	119.98	110.36
1	A	176	THR	N-CA-C	7.68	119.34	110.97
3	F	7	SER	N-CA-C	7.64	122.86	112.55
1	B	107	SER	N-CA-C	7.02	118.83	111.03
1	A	426	ILE	CB-CA-C	-6.33	103.77	111.88
1	A	426	ILE	N-CA-C	6.13	116.79	110.36
3	F	7	SER	CA-C-N	-5.99	112.35	119.84
3	F	7	SER	C-N-CA	-5.99	112.35	119.84
1	B	358	ALA	CA-C-N	-5.99	113.64	119.87
1	B	358	ALA	C-N-CA	-5.99	113.64	119.87
3	D	136	ASN	N-CA-C	5.79	118.39	109.07
1	A	176	THR	CB-CA-C	-5.67	102.22	110.96
3	D	7	SER	CA-C-N	-5.66	112.76	119.84
3	D	7	SER	C-N-CA	-5.66	112.76	119.84
1	B	266	GLY	CA-C-N	5.57	125.23	119.05
1	B	266	GLY	C-N-CA	5.57	125.23	119.05
1	A	427	ILE	CB-CA-C	-5.54	104.79	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	GLY	CA-C-N	5.52	125.62	119.32
1	A	266	GLY	C-N-CA	5.52	125.62	119.32
2	C	151	LYS	N-CA-C	5.33	117.92	109.50
3	F	124	LEU	N-CA-C	5.21	118.90	112.54
2	E	28	ASP	N-CA-C	-5.18	99.76	110.80
1	A	223	ILE	CB-CA-C	-5.08	105.20	111.70
1	B	309	ALA	CA-C-N	5.03	124.69	119.56
1	B	309	ALA	C-N-CA	5.03	124.69	119.56

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	3333	0	3484	123	0
1	B	3304	0	3457	100	0
2	C	1672	0	1654	33	0
2	E	1672	0	1654	35	0
3	D	1621	0	1546	45	0
3	F	1621	0	1546	35	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
All	All	13225	0	13341	339	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 13.

All (339) 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:28:ARG:HE	1:B:207:GLN:HG2	1.25	0.97
1:A:201:ILE:O	1:A:201:ILE:HG13	1.66	0.96
1:A:200:ILE:HD12	1:A:204:MET:HB2	1.50	0.93
1:A:422:ILE:HG23	1:A:423:LEU:N	1.80	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:MET:O	3:D:77:MET:HG3	1.68	0.91
3:F:95:GLN:OE1	3:F:95:GLN:N	2.05	0.89
1:A:422:ILE:CG2	1:A:423:LEU:N	2.36	0.88
3:D:79:ALA:O	3:D:81:ASP:N	2.04	0.88
1:A:422:ILE:CG2	1:A:423:LEU:H	1.87	0.88
3:D:95:GLN:OE1	3:D:95:GLN:N	2.08	0.87
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.59	0.84
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.15	0.81
1:A:421:LEU:C	1:A:424:PRO:HD2	2.07	0.80
1:A:200:ILE:HD12	1:A:204:MET:CB	2.11	0.80
3:F:1:ASP:OD2	3:F:1:ASP:N	2.16	0.78
1:A:201:ILE:O	1:A:201:ILE:CG1	2.30	0.77
1:A:200:ILE:CD1	1:A:204:MET:HG3	2.16	0.75
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.68	0.75
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.69	0.74
2:E:143:MET:HE3	2:E:190:THR:HG22	1.69	0.73
1:B:198:LEU:HD13	1:B:201:ILE:HD11	1.70	0.72
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.72	0.71
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.72	0.71
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.05	0.71
3:F:77:MET:HE3	3:F:103:LEU:HD21	1.73	0.71
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.74	0.69
2:E:130:TYR:CE2	3:F:123:GLN:HG3	2.27	0.69
1:A:360:MET:HE1	1:A:402:ILE:HD11	1.74	0.69
1:A:357:PHE:CZ	1:A:398:LEU:HD13	2.28	0.69
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.76	0.68
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.74	0.68
1:A:330:MET:HE1	1:A:370:ALA:HB1	1.76	0.68
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.75	0.67
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.28	0.67
1:A:200:ILE:HA	1:A:204:MET:HB2	1.76	0.67
1:B:212:LEU:HD12	1:B:212:LEU:H	1.60	0.66
3:D:49:ASP:O	3:D:51:SER:N	2.26	0.66
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.60	0.66
1:B:180:THR:HB	1:B:218:VAL:HA	1.77	0.65
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.77	0.65
1:B:360:MET:HE1	1:B:402:ILE:HG13	1.78	0.65
1:A:200:ILE:HD13	1:A:204:MET:HG3	1.78	0.65
3:D:76:THR:O	3:D:77:MET:C	2.39	0.65
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.77	0.65
1:A:422:ILE:HG22	1:A:423:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1:ASP:OD2	3:D:1:ASP:N	2.24	0.64
1:A:421:LEU:O	1:A:424:PRO:HD2	1.96	0.64
1:B:180:THR:HA	1:B:218:VAL:HG13	1.80	0.64
3:D:116:ILE:HD12	3:D:193:CYS:HB2	1.79	0.63
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.62	0.63
3:D:79:ALA:C	3:D:81:ASP:H	2.05	0.63
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.79	0.63
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.31	0.62
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.80	0.62
1:B:394:MET:HG2	1:B:412:VAL:HG22	1.81	0.62
3:D:89:GLN:O	3:D:95:GLN:HB2	1.99	0.62
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.65	0.62
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.81	0.62
1:A:320:ILE:CB	1:A:321:PRO:HD3	2.29	0.62
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.80	0.62
1:B:330:MET:HE1	1:B:370:ALA:HB1	1.81	0.61
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.65	0.61
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.30	0.61
3:D:60:ARG:NH2	3:D:80:GLU:OE1	2.26	0.61
2:C:39:GLN:HG3	2:C:44:GLY:O	2.00	0.60
3:F:38:LYS:O	3:F:41:THR:HG22	2.01	0.60
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.16	0.60
1:B:148:GLU:CD	1:B:148:GLU:H	2.08	0.60
1:B:243:LYS:HB3	2:E:31:ARG:HH21	1.65	0.60
1:A:73:ASP:OD1	1:A:73:ASP:N	2.34	0.60
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.36	0.60
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.82	0.60
3:D:12:SER:HA	3:D:104:GLU:O	2.02	0.60
1:A:71:THR:O	1:A:71:THR:OG1	2.21	0.59
1:A:357:PHE:CZ	1:A:398:LEU:CD1	2.85	0.59
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.28	0.59
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.85	0.58
3:D:79:ALA:C	3:D:81:ASP:N	2.60	0.58
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.86	0.58
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.39	0.58
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.32	0.58
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.86	0.58
1:A:200:ILE:HG22	1:A:201:ILE:N	2.19	0.57
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.86	0.57
1:B:336:ILE:O	1:B:340:ARG:HG3	2.05	0.57
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.85	0.57
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.37	0.57
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.87	0.57
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.87	0.57
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.87	0.56
1:A:272:TRP:O	1:A:276:MET:HB2	2.06	0.56
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.87	0.56
2:E:9:GLY:H	2:E:115:THR:HG21	1.70	0.56
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.87	0.56
1:A:219:PHE:HB3	1:B:430:LEU:CD1	2.35	0.56
3:F:77:MET:HE3	3:F:103:LEU:CD2	2.35	0.56
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.88	0.56
1:A:430:LEU:HD13	1:B:223:ILE:HD11	1.87	0.56
2:C:40:ALA:HB3	2:C:43:LYS:HB2	1.88	0.56
2:E:91:THR:HG23	2:E:118:THR:HA	1.89	0.55
1:A:360:MET:HG2	1:A:397:LEU:HD13	1.89	0.55
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.89	0.55
3:D:156:ASN:OD1	3:D:156:ASN:N	2.39	0.55
1:A:148:GLU:CD	1:A:148:GLU:H	2.15	0.54
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.23	0.54
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.23	0.54
1:A:115:ALA:HB1	1:A:178:LEU:HD21	1.90	0.54
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.06	0.54
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.43	0.54
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.88	0.54
1:B:356:ILE:HG22	4:B:501:F:F	1.98	0.54
1:B:394:MET:HG2	1:B:412:VAL:CG2	2.37	0.54
1:B:91:MET:HG2	1:B:292:VAL:O	2.07	0.54
1:A:174:ARG:O	1:A:178:LEU:HB2	2.08	0.54
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.89	0.54
1:B:38:MET:O	1:B:42:VAL:HG23	2.08	0.53
1:A:214:SER:O	1:A:218:VAL:HG23	2.09	0.53
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.43	0.53
1:A:94:TYR:OH	1:A:350:SER:OG	2.24	0.53
1:A:394:MET:HE2	1:A:412:VAL:HG22	1.89	0.53
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.91	0.53
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.91	0.53
1:B:107:SER:O	1:B:149:GLY:CA	2.57	0.53
3:D:75:ASN:C	3:D:77:MET:H	2.17	0.52
1:A:422:ILE:HG23	1:A:423:LEU:H	1.53	0.52
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:156:ASN:OD1	3:F:156:ASN:N	2.42	0.52
3:D:180:LEU:HD22	3:D:184:GLU:HG2	1.92	0.52
1:A:35:ILE:CG2	1:A:176:THR:HG21	2.39	0.52
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.45	0.52
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.92	0.52
1:B:87:ALA:O	1:B:91:MET:HG3	2.10	0.51
2:E:64:LEU:HB2	2:E:67:LYS:HB2	1.91	0.51
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.24	0.51
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.46	0.51
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.40	0.51
1:A:357:PHE:CE2	1:A:398:LEU:HD11	2.46	0.51
1:A:394:MET:HG2	1:A:412:VAL:HG22	1.92	0.51
1:B:241:VAL:HG22	1:B:324:THR:HG21	1.92	0.51
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.46	0.51
3:F:116:ILE:HD12	3:F:193:CYS:HB2	1.93	0.51
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.46	0.51
3:F:145:VAL:HG11	3:F:174:MET:HE1	1.92	0.51
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.92	0.51
3:D:8:PRO:O	3:D:101:THR:HG23	2.11	0.51
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.76	0.51
1:A:227:ILE:O	1:A:231:ILE:HG12	2.10	0.50
2:C:221:ARG:NH2	3:D:118:PRO:HB2	2.26	0.50
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.44	0.50
2:C:143:MET:HE3	2:C:190:THR:HG22	1.94	0.50
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.93	0.50
2:E:152:GLY:HA2	2:E:182:LEU:HD13	1.92	0.50
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.47	0.50
1:B:142:GLY:O	1:B:302:CYS:HB3	2.10	0.50
3:F:34:TRP:CG	3:F:72:LEU:HD12	2.46	0.50
1:B:53:PHE:O	1:B:57:VAL:HG23	2.11	0.50
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.94	0.50
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.47	0.50
1:B:148:GLU:OE1	1:B:357:PHE:HB3	2.12	0.50
1:A:360:MET:HE1	1:A:402:ILE:CD1	2.41	0.49
1:A:361:LEU:HD13	1:A:415:MET:HE1	1.94	0.49
1:B:107:SER:O	1:B:149:GLY:HA3	2.12	0.49
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.47	0.49
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.45	0.49
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.77	0.49
3:D:17:ASP:O	3:D:77:MET:HB3	2.13	0.49
2:C:135:GLY:O	2:C:137:ALA:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:GLN:HA	3:F:22:THR:O	2.13	0.49
1:A:183:ALA:HB2	1:A:200:ILE:HG12	1.94	0.49
1:A:212:LEU:HD12	1:A:212:LEU:H	1.77	0.49
1:A:75:TYR:HA	1:A:78:LEU:HD12	1.94	0.49
1:B:234:HIS:CD2	1:B:235:GLU:HG2	2.48	0.49
3:D:166:ASP:OD1	3:D:168:LYS:HB2	2.13	0.49
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.95	0.49
2:C:177:VAL:HG21	3:D:159:LEU:HD13	1.95	0.49
2:C:131:PRO:O	2:C:132:LEU:HD23	2.12	0.49
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.95	0.48
1:B:204:MET:HB3	1:B:204:MET:HE3	1.75	0.48
1:B:333:LEU:HD22	1:B:366:VAL:HG13	1.95	0.48
1:B:422:ILE:HA	1:B:425:MET:CE	2.43	0.48
2:E:30:SER:C	2:E:32:TYR:H	2.21	0.48
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.43	0.48
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.96	0.48
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.96	0.48
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.95	0.48
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.96	0.47
3:D:19:VAL:HG23	3:D:77:MET:CB	2.44	0.47
1:A:88:VAL:HA	1:A:91:MET:HE2	1.96	0.47
1:A:200:ILE:HD12	1:A:204:MET:CG	2.44	0.47
1:B:71:THR:O	1:B:71:THR:OG1	2.26	0.47
1:A:117:GLU:OE2	1:A:206:PRO:HB3	2.15	0.47
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.97	0.47
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.49	0.47
3:F:89:GLN:O	3:F:95:GLN:HB2	2.15	0.47
1:A:421:LEU:O	1:A:424:PRO:CD	2.62	0.47
1:A:91:MET:HG2	1:A:292:VAL:O	2.15	0.47
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.96	0.47
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.50	0.47
2:E:87:ARG:HH21	2:E:89:GLU:HG2	1.80	0.47
1:A:180:THR:CG2	1:A:221:GLY:HA3	2.45	0.46
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.96	0.46
1:B:422:ILE:HA	1:B:425:MET:HE2	1.97	0.46
1:A:409:ILE:HD13	1:A:426:ILE:HA	1.96	0.46
1:B:269:PHE:O	1:B:273:VAL:HG12	2.14	0.46
1:B:383:HIS:NE2	2:E:50:GLU:OE1	2.42	0.46
2:C:163:ASN:HD22	2:C:167:LEU:HD22	1.81	0.46
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.78	0.46
1:B:214:SER:O	1:B:218:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ILE:N	1:B:110:PRO:CD	2.78	0.46
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.68	0.46
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.96	0.46
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.97	0.46
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.74	0.46
1:B:100:TYR:O	1:B:126:ARG:NH1	2.44	0.46
1:B:316:GLY:O	1:B:319:LEU:HG	2.16	0.46
3:D:75:ASN:C	3:D:77:MET:N	2.74	0.46
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.98	0.46
1:A:26:LEU:HB3	1:B:442:LYS:HZ3	1.80	0.45
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.81	0.45
1:A:219:PHE:HB3	1:B:430:LEU:HD11	1.97	0.45
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.98	0.45
1:A:394:MET:HE3	1:A:415:MET:HE3	1.98	0.45
2:E:135:GLY:O	2:E:137:ALA:N	2.45	0.45
3:F:107:ARG:NH2	3:F:110:ALA:HB2	2.31	0.45
1:A:320:ILE:CB	1:A:321:PRO:CD	2.95	0.45
1:B:229:TYR:O	1:B:233:ASN:HB2	2.17	0.45
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.52	0.45
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.51	0.45
1:A:200:ILE:CD1	1:A:204:MET:CG	2.92	0.45
1:A:270:ASN:O	1:A:273:VAL:HG13	2.16	0.45
1:B:73:ASP:OD1	1:B:73:ASP:N	2.40	0.45
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.52	0.45
1:A:158:ILE:O	1:A:162:VAL:HG13	2.18	0.44
1:A:250:ASN:ND2	1:A:382:TYR:HE2	2.16	0.44
1:A:313:SER:OG	1:A:314:GLY:N	2.50	0.44
2:C:18:LEU:HD11	2:C:117:VAL:HG22	1.99	0.44
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.52	0.44
2:E:16:GLY:O	2:E:86:VAL:HG23	2.17	0.44
2:C:130:TYR:CZ	3:D:123:GLN:HG3	2.51	0.44
2:E:51:ILE:CD1	2:E:72:ARG:HG2	2.48	0.44
1:A:35:ILE:HG23	1:A:176:THR:HG21	2.00	0.44
2:E:65:LYS:H	2:E:65:LYS:HG3	1.60	0.44
2:C:217:LYS:HE2	2:C:219:VAL:HG12	2.00	0.44
1:A:423:LEU:N	1:A:424:PRO:CD	2.81	0.44
1:B:224:MET:O	1:B:228:MET:HG2	2.18	0.44
2:C:40:ALA:HB3	2:C:43:LYS:CB	2.48	0.44
1:B:388:THR:HG22	1:B:421:LEU:HD11	2.00	0.44
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.88	0.44
1:B:274:LEU:O	1:B:277:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.00	0.43
1:A:420:GLN:H	1:A:420:GLN:HG3	1.47	0.43
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.26	0.43
2:C:16:GLY:O	2:C:86:VAL:HG23	2.17	0.43
2:E:149:LEU:HD13	3:F:132:VAL:HG21	1.99	0.43
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.71	0.43
2:C:123:LYS:NZ	2:C:123:LYS:HB3	2.34	0.43
3:D:19:VAL:HG23	3:D:77:MET:HB2	2.01	0.43
2:E:68:PHE:CE2	2:E:83:ILE:HG23	2.53	0.43
3:F:139:TYR:CD2	3:F:140:PRO:HA	2.54	0.43
1:A:139:LEU:HD21	1:A:145:LEU:HB2	2.00	0.43
1:A:243:LYS:HD2	1:A:420:GLN:NE2	2.33	0.43
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.82	0.43
1:A:59:TRP:O	1:A:63:GLN:HG2	2.19	0.43
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.53	0.43
1:B:174:ARG:O	1:B:178:LEU:HB2	2.18	0.43
1:B:206:PRO:HG2	1:B:211:THR:HG21	2.01	0.43
3:D:34:TRP:HB2	3:D:47:ILE:HB	2.01	0.43
2:E:195:SER:O	2:E:199:GLU:HB3	2.19	0.43
3:F:34:TRP:CD2	3:F:72:LEU:HD12	2.53	0.43
1:B:75:TYR:O	1:B:79:LEU:HG	2.18	0.43
1:B:332:MET:O	1:B:336:ILE:HG13	2.19	0.43
3:D:125:THR:HG22	3:D:125:THR:O	2.18	0.43
1:A:430:LEU:HD11	1:B:219:PHE:HB3	2.00	0.43
1:B:77:LEU:O	1:B:81:VAL:HG13	2.19	0.43
1:B:337:PHE:O	1:B:341:VAL:HG23	2.19	0.43
2:C:143:MET:HB3	2:C:190:THR:CG2	2.49	0.43
1:A:216:LYS:O	1:A:220:ILE:HG13	2.19	0.42
2:C:30:SER:C	2:C:32:TYR:H	2.26	0.42
3:D:174:MET:HE2	3:D:174:MET:HB3	1.81	0.42
2:E:61:THR:O	2:E:63:SER:N	2.52	0.42
1:A:61:GLN:HG2	1:A:64:ARG:HH21	1.85	0.42
1:A:314:GLY:O	1:A:340:ARG:NH2	2.52	0.42
1:B:369:THR:CG2	1:B:373:MET:HE3	2.49	0.42
3:D:76:THR:O	3:D:77:MET:O	2.37	0.42
3:D:191:TYR:HB2	3:D:208:PHE:CE2	2.53	0.42
1:A:37:PHE:CD2	1:A:38:MET:HE2	2.54	0.42
1:B:98:ARG:HB3	1:B:288:ILE:HG13	2.02	0.42
1:A:74:ASN:HB3	1:A:77:LEU:HB3	2.02	0.42
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.37	0.42
2:E:47:TRP:CE2	3:F:95:GLN:NE2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HA	1:A:160:ARG:HD2	1.63	0.42
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.54	0.42
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.55	0.42
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.89	0.42
1:A:244:LEU:HD11	1:A:324:THR:HG22	2.02	0.42
1:B:199:PHE:CD1	1:B:407:THR:HG21	2.55	0.42
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.54	0.42
3:F:7:SER:HB3	3:F:22:THR:HB	2.02	0.42
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.27	0.42
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.54	0.41
1:A:320:ILE:HB	1:A:321:PRO:CD	2.41	0.41
1:B:98:ARG:CB	1:B:288:ILE:HG13	2.50	0.41
1:B:305:LEU:HA	1:B:308:VAL:HG22	2.02	0.41
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.54	0.41
1:B:158:ILE:O	1:B:162:VAL:HG13	2.20	0.41
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.66	0.41
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.20	0.41
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.56	0.41
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.55	0.41
1:A:136:LEU:HA	1:A:136:LEU:HD12	1.76	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD12	1.82	0.41
2:E:103:TYR:HD2	3:F:31:TYR:CE2	2.39	0.41
1:A:18:ARG:O	1:A:22:ILE:HG13	2.21	0.41
1:A:257:ILE:O	1:A:261:ILE:HG13	2.21	0.41
2:C:178:LEU:HD13	2:C:183:TYR:CZ	2.54	0.41
2:E:130:TYR:HD2	2:E:149:LEU:HD23	1.85	0.41
1:A:172:GLU:N	1:A:212:LEU:HD13	2.36	0.41
1:B:255:TYR:CE2	1:B:424:PRO:HB3	2.55	0.41
3:D:77:MET:O	3:D:77:MET:CG	2.51	0.41
2:E:105:TYR:CD2	3:F:91:SER:HA	2.56	0.41
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.21	0.41
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.55	0.41
1:B:103:GLU:H	1:B:103:GLU:HG3	1.40	0.41
1:B:234:HIS:HD1	1:B:234:HIS:H	1.68	0.41
1:B:330:MET:O	1:B:334:VAL:HG23	2.20	0.41
1:B:231:ILE:HB	1:B:232:PHE:HD1	1.84	0.41
1:B:421:LEU:C	1:B:424:PRO:HD2	2.45	0.41
3:D:6:GLN:HA	3:D:22:THR:O	2.20	0.41
3:D:166:ASP:OD1	3:D:168:LYS:N	2.54	0.41
1:B:90:ALA:O	1:B:94:TYR:HD1	2.04	0.40
2:E:65:LYS:HB2	2:E:66:ASP:H	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.56	0.40
2:E:94:TYR:O	2:E:114:GLY:HA2	2.22	0.40
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.36	0.40
1:A:234:HIS:CD2	1:A:235:GLU:HG2	2.56	0.40
1:B:131:LYS:HG3	1:B:150:PRO:HA	2.03	0.40
3:D:180:LEU:HD22	3:D:184:GLU:CG	2.51	0.40
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.86	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	442/446 (99%)	411 (93%)	29 (7%)	2 (0%)	24	51
1	B	439/446 (98%)	410 (93%)	28 (6%)	1 (0%)	43	70
2	C	219/222 (99%)	199 (91%)	16 (7%)	4 (2%)	6	22
2	E	219/222 (99%)	196 (90%)	18 (8%)	5 (2%)	5	17
3	D	209/211 (99%)	188 (90%)	18 (9%)	3 (1%)	9	28
3	F	209/211 (99%)	194 (93%)	14 (7%)	1 (0%)	24	51
All	All	1737/1758 (99%)	1598 (92%)	123 (7%)	16 (1%)	14	38

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	137	ALA
3	D	50	THR
3	D	77	MET
3	D	80	GLU
2	E	65	LYS

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Mol	Chain	Res	Type
2	E	137	ALA
2	C	65	LYS
1	A	202	GLU
2	C	136	SER
2	E	62	PRO
2	E	136	SER
2	E	31	ARG
3	F	67	GLY
1	B	144	VAL
1	A	422	ILE
2	C	62	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/337 (99%)	297 (89%)	38 (11%)	5	17
1	B	332/337 (98%)	299 (90%)	33 (10%)	7	22
2	C	181/182 (100%)	159 (88%)	22 (12%)	5	14
2	E	181/182 (100%)	161 (89%)	20 (11%)	6	18
3	D	185/185 (100%)	171 (92%)	14 (8%)	12	33
3	F	185/185 (100%)	170 (92%)	15 (8%)	11	30
All	All	1399/1408 (99%)	1257 (90%)	142 (10%)	7	21

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	65	MET
1	A	70	HIS
1	A	71	THR
1	A	73	ASP
1	A	78	LEU
1	A	79	LEU

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	96	LEU
1	A	103	GLU
1	A	111	GLU
1	A	136	LEU
1	A	148	GLU
1	A	162	VAL
1	A	171	ASP
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	222	VAL
1	A	241	VAL
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
1	A	320	ILE
1	A	391	ILE
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
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	81	VAL
1	B	103	GLU
1	B	109	ILE
1	B	131	LYS
1	B	136	LEU
1	B	139	LEU
1	B	148	GLU

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Mol	Chain	Res	Type
1	B	162	VAL
1	B	180	THR
1	B	200	ILE
1	B	201	ILE
1	B	204	MET
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	222	VAL
1	B	230	ARG
1	B	241	VAL
1	B	244	LEU
1	B	251	THR
1	B	273	VAL
1	B	346	LEU
1	B	391	ILE
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	444	LEU
1	B	453	LEU
2	C	2	VAL
2	C	5	LEU
2	C	30	SER
2	C	43	LYS
2	C	55	SER
2	C	65	LYS
2	C	66	ASP
2	C	72	ARG
2	C	83	ILE
2	C	88	SER
2	C	96	CYS
2	C	98	ARG
2	C	120	SER
2	C	123	LYS
2	C	144	VAL
2	C	148	CYS
2	C	151	LYS
2	C	177	VAL
2	C	198	SER
2	C	200	THR

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Mol	Chain	Res	Type
2	C	204	ASN
2	C	214	VAL
3	D	1	ASP
3	D	27	SER
3	D	36	GLN
3	D	76	THR
3	D	77	MET
3	D	80	GLU
3	D	106	LEU
3	D	156	ASN
3	D	170	SER
3	D	176	SER
3	D	190	SER
3	D	192	THR
3	D	201	THR
3	D	206	LYS
2	E	2	VAL
2	E	5	LEU
2	E	6	GLU
2	E	21	SER
2	E	30	SER
2	E	43	LYS
2	E	65	LYS
2	E	72	ARG
2	E	83	ILE
2	E	87	ARG
2	E	96	CYS
2	E	98	ARG
2	E	115	THR
2	E	144	VAL
2	E	151	LYS
2	E	156	GLU
2	E	157	PRO
2	E	167	LEU
2	E	188	SER
2	E	200	THR
3	F	1	ASP
3	F	2	ILE
3	F	6	GLN
3	F	22	THR
3	F	27	SER
3	F	73	THR

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Mol	Chain	Res	Type
3	F	74	ILE
3	F	106	LEU
3	F	116	ILE
3	F	125	THR
3	F	131	VAL
3	F	156	ASN
3	F	170	SER
3	F	190	SER
3	F	201	THR

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	24	GLN
1	A	61	GLN
1	A	63	GLN
1	A	175	HIS
1	A	207	GLN
1	A	281	HIS
1	A	284	HIS
1	A	420	GLN
1	B	61	GLN
1	B	119	GLN
1	B	207	GLN
2	C	163	ASN
3	D	36	GLN
3	D	188	HIS
3	D	209	ASN
2	E	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	444/446 (99%)	0.29	29 (6%)	25 20	33, 53, 84, 124	0
1	B	441/446 (98%)	0.31	30 (6%)	23 18	36, 57, 92, 133	0
2	C	221/222 (99%)	0.01	12 (5%)	31 24	25, 51, 86, 119	0
2	E	221/222 (99%)	-0.01	5 (2%)	61 52	32, 53, 90, 123	0
3	D	211/211 (100%)	0.42	16 (7%)	20 16	33, 63, 87, 103	0
3	F	211/211 (100%)	-0.10	4 (1%)	66 58	29, 48, 100, 124	0
All	All	1749/1758 (99%)	0.19	96 (5%)	30 24	25, 54, 92, 133	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	PHE	7.6
3	D	39	SER	7.0
1	B	95	PHE	6.5
1	A	447	ALA	5.6
3	D	20	THR	5.4
1	A	168	LEU	5.4
1	B	288	ILE	4.6
1	B	72	ALA	4.3
3	D	82	ALA	4.2
3	D	167	SER	4.2
3	F	127	GLY	4.1
1	B	104	ALA	4.0
1	B	445	TYR	4.0
3	D	69	SER	4.0
1	A	376	VAL	3.9
2	C	140	ALA	3.8
1	A	377	GLU	3.8
1	B	73	ASP	3.7
3	D	71	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	380	PRO	3.7
1	A	460	GLN	3.6
1	B	165	ILE	3.6
1	A	212	LEU	3.5
1	A	235	GLU	3.5
2	E	31	ARG	3.5
1	A	167	ARG	3.4
2	E	66	ASP	3.4
2	C	139	ALA	3.4
3	F	128	GLY	3.3
1	B	398	LEU	3.3
2	C	141	ALA	3.3
1	A	444	LEU	3.3
1	A	23	ARG	3.3
1	B	307	PHE	3.2
2	C	43	LYS	3.2
1	A	378	LEU	3.2
2	C	199	GLU	3.2
1	A	234	HIS	3.2
1	A	448	ILE	3.2
1	A	72	ALA	3.1
1	A	445	TYR	3.1
1	A	386	ALA	3.1
2	C	44	GLY	3.1
1	B	199	PHE	3.0
3	D	70	TYR	3.0
1	A	165	ILE	3.0
1	B	70	HIS	2.9
3	F	155	GLN	2.9
2	C	42	GLY	2.9
1	B	186	LEU	2.8
1	A	169	LYS	2.8
3	D	22	THR	2.7
3	D	40	GLY	2.7
1	B	366	VAL	2.7
1	B	402	ILE	2.7
1	B	411	LEU	2.7
3	D	93	HIS	2.7
3	D	64	SER	2.7
1	A	258	LEU	2.7
1	A	180	THR	2.7
2	C	41	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	2.7
1	A	166	PHE	2.6
1	A	288	ILE	2.6
2	E	139	ALA	2.6
2	E	221	ARG	2.6
3	F	153	GLU	2.5
1	B	183	ALA	2.5
1	B	287	ASN	2.5
1	B	353	PRO	2.4
1	B	25	LEU	2.4
2	C	31	ARG	2.3
1	B	34	ALA	2.3
1	B	97	VAL	2.3
1	B	83	PHE	2.2
1	A	99	LYS	2.2
1	B	96	LEU	2.2
1	A	62	ASN	2.2
3	D	140	PRO	2.2
1	B	253	TRP	2.2
1	B	354	GLY	2.2
3	D	63	GLY	2.2
1	B	168	LEU	2.2
1	A	170	GLY	2.1
1	A	423	LEU	2.1
1	B	367	LEU	2.1
2	C	40	ALA	2.1
1	B	289	THR	2.1
1	A	352	ALA	2.1
1	A	27	GLU	2.1
2	E	140	ALA	2.0
3	D	49	ASP	2.0
3	D	105	ILE	2.0
2	C	179	GLN	2.0
3	D	121	SER	2.0
2	C	8	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
4	F	A	501	1/1	0.89	0.16	47,47,47,47	0
4	F	B	501	1/1	0.94	0.18	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.