



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:06 PM GMT

PDB ID : 4KJQ
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

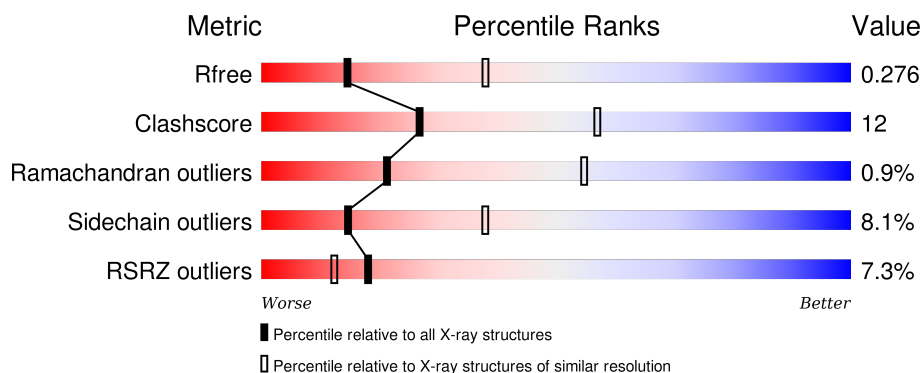
1 Overall quality at a glance

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}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>7%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
1	B	446	<div> <div>6%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
2	C	222	<div> <div>7%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
2	E	222	<div> <div>3%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
3	D	211	<div> <div>11%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F	A	501	-	-	-	X
4	F	B	501	-	-	-	X

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			

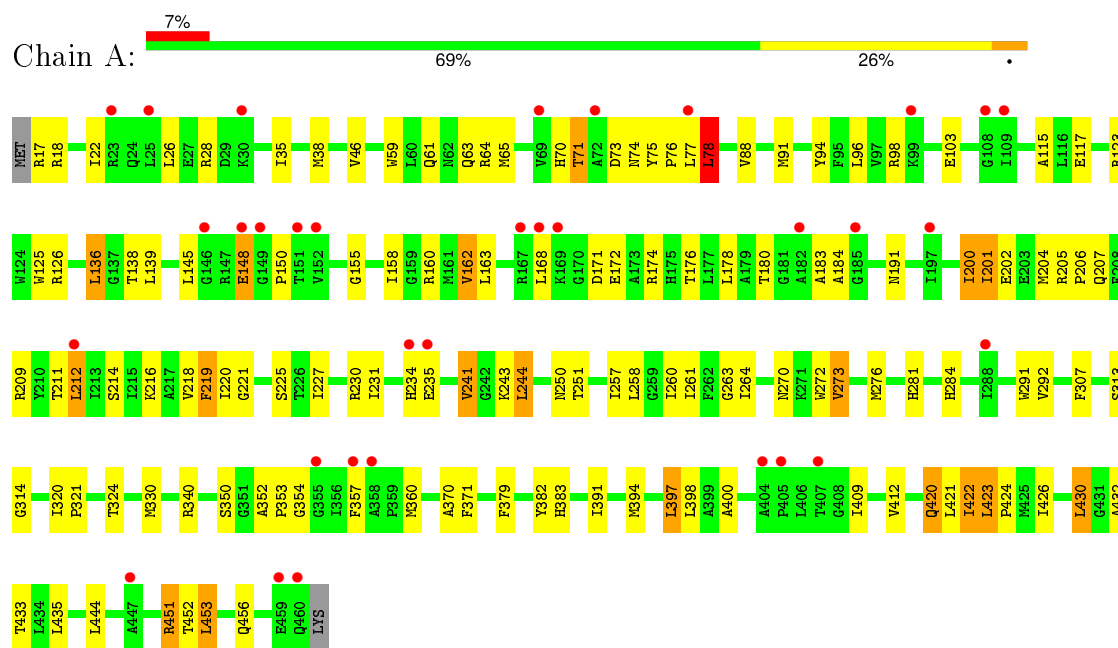
- Molecule 4 is FLUORIDE ION (three-letter code: F) (formula: F).

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

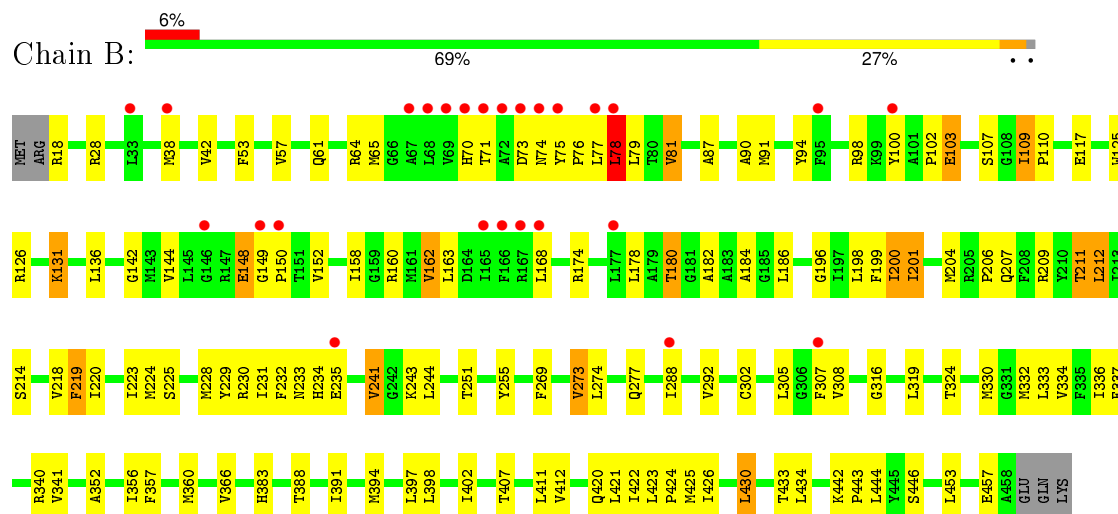
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

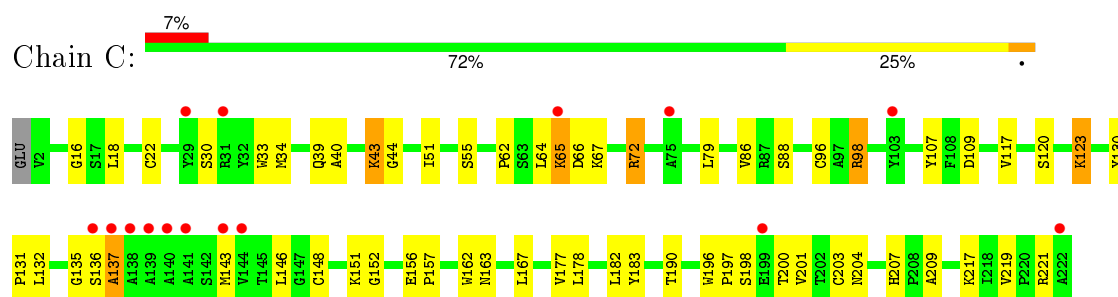
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



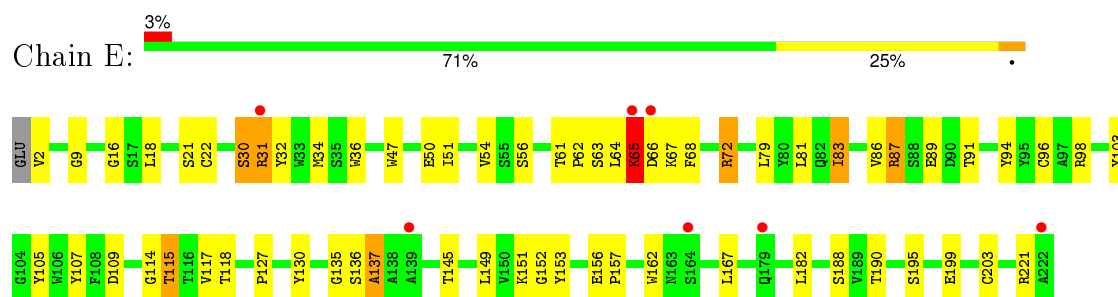
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



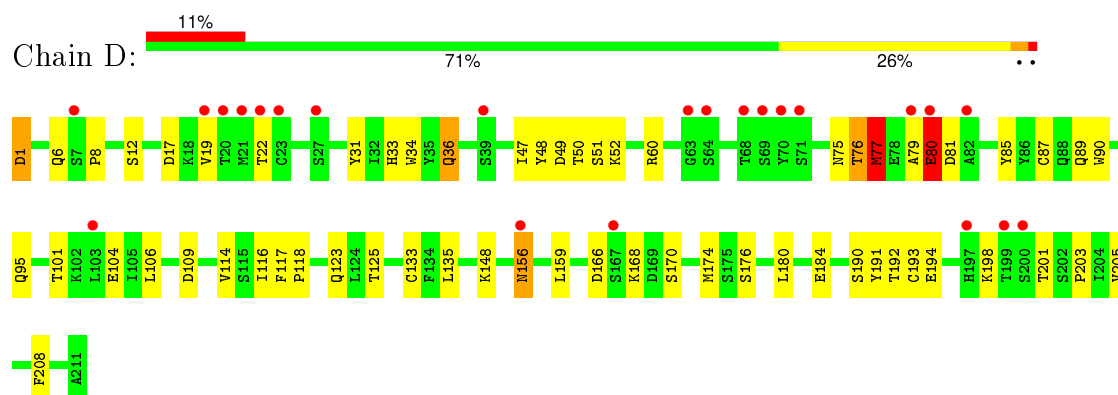
- Molecule 2: Fab, heavy chain



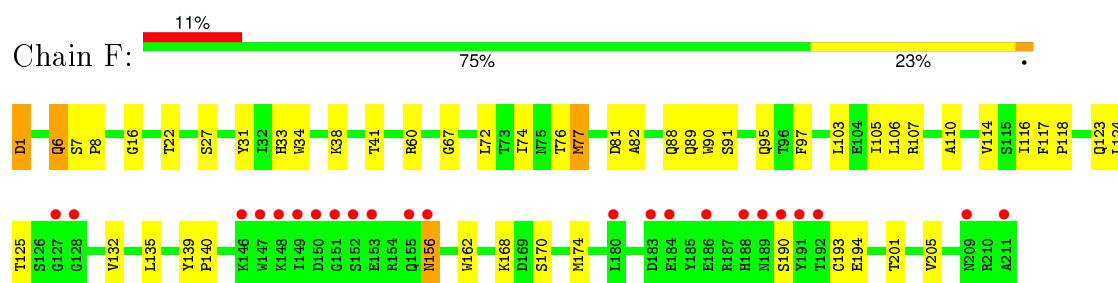
• Molecule 2: Fab, heavy chain



• 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 39.36 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.37-2.88) 99.4 (39.36-2.88)	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 0.234 , 0.276	Depositor DCC
R_{free} test set	3317 reflections (5.34%)	DCC
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 , 35.1	EDS
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 65430 reflections (0.002%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.46	0/3405	0.63	1/4621 (0.0%)
1	B	0.43	0/3376	0.60	1/4583 (0.0%)
2	C	0.50	0/1721	0.64	0/2355
2	E	0.47	0/1721	0.62	0/2355
3	D	0.46	0/1660	0.62	0/2257
3	F	0.46	0/1660	0.63	1/2257 (0.0%)
All	All	0.46	0/13543	0.62	3/18428 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	LEU	CA-CB-CG	6.72	130.75	115.30
1	B	78	LEU	CA-CB-CG	5.88	128.83	115.30
3	F	124	LEU	CB-CA-C	-5.35	100.03	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3484	115	0
1	B	3304	0	3457	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1672	0	1654	31	0
2	E	1672	0	1654	35	0
3	D	1621	0	1546	45	0
3	F	1621	0	1546	32	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
All	All	13225	0	13341	320	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 12.

All (320) 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:HG13	1:A:201:ILE:O	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
3:D:77:MET:O	3:D:77:MET:HG3	1.68	0.91
3:F:95:GLN:N	3:F:95:GLN:OE1	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:N	3:D:95:GLN:OE1	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: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:CG1	1:A:201:ILE:O	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
1:A:421:LEU:C	1:A:424:PRO:HD2	2.07	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
2:E:130:TYR:CE2	3:F:123:GLN:HG3	2.27	0.69
1:A:430:LEU:HD21	1:B:220:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.74	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:H	1:B:212:LEU:HD12	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:A:421:LEU:O	1:A:424:PRO:HD2	1.96	0.66
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.77	0.65
1:B:180:THR:HB	1:B:218:VAL:HA	1.77	0.65
1:A:200:ILE:HD13	1:A:204:MET:HG3	1.78	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
3:D:1:ASP:N	3:D:1:ASP:OD2	2.24	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:F:82:ALA:HB2	3:F:105:ILE:HD11	1.79	0.63
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.80	0.62
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.31	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: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
3:D:76:THR:O	3:D:77:MET:C	2.39	0.60
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.16	0.60
1:B:243:LYS:HB3	2:E:31:ARG:HH21	1.65	0.60
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.36	0.60
1:A:73:ASP:OD1	1:A:73:ASP:N	2.34	0.60
3:D:12:SER:HA	3:D:104:GLU:O	2.02	0.60
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.82	0.60
1:A:71:THR:OG1	1:A:71:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.85	0.58
3:D:79:ALA:C	3:D:81:ASP:H	2.05	0.58
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.39	0.58
2:E:145:THR:HG1	2:E:190:THR:HG1	1.50	0.58
1:B:422:ILE:HA	1:B:425:MET:HE2	1.85	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:A:94:TYR:HH	1:A:350:SER:HG	1.44	0.57
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.85	0.57
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.20	0.57
1:B:336:ILE:O	1:B:340:ARG:HG3	2.05	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:A:423:LEU:HB3	1:A:424:PRO:HD3	1.87	0.56
1:A:272:TRP:O	1:A:276:MET:HB2	2.06	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
1:A:430:LEU:HD13	1:B:223:ILE:HD11	1.87	0.56
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.88	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:B:148:GLU:CD	1:B:148:GLU:H	2.08	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:N	3:D:156:ASN:OD1	2.39	0.55
3:F:77:MET:HE3	3:F:103:LEU:HD21	1.90	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
3:D:79:ALA:C	3:D:81:ASP:N	2.60	0.54
1:B:394:MET:HG2	1:B:412:VAL:CG2	2.37	0.54
1:B:356:ILE:HG22	4:B:501:F:F	1.98	0.54
1:B:91:MET:HG2	1:B:292:VAL:O	2.07	0.54
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:O	1:A:178:LEU:HB2	2.08	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
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.91	0.53
1:B:107:SER:O	1:B:149:GLY:CA	2.57	0.53
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.91	0.53
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
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
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.92	0.52
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.45	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
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.46	0.51
1:A:357:PHE:CE2	1:A:398:LEU:HD11	2.46	0.51
1:B:241:VAL:HG22	1:B:324:THR:HG21	1.92	0.51
3:F:116:ILE:HD12	3:F:193:CYS:HB2	1.93	0.51
1:A:394:MET:HG2	1:A:412:VAL:HG22	1.92	0.51
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.46	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: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
3:F:34:TRP:CG	3:F:72:LEU:HD12	2.46	0.50
1:B:142:GLY:O	1:B:302:CYS:HB3	2.10	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:148:GLU:H	1:A:148:GLU:CD	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:GLN:HG2	1:B:28:ARG:HE	1.77	0.49
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.45	0.49
3:D:17:ASP:O	3:D:77:MET:HB3	2.13	0.49
3:F:6:GLN:HA	3:F:22:THR:O	2.13	0.49
2:C:135:GLY:O	2:C:137:ALA:N	2.42	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
3:D:166:ASP:OD1	3:D:168:LYS:HB2	2.13	0.49
1:A:88:VAL:HA	1:A:91:MET:HE2	1.95	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
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:422:ILE:HA	1:B:425:MET:CE	2.43	0.48
1:B:333:LEU:HD22	1:B:366:VAL:HG13	1.95	0.48
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.43	0.48
3:D:75:ASN:C	3:D:77:MET:H	2.17	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:200:ILE:HD12	1:A:204:MET:CG	2.44	0.47
1:B:71:THR:OG1	1:B:71:THR:O	2.26	0.47
3:F:89:GLN:O	3:F:95:GLN:HB2	2.15	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
1:A:421:LEU:O	1:A:424:PRO:CD	2.62	0.47
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.96	0.47
1:A:91:MET:HG2	1:A:292:VAL:O	2.15	0.47
3:D:135:LEU:HD12	3:D:174:MET:HE2	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
2:C:163:ASN:HD22	2:C:167:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.78	0.46
1:B:269:PHE:O	1:B:273:VAL:HG12	2.14	0.46
1:A:409:ILE:HD13	1:A:426:ILE:HA	1.96	0.46
1:B:383:HIS:NE2	2:E:50:GLU:OE1	2.42	0.46
1:B:214:SER:O	1:B:218:VAL:HG23	2.16	0.46
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
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.74	0.46
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.97	0.46
1:B:100:TYR:O	1:B:126:ARG:NH1	2.44	0.46
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.98	0.46
1:B:316:GLY:O	1:B:319:LEU:HG	2.16	0.46
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
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
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.51	0.45
1:A:320:ILE:CB	1:A:321:PRO:CD	2.95	0.45
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.52	0.45
1:B:229:TYR:O	1:B:233:ASN:HB2	2.17	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
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.52	0.45
1:B:73:ASP:OD1	1:B:73:ASP:N	2.40	0.45
1:A:313:SER:OG	1:A:314:GLY:N	2.50	0.45
1:A:250:ASN:ND2	1:A:382:TYR:HE2	2.16	0.44
1:A:158:ILE:O	1:A:162:VAL:HG13	2.18	0.44
2:E:16:GLY:O	2:E:86:VAL:HG23	2.17	0.44
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.52	0.44
2:C:18:LEU:HD11	2:C:117:VAL:HG22	1.99	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:HG3	2:E:65:LYS:H	1.60	0.44
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.99	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
2:C:40:ALA:HB3	2:C:43:LYS:CB	2.48	0.44
1:A:26:LEU:HB3	1:B:442:LYS:HZ2	1.83	0.44
1:B:224:MET:O	1:B:228:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.88	0.44
1:B:388:THR:HG22	1:B:421:LEU:HD11	2.00	0.44
1:B:274:LEU:O	1:B:277:GLN:HB2	2.18	0.43
2:E:30:SER:C	2:E:32:TYR:H	2.21	0.43
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.00	0.43
2:E:149:LEU:HD13	3:F:132:VAL:HG21	1.99	0.43
2:C:16:GLY:O	2:C:86:VAL:HG23	2.17	0.43
1:A:420:GLN:HG3	1:A:420:GLN:H	1.47	0.43
3:D:19:VAL:HG23	3:D:77:MET:HB2	2.01	0.43
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.71	0.43
2:E:68:PHE:CE2	2:E:83:ILE:HG23	2.53	0.43
2:C:123:LYS:HB3	2:C:123:LYS:NZ	2.34	0.43
3:F:139:TYR:CD2	3:F:140:PRO:HA	2.54	0.43
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.82	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
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.53	0.43
1:A:59:TRP:O	1:A:63:GLN:HG2	2.19	0.43
3:F:34:TRP:CD2	3:F:72:LEU:HD12	2.53	0.43
3:D:34:TRP:HB2	3:D:47:ILE:HB	2.01	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
2:E:195:SER:O	2:E:199:GLU:HB3	2.19	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
2:C:143:MET:HB3	2:C:190:THR:CG2	2.49	0.43
1:B:337:PHE:O	1:B:341:VAL:HG23	2.19	0.43
1:A:216:LYS:O	1:A:220:ILE:HG13	2.19	0.42
2:E:61:THR:O	2:E:63:SER:N	2.52	0.42
3:D:76:THR:O	3:D:77:MET:O	2.37	0.42
1:A:314:GLY:O	1:A:340:ARG:NH2	2.52	0.42
1:A:61:GLN:HG2	1:A:64:ARG:HH21	1.85	0.42
3:D:191:TYR:HB2	3:D:208:PHE:CE2	2.53	0.42
1:B:98:ARG:HB3	1:B:288:ILE:HG13	2.02	0.42
2:E:47:TRP:CE2	3:F:95:GLN:NE2	2.86	0.42
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.37	0.42
1:A:74:ASN:HB3	1:A:77:LEU:HB3	2.02	0.42
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.54	0.42
1:A:160:ARG:HD2	1:A:160:ARG:HA	1.63	0.42
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.89	0.42
3:F:7:SER:HB3	3:F:22:THR:HB	2.02	0.42
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.54	0.42
1:B:199:PHE:CD1	1:B:407:THR:HG21	2.55	0.42
1:A:244:LEU:HD11	1:A:324:THR:HG22	2.02	0.42
1:A:320:ILE:HB	1:A:321:PRO:CD	2.41	0.41
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.54	0.41
1:B:98:ARG:CB	1:B:288:ILE:HG13	2.50	0.41
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.54	0.41
1:B:305:LEU:HA	1:B:308:VAL:HG22	2.02	0.41
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.20	0.41
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.66	0.41
1:B:158:ILE:O	1:B:162:VAL:HG13	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:178:LEU:HD12	1:A:178:LEU:HA	1.82	0.41
2:E:103:TYR:HD2	3:F:31:TYR:CE2	2.39	0.41
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.76	0.41
2:E:130:TYR:HD2	2:E:149:LEU:HD23	1.85	0.41
1:A:18:ARG:O	1:A:22:ILE:HG13	2.21	0.41
2:C:178:LEU:HD13	2:C:183:TYR:CZ	2.54	0.41
1:A:257:ILE:O	1:A:261:ILE:HG13	2.21	0.41
3:D:77:MET:O	3:D:77:MET:CG	2.51	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
2:E:105:TYR:CD2	3:F:91:SER:HA	2.56	0.41
3:D:75:ASN:C	3:D:77:MET:N	2.74	0.41
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.21	0.41
1:B:234:HIS:HD1	1:B:234:HIS:H	1.68	0.41
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.55	0.41
1:B:103:GLU:HG3	1:B:103:GLU:H	1.40	0.41
1:B:330:MET:O	1:B:334:VAL:HG23	2.20	0.41
3:D:166:ASP:OD1	3:D:168:LYS:N	2.54	0.41
1:B:231:ILE:HB	1:B:232:PHE:HD1	1.84	0.41
3:D:6:GLN:HA	3:D:22:THR:O	2.20	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
2:E:94:TYR:O	2:E:114:GLY:HA2	2.22	0.40
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:330:MET:CE	1:A:370:ALA:HB1	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%)	34	69
1	B	439/446 (98%)	410 (93%)	28 (6%)	1 (0%)	52	83
2	C	219/222 (99%)	199 (91%)	16 (7%)	4 (2%)	11	35
2	E	219/222 (99%)	196 (90%)	18 (8%)	5 (2%)	8	28
3	D	209/211 (99%)	188 (90%)	18 (9%)	3 (1%)	14	42
3	F	209/211 (99%)	194 (93%)	14 (7%)	1 (0%)	34	69
All	All	1737/1758 (99%)	1598 (92%)	123 (7%)	16 (1%)	21	55

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
2	E	137	ALA

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Mol	Chain	Res	Type
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 [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	335/337 (99%)	304 (91%)	31 (9%)	11	30
1	B	332/337 (98%)	304 (92%)	28 (8%)	14	36
2	C	181/182 (100%)	165 (91%)	16 (9%)	12	33
2	E	181/182 (100%)	167 (92%)	14 (8%)	16	40
3	D	185/185 (100%)	172 (93%)	13 (7%)	19	46
3	F	185/185 (100%)	173 (94%)	12 (6%)	21	50
All	All	1399/1408 (99%)	1285 (92%)	114 (8%)	15	38

All (114) 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	78	LEU
1	A	96	LEU
1	A	103	GLU
1	A	136	LEU

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Mol	Chain	Res	Type
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	241	VAL
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
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	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	148	GLU
1	B	162	VAL
1	B	180	THR
1	B	200	ILE
1	B	201	ILE
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	230	ARG
1	B	241	VAL
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	251	THR
1	B	273	VAL
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	430	LEU
1	B	433	THR
1	B	444	LEU
1	B	453	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	88	SER
2	C	96	CYS
2	C	98	ARG
2	C	120	SER
2	C	123	LYS
2	C	148	CYS
2	C	151	LYS
2	C	198	SER
2	C	200	THR
2	C	204	ASN
3	D	1	ASP
3	D	36	GLN
3	D	76	THR
3	D	77	MET
3	D	80	GLU
3	D	106	LEU
3	D	133	CYS
3	D	156	ASN
3	D	170	SER
3	D	176	SER
3	D	190	SER
3	D	201	THR
3	D	203	PRO
2	E	2	VAL
2	E	21	SER
2	E	30	SER
2	E	65	LYS

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Mol	Chain	Res	Type
2	E	72	ARG
2	E	83	ILE
2	E	87	ARG
2	E	96	CYS
2	E	115	THR
2	E	151	LYS
2	E	156	GLU
2	E	157	PRO
2	E	167	LEU
2	E	188	SER
3	F	1	ASP
3	F	6	GLN
3	F	27	SER
3	F	74	ILE
3	F	77	MET
3	F	106	LEU
3	F	125	THR
3	F	156	ASN
3	F	168	LYS
3	F	170	SER
3	F	190	SER
3	F	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	284	HIS
1	B	119	GLN
2	C	163	ASN
2	C	172	HIS
3	D	36	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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%)	0.38	33 (7%) 17 12	33, 53, 84, 124	0
1	B	441/446 (98%)	0.20	26 (5%) 26 20	36, 57, 92, 133	0
2	C	221/222 (99%)	0.06	15 (6%) 20 15	25, 51, 86, 119	0
2	E	221/222 (99%)	-0.09	7 (3%) 51 45	32, 53, 90, 123	0
3	D	211/211 (100%)	0.35	23 (10%) 7 4	33, 63, 87, 103	0
3	F	211/211 (100%)	0.20	23 (10%) 7 4	29, 48, 100, 124	0
All	All	1749/1758 (99%)	0.21	127 (7%) 18 12	25, 54, 92, 133	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	GLN	9.4
1	A	72	ALA	8.1
1	B	72	ALA	8.0
1	B	70	HIS	6.2
1	A	168	LEU	5.9
1	B	73	ASP	5.7
3	D	20	THR	5.4
1	B	71	THR	5.3
1	B	307	PHE	5.1
1	B	168	LEU	4.7
1	B	68	LEU	4.3
3	F	155	GLN	4.1
3	F	192	THR	4.1
2	E	66	ASP	4.0
3	D	70	TYR	3.9
3	F	127	GLY	3.8
2	C	141	ALA	3.8
1	B	95	PHE	3.7
3	F	153	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	165	ILE	3.6
3	D	21	MET	3.6
3	D	22	THR	3.6
1	B	74	ASN	3.6
3	F	152	SER	3.6
3	F	151	GLY	3.6
1	A	69	VAL	3.6
1	B	67	ALA	3.6
1	B	69	VAL	3.5
3	F	156	ASN	3.5
3	F	149	ILE	3.5
2	E	65	LYS	3.4
1	A	77	LEU	3.4
2	C	139	ALA	3.3
1	A	288	ILE	3.3
3	D	82	ALA	3.3
1	A	23	ARG	3.3
1	B	75	TYR	3.3
3	F	147	TRP	3.2
2	C	29	TYR	3.2
1	A	459	GLU	3.2
3	D	200	SER	3.2
2	C	65	LYS	3.2
3	F	180	LEU	3.1
3	F	128	GLY	3.0
1	A	234	HIS	3.0
3	D	19	VAL	3.0
1	B	78	LEU	3.0
1	A	235	GLU	3.0
3	D	39	SER	3.0
2	C	144	VAL	3.0
2	E	222	ALA	3.0
1	A	149	GLY	2.9
2	C	136	SER	2.9
3	F	191	TYR	2.9
3	D	79	ALA	2.9
1	B	166	PHE	2.9
2	C	140	ALA	2.9
2	E	139	ALA	2.9
2	E	31	ARG	2.8
3	D	7	SER	2.8
1	A	146	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	23	CYS	2.8
3	D	63	GLY	2.8
3	F	211	ALA	2.8
3	D	103	LEU	2.8
3	D	69	SER	2.7
3	D	199	THR	2.7
1	A	152	VAL	2.7
1	A	109	ILE	2.7
3	F	209	ASN	2.7
1	A	169	LYS	2.7
3	D	68	THR	2.7
1	A	358	ALA	2.7
3	D	27	SER	2.6
3	F	150	ASP	2.6
2	C	138	ALA	2.6
3	D	197	HIS	2.6
1	A	148	GLU	2.5
3	F	184	GLU	2.5
1	B	33	LEU	2.5
1	B	167	ARG	2.5
2	C	137	ALA	2.5
1	A	108	GLY	2.4
1	A	185	GLY	2.4
3	D	71	SER	2.4
1	A	407	THR	2.4
1	A	30	LYS	2.3
2	C	103	TYR	2.3
1	A	182	ALA	2.3
1	B	100	TYR	2.3
3	F	189	ASN	2.3
3	D	167	SER	2.3
3	F	146	LYS	2.3
3	D	80	GLU	2.3
2	C	31	ARG	2.3
1	A	212	LEU	2.3
1	B	149	GLY	2.3
1	A	405	PRO	2.3
3	F	183	ASP	2.2
2	C	199	GLU	2.2
1	A	167	ARG	2.2
1	B	235	GLU	2.2
3	F	188	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	404	ALA	2.2
3	F	190	SER	2.2
2	C	143	MET	2.2
1	B	38	MET	2.2
1	B	77	LEU	2.2
1	A	447	ALA	2.2
3	D	64	SER	2.1
1	B	288	ILE	2.1
1	A	151	THR	2.1
1	B	146	GLY	2.1
2	E	179	GLN	2.1
3	F	186	GLU	2.1
3	F	148	LYS	2.1
2	E	164	SER	2.1
1	A	99	LYS	2.1
1	B	150	PRO	2.1
1	A	357	PHE	2.1
1	A	25	LEU	2.0
1	B	177	LEU	2.0
2	C	75	ALA	2.0
1	A	197	ILE	2.0
1	A	355	GLY	2.0
2	C	222	ALA	2.0
3	D	156	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	F	B	501	1/1	0.94	0.36	3.10	43,43,43,43	0
4	F	A	501	1/1	0.93	0.53	2.10	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.