



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 2FEC / pdb_00002fec
Title : Structure of the E203Q mutant of the Cl⁻/H⁺ exchanger CLC-ec1 from E.Coli
Authors : Accardi, A.; Walden, M.P.; Nguitragool, W.; Jayaram, H.; Williams, C.;
Miller, C.
Deposited on : 2005-12-15
Resolution : 3.97 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

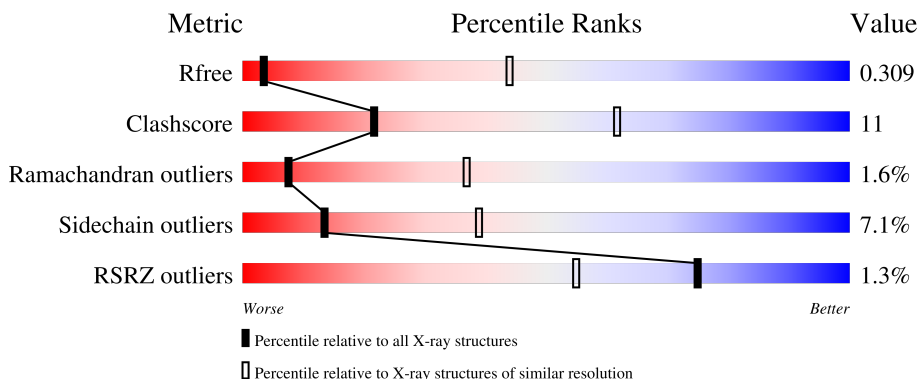
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 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.



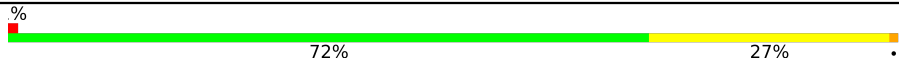
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	465	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 71% 22% • 5%</p>
1	B	465	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 66% 25% • 5%</p>
2	I	222	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 70% 28% •</p>
2	J	222	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 69% 28% •</p>
3	L	211	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 64% 34% •</p>

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Mol	Chain	Length	Quality of chain
3	O	211	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into two segments: a green segment on the left representing 72% and a yellow segment on the right representing 27%. A small red square is at the start of the bar, and a small black dot is at the end. A '%' symbol is positioned above the start of the bar.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13223 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
			Total	C	N	O	S			
1	A	444	3333	2190	561	562	20	0	0	0
1	B	441	3304	2174	554	556	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	GLN	GLU	engineered mutation	UNP P37019
B	203	GLN	GLU	engineered mutation	UNP P37019

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

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

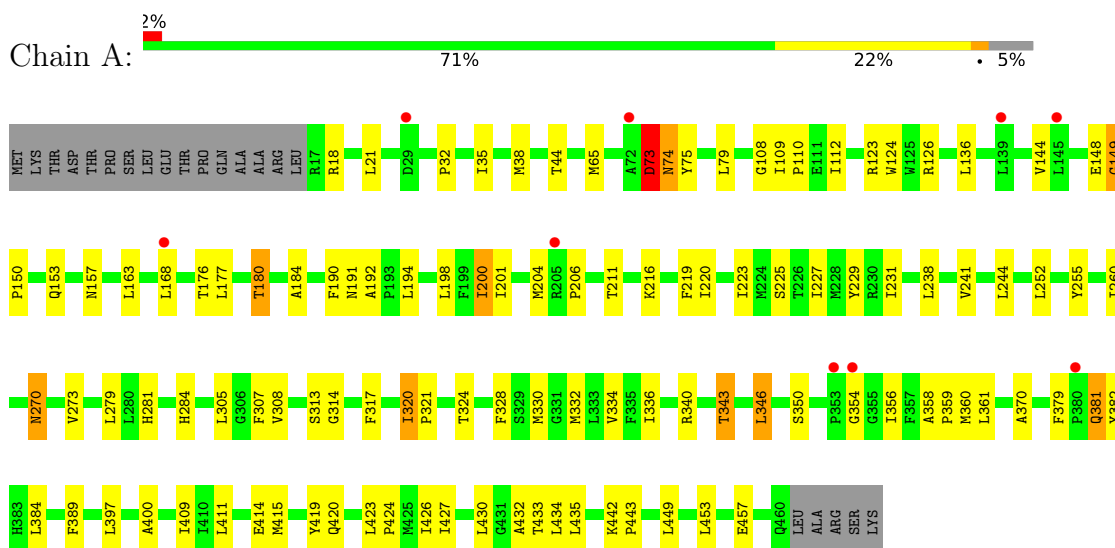
- Molecule 3 is a protein called Fab fragment, light chain.

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

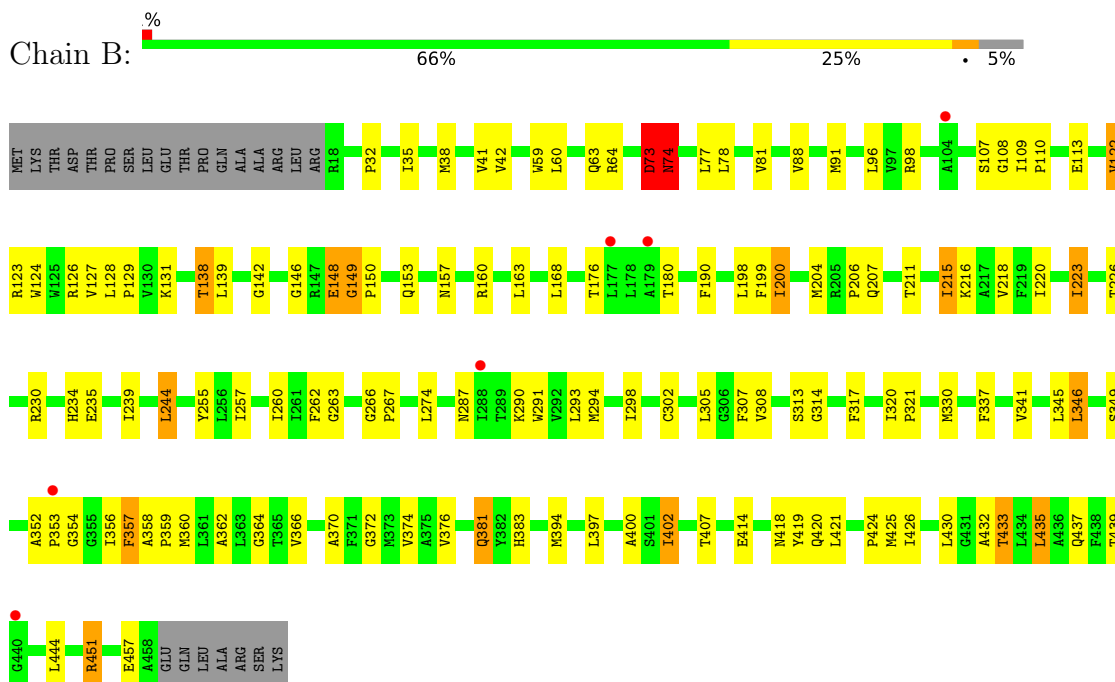
3 Residue-property plots i

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.

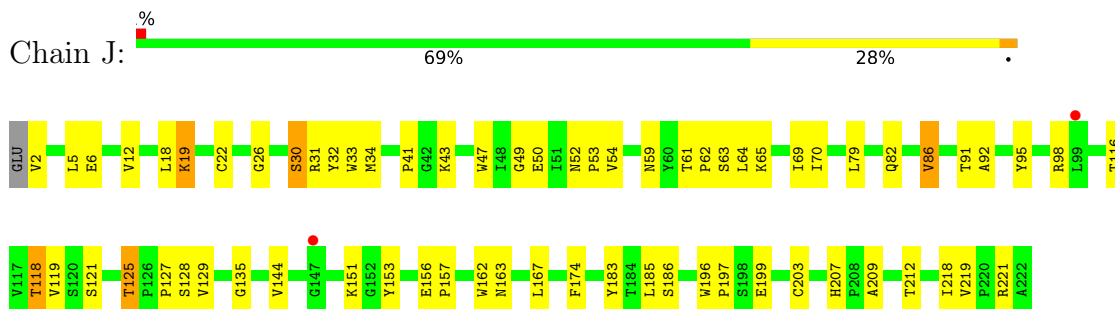
- Molecule 1: H(+)/Cl(-) exchange transporter clcA



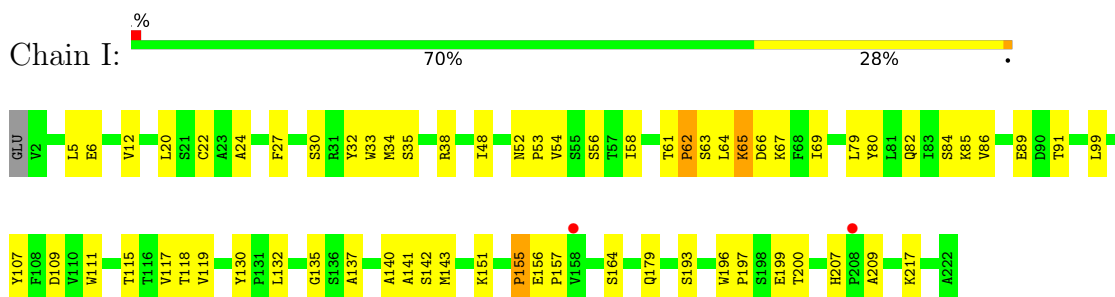
- Molecule 1: H(+)/Cl(-) exchange transporter clcA



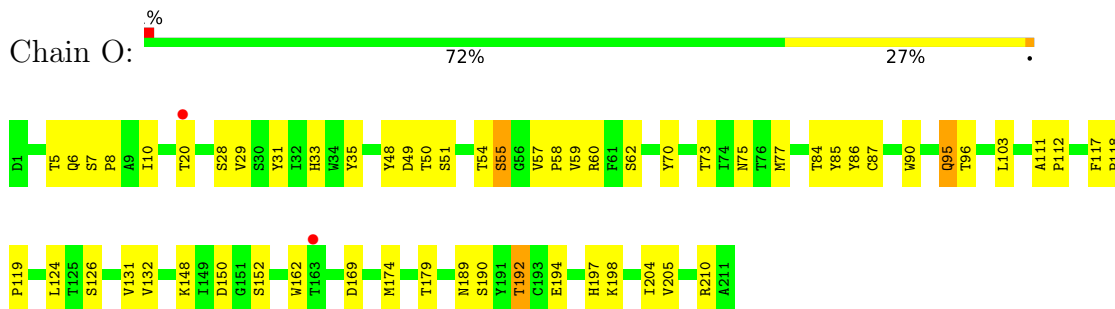
- Molecule 2: Fab fragment, heavy chain



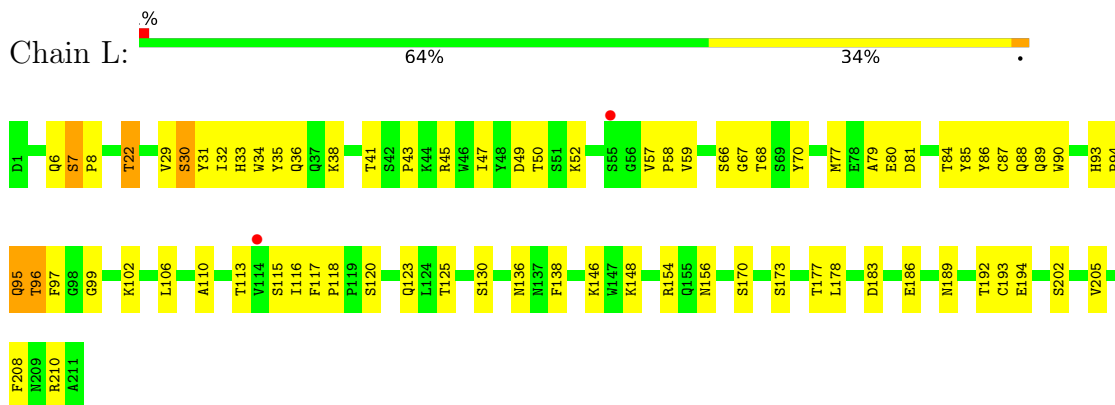
- Molecule 2: Fab fragment, heavy chain



- Molecule 3: Fab fragment, light chain



- Molecule 3: Fab fragment, light chain



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.31Å 98.50Å 170.41Å 90.00° 131.51° 90.00°	Depositor
Resolution (Å)	128.04 – 3.97 127.61 – 3.97	Depositor EDS
% Data completeness (in resolution range)	97.8 (128.04-3.97) 97.7 (127.61-3.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 3.99Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.269 , 0.326 0.253 , 0.309	Depositor DCC
R_{free} test set	1258 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	141.0	Xtrriage
Anisotropy	0.433	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	2/3405 (0.1%)	0.87	0/4621
1	B	0.63	2/3376 (0.1%)	0.90	0/4583
2	I	0.53	0/1721	0.80	0/2355
2	J	0.69	4/1721 (0.2%)	0.84	5/2355 (0.2%)
3	L	0.49	0/1660	0.81	2/2257 (0.1%)
3	O	0.51	0/1660	0.86	2/2257 (0.1%)
All	All	0.57	8/13543 (0.1%)	0.86	9/18428 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	ASP	C-O	15.48	1.43	1.24
2	J	19	LYS	CE-NZ	11.39	1.83	1.49
2	J	199	GLU	CD-OE2	7.87	1.40	1.25
1	B	73	ASP	C-N	7.40	1.44	1.33
2	J	199	GLU	CD-OE1	7.22	1.39	1.25
1	A	73	ASP	C-N	7.11	1.43	1.33
2	J	19	LYS	CD-CE	7.06	1.73	1.52
1	A	320	ILE	CA-CB	5.07	1.56	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	111	ALA	CA-C-N	7.24	127.23	119.78
3	O	111	ALA	C-N-CA	7.24	127.23	119.78
2	J	65	LYS	N-CA-C	5.53	119.12	112.38
2	J	64	LEU	N-CA-C	5.42	116.92	110.19
2	J	19	LYS	CD-CE-NZ	-5.36	94.75	111.90
2	J	125	THR	CA-C-N	5.04	123.34	119.66
2	J	125	THR	C-N-CA	5.04	123.34	119.66
3	L	202	SER	CA-C-N	5.01	126.10	119.84
3	L	202	SER	C-N-CA	5.01	126.10	119.84

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	3486	67	0
1	B	3304	0	3459	94	0
2	I	1672	0	1654	34	0
2	J	1672	0	1654	36	0
3	L	1621	0	1546	48	0
3	O	1621	0	1546	31	0
All	All	13223	0	13345	288	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 11.

All (288) 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)
2:J:19:LYS:NZ	2:J:19:LYS:CE	1.83	1.41
3:L:7:SER:HB3	3:L:8:PRO:HD3	1.41	1.00
3:L:146:LYS:HB3	3:L:194:GLU:HB2	1.44	1.00
1:B:381:GLN:H	1:B:381:GLN:HE21	1.15	0.92
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.59	0.84
1:B:148:GLU:CD	1:B:148:GLU:H	1.93	0.77
3:O:6:GLN:HE22	3:O:86:TYR:HA	1.52	0.74
1:A:38:MET:HB3	1:A:177:LEU:HD11	1.69	0.74
1:A:381:GLN:H	1:A:381:GLN:NE2	1.85	0.74
1:B:381:GLN:HE21	1:B:381:GLN:N	1.86	0.72
3:L:7:SER:CB	3:L:8:PRO:HD3	2.19	0.72
3:L:36:GLN:HG3	3:L:85:TYR:CE2	2.25	0.71
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.73	0.70
1:B:381:GLN:H	1:B:381:GLN:NE2	1.88	0.69
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.75	0.69
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.75	0.69
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:148:LYS:HB2	3:O:192:THR:OG1	1.95	0.67
2:J:91:THR:HG23	2:J:118:THR:HA	1.76	0.66
3:L:6:GLN:HG3	3:L:99:GLY:H	1.61	0.66
1:A:148:GLU:CD	1:A:148:GLU:H	2.03	0.66
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.78	0.65
1:B:239:ILE:HD13	1:B:394:MET:HE1	1.78	0.65
1:A:227:ILE:O	1:A:231:ILE:HG12	1.97	0.64
3:L:34:TRP:HB2	3:L:47:ILE:HB	1.80	0.64
1:A:144:VAL:HG21	1:A:343:THR:HB	1.80	0.64
3:O:29:VAL:HG23	3:O:70:TYR:HE1	1.63	0.63
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.79	0.63
2:J:207:HIS:CE1	2:J:209:ALA:HB3	2.35	0.62
2:I:130:TYR:HB3	3:L:120:SER:OG	2.00	0.62
2:J:19:LYS:NZ	2:J:19:LYS:CD	2.62	0.62
2:J:156:GLU:OE1	2:J:157:PRO:HA	2.00	0.62
3:L:7:SER:HB2	3:L:22:THR:HB	1.81	0.61
2:I:91:THR:HA	2:I:117:VAL:O	2.00	0.61
2:J:33:TRP:CZ2	2:J:52:ASN:HB3	2.35	0.61
1:A:384:LEU:HD22	1:A:389:PHE:HE1	1.64	0.60
1:B:298:ILE:HG12	1:B:346:LEU:HD23	1.84	0.60
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.84	0.60
3:L:6:GLN:HE22	3:L:86:TYR:HA	1.67	0.60
3:O:124:LEU:C	3:O:126:SER:H	2.10	0.59
3:L:7:SER:HB3	3:L:8:PRO:CD	2.24	0.59
1:B:176:THR:O	1:B:180:THR:HG23	2.02	0.59
2:I:91:THR:HG23	2:I:118:THR:HA	1.84	0.59
1:B:113:GLU:HG3	1:B:204:MET:SD	2.42	0.59
1:B:180:THR:HG22	1:B:218:VAL:HA	1.84	0.59
3:O:194:GLU:HG2	3:O:205:VAL:HG12	1.84	0.59
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.85	0.59
3:L:88:GLN:HB2	3:L:97:PHE:CD1	2.38	0.59
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.85	0.58
3:L:194:GLU:HG2	3:L:205:VAL:HG12	1.83	0.58
1:A:313:SER:OG	1:A:314:GLY:N	2.36	0.58
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.86	0.58
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.85	0.58
1:A:409:ILE:HD13	1:A:426:ILE:HA	1.86	0.58
3:L:38:LYS:O	3:L:41:THR:HG22	2.04	0.58
1:B:360:MET:HE1	1:B:402:ILE:HG22	1.84	0.57
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.85	0.57
2:I:91:THR:OG1	2:I:119:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:O	1:A:180:THR:HG23	2.05	0.57
1:B:362:ALA:O	1:B:366:VAL:HG23	2.04	0.57
3:O:95:GLN:N	3:O:95:GLN:CD	2.63	0.57
3:L:136:ASN:HD22	3:L:173:SER:HB3	1.68	0.57
1:B:148:GLU:HG2	1:B:357:PHE:HB3	1.86	0.57
3:L:31:TYR:HA	3:L:50:THR:OG1	2.04	0.56
2:J:34:MET:HB3	2:J:79:LEU:HD22	1.86	0.56
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.88	0.56
2:J:30:SER:C	2:J:32:TYR:H	2.14	0.56
1:B:38:MET:HA	1:B:41:VAL:HG12	1.86	0.56
2:I:69:ILE:HB	2:I:82:GLN:HB2	1.87	0.56
3:L:146:LYS:HB3	3:L:194:GLU:CB	2.29	0.56
3:L:66:SER:HA	3:L:70:TYR:CZ	2.41	0.56
3:O:95:GLN:CD	3:O:95:GLN:H	2.13	0.56
3:L:89:GLN:HE21	3:L:96:THR:H	1.52	0.56
2:I:24:ALA:HB1	2:I:27:PHE:CE1	2.40	0.55
3:L:93:HIS:CG	3:L:94:PRO:HA	2.42	0.55
3:O:6:GLN:NE2	3:O:87:CYS:H	2.04	0.55
3:L:79:ALA:C	3:L:81:ASP:H	2.15	0.55
1:A:73:ASP:O	1:A:74:ASN:C	2.50	0.55
2:J:61:THR:O	2:J:63:SER:N	2.40	0.55
1:B:59:TRP:O	1:B:63:GLN:HG2	2.08	0.54
2:I:141:ALA:O	2:I:193:SER:HB2	2.08	0.54
1:A:184:ALA:HB1	1:A:225:SER:HB3	1.89	0.54
1:B:402:ILE:HG13	1:B:402:ILE:O	2.05	0.54
2:J:127:PRO:HD2	2:J:212:THR:HG21	1.89	0.53
1:A:194:LEU:CD2	1:B:426:ILE:HD11	2.39	0.53
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.91	0.53
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.73	0.53
3:L:115:SER:HB3	3:L:117:PHE:HE1	1.74	0.53
1:A:112:ILE:HD11	1:A:153:GLN:HG3	1.91	0.53
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.90	0.53
3:O:31:TYR:HA	3:O:50:THR:OG1	2.08	0.53
2:J:6:GLU:HA	2:J:22:CYS:HA	1.90	0.53
2:I:84:SER:HB3	2:I:85:LYS:HE2	1.91	0.52
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.74	0.52
3:L:95:GLN:CD	3:L:95:GLN:N	2.68	0.52
1:A:414:GLU:HG2	1:B:419:TYR:CE1	2.44	0.52
2:J:49:GLY:HA3	2:J:70:ILE:HD12	1.90	0.52
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.91	0.52
1:B:274:LEU:HB3	1:B:451:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:31:TYR:HB3	3:O:49:ASP:OD1	2.09	0.52
1:B:360:MET:HE1	1:B:402:ILE:CG2	2.40	0.52
3:L:29:VAL:HG23	3:L:70:TYR:CE1	2.45	0.52
2:J:33:TRP:CH2	2:J:52:ASN:HB3	2.45	0.52
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.90	0.52
2:I:207:HIS:CE1	2:I:209:ALA:HB3	2.45	0.52
1:B:73:ASP:O	1:B:74:ASN:C	2.53	0.52
2:I:61:THR:OG1	2:I:62:PRO:HD2	2.09	0.52
2:I:63:SER:OG	2:I:64:LEU:N	2.43	0.51
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.39	0.51
1:B:305:LEU:C	1:B:307:PHE:H	2.17	0.51
3:L:36:GLN:O	3:L:43:PRO:HA	2.11	0.51
1:A:148:GLU:O	1:A:149:GLY:C	2.53	0.51
1:B:337:PHE:O	1:B:341:VAL:HG23	2.11	0.51
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.91	0.51
1:A:336:ILE:O	1:A:340:ARG:HG3	2.09	0.51
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.46	0.51
2:J:69:ILE:HB	2:J:82:GLN:HB2	1.92	0.50
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.75	0.50
3:O:90:TRP:CG	3:O:95:GLN:HB3	2.47	0.50
2:J:49:GLY:HA3	2:J:70:ILE:CD1	2.42	0.50
2:I:107:TYR:HB3	3:L:33:HIS:CD2	2.47	0.50
3:L:30:SER:HA	3:L:70:TYR:OH	2.11	0.50
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.93	0.50
3:L:6:GLN:NE2	3:L:87:CYS:H	2.09	0.50
3:O:189:ASN:HD22	3:O:210:ARG:HB2	1.77	0.50
3:L:186:GLU:HG2	3:L:210:ARG:NH1	2.27	0.50
3:O:162:TRP:CD1	3:O:174:MET:HG3	2.46	0.49
3:L:7:SER:CB	3:L:8:PRO:CD	2.89	0.49
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.94	0.49
1:B:32:PRO:HD2	1:B:35:ILE:HD12	1.94	0.49
3:L:115:SER:HB3	3:L:117:PHE:CE1	2.48	0.49
3:L:115:SER:CB	3:L:117:PHE:HE1	2.25	0.49
2:I:109:ASP:HA	3:L:45:ARG:HD3	1.94	0.49
1:B:287:ASN:HD22	1:B:290:LYS:H	1.59	0.49
2:J:163:ASN:HD22	2:J:167:LEU:HB2	1.77	0.49
2:I:34:MET:HB3	2:I:79:LEU:HD22	1.95	0.49
1:B:421:LEU:O	1:B:425:MET:HG3	2.12	0.48
2:I:52:ASN:HD21	2:I:56:SER:H	1.61	0.48
3:L:123:GLN:NE2	3:L:130:SER:H	2.10	0.48
1:A:108:GLY:O	1:A:112:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.95	0.48
2:J:207:HIS:HE1	2:J:209:ALA:HB3	1.76	0.48
1:B:257:ILE:HA	1:B:260:ILE:HD12	1.95	0.48
3:O:197:HIS:CG	3:O:198:LYS:H	2.32	0.48
2:I:61:THR:O	2:I:63:SER:N	2.47	0.48
1:B:370:ALA:O	1:B:374:VAL:HG23	2.14	0.48
3:O:60:ARG:HB2	3:O:75:ASN:O	2.13	0.48
3:L:110:ALA:O	3:L:138:PHE:HA	2.14	0.48
1:A:252:LEU:HD22	1:A:427:ILE:HD12	1.95	0.48
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.44	0.47
3:L:118:PRO:HB3	3:L:208:PHE:CE1	2.48	0.47
1:A:419:TYR:CE1	1:B:414:GLU:HG2	2.49	0.47
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.95	0.47
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.50	0.47
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.49	0.47
1:B:148:GLU:HG3	1:B:190:PHE:CZ	2.49	0.47
1:B:148:GLU:O	1:B:149:GLY:C	2.57	0.47
2:I:6:GLU:HA	2:I:22:CYS:HA	1.96	0.47
2:I:38:ARG:HG2	2:I:48:ILE:HD11	1.96	0.47
1:B:148:GLU:OE2	1:B:358:ALA:HB2	2.14	0.47
2:J:41:PRO:HD3	2:J:92:ALA:HA	1.96	0.47
1:A:346:LEU:O	1:A:350:SER:HB3	2.14	0.47
2:I:52:ASN:HB2	2:I:53:PRO:CD	2.45	0.47
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.97	0.47
2:J:49:GLY:HA2	2:J:59:ASN:O	2.14	0.47
2:J:174:PHE:HD2	2:J:186:SER:O	1.97	0.47
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.95	0.47
1:A:384:LEU:HD22	1:A:389:PHE:CE1	2.49	0.47
3:O:148:LYS:HA	3:O:152:SER:O	2.15	0.47
1:A:109:ILE:N	1:A:110:PRO:CD	2.77	0.47
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.50	0.47
2:J:47:TRP:HZ2	2:J:50:GLU:HG2	1.79	0.47
2:J:127:PRO:HB3	2:J:153:TYR:HB3	1.97	0.47
2:I:111:TRP:HE1	3:L:35:TYR:HE2	1.63	0.47
3:O:77:MET:SD	3:O:103:LEU:HD21	2.56	0.46
2:I:24:ALA:HB1	2:I:27:PHE:HE1	1.80	0.46
2:J:2:VAL:HA	2:J:26:GLY:HA3	1.97	0.46
1:B:38:MET:O	1:B:42:VAL:HG23	2.15	0.46
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.64	0.46
1:A:411:LEU:HG	1:A:415:MET:HE2	1.97	0.46
3:L:130:SER:HA	3:L:178:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:148:LYS:HB2	3:L:192:THR:HG1	1.80	0.46
1:B:88:VAL:HA	1:B:91:MET:HE3	1.98	0.46
3:L:123:GLN:HE22	3:L:130:SER:H	1.63	0.46
3:L:148:LYS:HB2	3:L:192:THR:OG1	2.15	0.46
1:B:230:ARG:O	1:B:234:HIS:HB3	2.16	0.46
1:B:263:GLY:O	1:B:267:PRO:HD3	2.16	0.46
2:I:30:SER:C	2:I:32:TYR:H	2.23	0.46
3:L:90:TRP:CD2	3:L:95:GLN:HB3	2.50	0.46
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.97	0.46
1:A:358:ALA:HA	1:A:361:LEU:HD12	1.98	0.46
1:B:60:LEU:O	1:B:64:ARG:HG3	2.17	0.45
1:A:194:LEU:HD21	1:B:426:ILE:HD11	1.97	0.45
1:B:109:ILE:N	1:B:110:PRO:CD	2.79	0.45
2:J:196:TRP:CG	2:J:197:PRO:HA	2.50	0.45
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.97	0.45
2:I:135:GLY:C	2:I:137:ALA:H	2.23	0.45
1:B:313:SER:OG	1:B:314:GLY:N	2.50	0.45
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.99	0.45
1:A:381:GLN:NE2	1:A:381:GLN:N	2.62	0.45
2:J:33:TRP:CE2	2:J:52:ASN:HB3	2.52	0.45
3:O:197:HIS:CG	3:O:198:LYS:N	2.85	0.45
2:I:65:LYS:HB2	2:I:66:ASP:H	1.65	0.45
1:A:305:LEU:C	1:A:307:PHE:H	2.26	0.44
1:B:190:PHE:CE2	1:B:317:PHE:HZ	2.35	0.44
2:I:20:LEU:O	2:I:80:TYR:HA	2.17	0.44
1:B:320:ILE:HB	1:B:321:PRO:HD3	2.00	0.44
3:O:124:LEU:C	3:O:126:SER:N	2.75	0.44
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.81	0.44
1:B:215:ILE:H	1:B:215:ILE:HG13	1.51	0.44
2:I:200:THR:HG23	2:I:217:LYS:HE3	1.98	0.44
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.53	0.44
1:B:383:HIS:HD2	2:I:33:TRP:CZ3	2.36	0.44
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.99	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.18	0.44
2:J:52:ASN:HB2	2:J:53:PRO:HD2	2.00	0.44
3:O:35:TYR:O	3:O:85:TYR:HA	2.18	0.44
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.53	0.43
1:B:142:GLY:O	1:B:302:CYS:HB3	2.18	0.43
1:B:180:THR:CG2	1:B:218:VAL:HA	2.48	0.43
2:I:65:LYS:H	2:I:65:LYS:HG3	1.52	0.43
2:I:196:TRP:CG	2:I:197:PRO:HA	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:49:ASP:HB2	3:L:52:LYS:HD2	2.00	0.43
1:B:78:LEU:HA	1:B:81:VAL:HG22	2.01	0.43
2:I:155:PRO:HB2	2:I:156:GLU:H	1.70	0.43
2:J:163:ASN:HD21	2:J:167:LEU:HD22	1.82	0.43
1:B:345:LEU:O	1:B:349:SER:HB2	2.17	0.43
2:J:86:VAL:HG12	2:J:119:VAL:HG21	2.01	0.43
1:B:148:GLU:CD	1:B:148:GLU:N	2.68	0.43
3:L:57:VAL:HA	3:L:58:PRO:HD2	1.86	0.43
3:L:116:ILE:HD13	3:L:193:CYS:HB2	2.01	0.43
1:B:199:PHE:HA	1:B:407:THR:OG1	2.19	0.43
3:O:117:PHE:HA	3:O:118:PRO:HD3	1.92	0.43
3:O:150:ASP:HA	3:O:190:SER:HB3	2.01	0.43
1:B:234:HIS:HD1	1:B:235:GLU:HG2	1.84	0.42
1:B:266:GLY:HA3	1:B:400:ALA:HB1	2.01	0.42
3:L:154:ARG:HH21	3:L:156:ASN:HB2	1.84	0.42
1:A:241:VAL:HG11	1:A:324:THR:HG21	2.01	0.42
1:A:328:PHE:HD1	1:A:332:MET:HG2	1.84	0.42
1:A:356:ILE:O	1:A:360:MET:HG3	2.19	0.42
1:B:262:PHE:HZ	1:B:364:GLY:HA2	1.84	0.42
3:O:62:SER:OG	3:O:73:THR:HB	2.19	0.42
2:I:132:LEU:HB3	3:L:117:PHE:CD2	2.54	0.42
1:A:32:PRO:HD2	1:A:35:ILE:HD12	2.01	0.42
1:B:330:MET:HE3	1:B:330:MET:HA	2.01	0.42
3:O:112:PRO:HG2	3:O:204:ILE:HD12	2.01	0.42
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.85	0.42
3:O:33:HIS:ND1	3:O:48:TYR:HB2	2.35	0.42
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.35	0.42
1:A:330:MET:HE1	1:A:370:ALA:HB1	2.02	0.42
3:O:54:THR:HG22	3:O:55:SER:N	2.35	0.42
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.35	0.42
2:J:12:VAL:HG11	2:J:18:LEU:HD22	2.01	0.42
2:J:30:SER:O	2:J:32:TYR:N	2.53	0.41
2:J:156:GLU:HG2	2:J:183:TYR:CE1	2.55	0.41
1:B:108:GLY:H	1:B:110:PRO:HD2	1.85	0.41
1:B:131:LYS:HD3	1:B:153:GLN:NE2	2.35	0.41
1:B:421:LEU:C	1:B:424:PRO:HD2	2.45	0.41
2:J:196:TRP:CD1	2:J:197:PRO:HA	2.55	0.41
2:I:67:LYS:HA	2:I:67:LYS:HD2	1.89	0.41
1:A:192:ALA:HB1	1:A:414:GLU:OE2	2.20	0.41
3:L:117:PHE:HA	3:L:118:PRO:HD3	1.76	0.41
1:A:191:ASN:O	1:A:191:ASN:CG	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:VAL:HB	1:B:160:ARG:HG2	2.03	0.41
3:O:58:PRO:HB2	3:O:60:ARG:HG2	2.02	0.41
1:A:194:LEU:HD23	1:B:426:ILE:HD11	2.01	0.41
1:A:423:LEU:HD11	1:B:226:THR:HG21	2.03	0.41
1:B:127:VAL:O	1:B:128:LEU:C	2.63	0.41
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.56	0.41
2:J:162:TRP:CZ3	2:J:203:CYS:HB3	2.55	0.41
2:I:35:SER:HB2	2:I:99:LEU:HD11	2.01	0.41
1:A:216:LYS:HE2	1:B:433:THR:HG22	2.02	0.41
1:B:294:MET:HE2	1:B:294:MET:HB3	1.93	0.41
2:J:30:SER:C	2:J:32:TYR:N	2.79	0.41
1:B:244:LEU:HB2	1:B:418:ASN:OD1	2.20	0.40
1:B:372:GLY:O	1:B:376:VAL:HG23	2.21	0.40
3:L:93:HIS:ND1	3:L:94:PRO:HA	2.36	0.40
2:I:89:GLU:OE1	2:I:89:GLU:N	2.54	0.40
1:B:138:THR:HG21	1:B:352:ALA:HB1	2.03	0.40
1:B:200:ILE:HA	1:B:204:MET:HB2	2.03	0.40
3:O:29:VAL:HG23	3:O:70:TYR:CE1	2.50	0.40
3:O:118:PRO:HA	3:O:119:PRO:HD2	1.96	0.40
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.22	0.40
1:B:418:ASN:O	1:B:419:TYR:C	2.64	0.40
2:J:6:GLU:OE2	2:J:95:TYR:HA	2.21	0.40
2:J:135:GLY:HA2	2:J:221:ARG:HE	1.87	0.40
3:O:57:VAL:HA	3:O:58:PRO:HD2	1.87	0.40
3:O:7:SER:HB3	3:O:8:PRO:HD3	2.03	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	442/465 (95%)	411 (93%)	25 (6%)	6 (1%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	439/465 (94%)	406 (92%)	29 (7%)	4 (1%)	14	48
2	I	219/222 (99%)	192 (88%)	20 (9%)	7 (3%)	3	25
2	J	219/222 (99%)	193 (88%)	24 (11%)	2 (1%)	14	48
3	L	209/211 (99%)	181 (87%)	22 (10%)	6 (3%)	3	26
3	O	209/211 (99%)	181 (87%)	25 (12%)	3 (1%)	9	39
All	All	1737/1796 (97%)	1564 (90%)	145 (8%)	28 (2%)	7	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	B	73	ASP
3	O	55	SER
3	L	7	SER
1	A	74	ASN
1	B	74	ASN
2	J	62	PRO
2	I	62	PRO
2	I	65	LYS
2	J	31	ARG
2	I	140	ALA
3	L	59	VAL
3	L	170	SER
1	A	149	GLY
3	O	51	SER
3	O	169	ASP
2	I	142	SER
3	L	80	GLU
3	L	102	LYS
1	B	149	GLY
2	I	164	SER
3	L	67	GLY
1	A	206	PRO
1	B	206	PRO
1	A	443	PRO
1	A	201	ILE
2	I	155	PRO
2	I	157	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/353 (95%)	315 (94%)	20 (6%)	17	43
1	B	332/353 (94%)	305 (92%)	27 (8%)	11	34
2	I	181/182 (100%)	171 (94%)	10 (6%)	19	45
2	J	181/182 (100%)	164 (91%)	17 (9%)	8	29
3	L	185/185 (100%)	171 (92%)	14 (8%)	12	37
3	O	185/185 (100%)	173 (94%)	12 (6%)	15	41
All	All	1399/1440 (97%)	1299 (93%)	100 (7%)	13	39

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	44	THR
1	A	65	MET
1	A	136	LEU
1	A	180	THR
1	A	200	ILE
1	A	211	THR
1	A	238	LEU
1	A	244	LEU
1	A	270	ASN
1	A	279	LEU
1	A	334	VAL
1	A	343	THR
1	A	346	LEU
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	433	THR
1	A	442	LYS
1	A	457	GLU
1	B	73	ASP
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	96	LEU
1	B	107	SER
1	B	122	VAL
1	B	138	THR
1	B	139	LEU
1	B	148	GLU
1	B	200	ILE
1	B	207	GLN
1	B	211	THR
1	B	215	ILE
1	B	223	ILE
1	B	244	LEU
1	B	293	LEU
1	B	346	LEU
1	B	357	PHE
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	435	LEU
1	B	437	GLN
1	B	439	THR
1	B	444	LEU
1	B	451	ARG
2	J	5	LEU
2	J	30	SER
2	J	43	LYS
2	J	54	VAL
2	J	86	VAL
2	J	98	ARG
2	J	116	THR
2	J	118	THR
2	J	121	SER
2	J	125	THR
2	J	128	SER
2	J	129	VAL
2	J	144	VAL
2	J	151	LYS
2	J	185	LEU
2	J	218	ILE
2	J	219	VAL

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Mol	Chain	Res	Type
3	O	5	THR
3	O	10	ILE
3	O	20	THR
3	O	28	SER
3	O	59	VAL
3	O	84	THR
3	O	95	GLN
3	O	96	THR
3	O	131	VAL
3	O	132	VAL
3	O	179	THR
3	O	192	THR
2	I	5	LEU
2	I	12	VAL
2	I	54	VAL
2	I	58	ILE
2	I	86	VAL
2	I	115	THR
2	I	143	MET
2	I	151	LYS
2	I	179	GLN
2	I	199	GLU
3	L	22	THR
3	L	30	SER
3	L	32	ILE
3	L	68	THR
3	L	77	MET
3	L	84	THR
3	L	95	GLN
3	L	96	THR
3	L	106	LEU
3	L	113	THR
3	L	125	THR
3	L	177	THR
3	L	183	ASP
3	L	189	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	234	HIS
1	A	327	ASN
1	A	381	GLN
1	A	420	GLN
1	B	62	ASN
1	B	74	ASN
1	B	157	ASN
1	B	175	HIS
1	B	287	ASN
1	B	318	ASN
1	B	327	ASN
1	B	381	GLN
1	B	383	HIS
2	J	163	ASN
2	J	179	GLN
2	J	207	HIS
3	O	6	GLN
3	O	36	GLN
3	O	189	ASN
2	I	82	GLN
2	I	172	HIS
3	L	6	GLN
3	L	36	GLN
3	L	37	GLN
3	L	89	GLN
3	L	123	GLN
3	L	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	444/465 (95%)	-0.03	9 (2%) 65 46	117, 150, 183, 202	0
1	B	441/465 (94%)	0.07	6 (1%) 73 53	121, 158, 194, 210	0
2	I	221/222 (99%)	0.14	2 (0%) 81 62	131, 162, 185, 194	0
2	J	221/222 (99%)	0.10	2 (0%) 81 62	131, 146, 169, 176	0
3	L	211/211 (100%)	-0.11	2 (0%) 81 62	115, 139, 188, 197	0
3	O	211/211 (100%)	0.03	2 (0%) 81 62	152, 167, 181, 183	0
All	All	1749/1796 (97%)	0.03	23 (1%) 75 55	115, 156, 185, 210	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	GLY	5.1
3	L	114	VAL	5.1
1	A	145	LEU	4.6
2	J	147	GLY	4.4
1	B	353	PRO	4.1
1	A	139	LEU	4.0
1	B	179	ALA	3.4
1	A	29	ASP	3.4
1	A	168	LEU	3.1
3	L	55	SER	3.1
1	A	380	PRO	2.9
1	A	72	ALA	2.8
1	B	440	GLY	2.7
1	B	104	ALA	2.6
1	B	177	LEU	2.6
3	O	163	THR	2.5
2	I	208	PRO	2.4
1	A	205	ARG	2.2
3	O	20	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	158	VAL	2.1
2	J	99	LEU	2.1
1	B	288	ILE	2.1
1	A	353	PRO	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.