



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:27 AM UTC

PDB ID : 2FED / pdb_00002fed
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 : 3.32 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

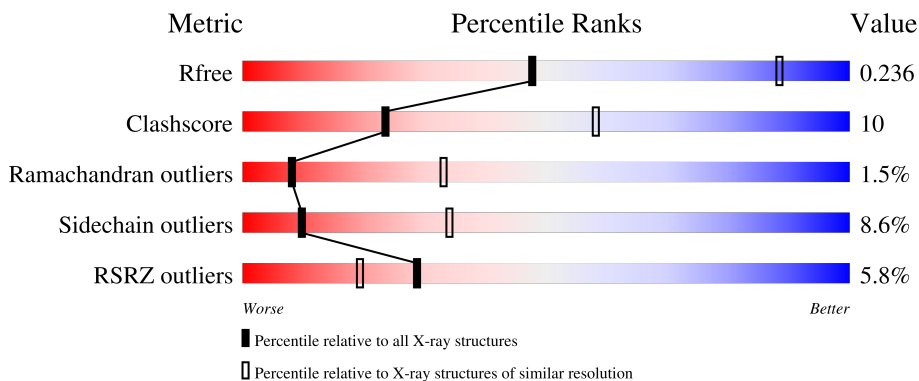
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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.



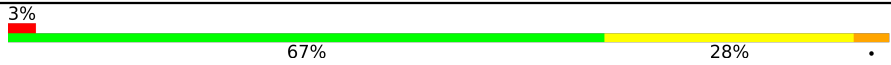
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	
1	B	465	
2	C	222	
2	E	222	
3	D	211	

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Mol	Chain	Length	Quality of chain
3	F	211	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '67%', and a yellow segment on the right labeled '28%'. A small black dot is visible at the far right end 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	C	221	1672	1077	274	315	6	0	0	0
2	E	221	1672	1077	274	315	6	0	0	0

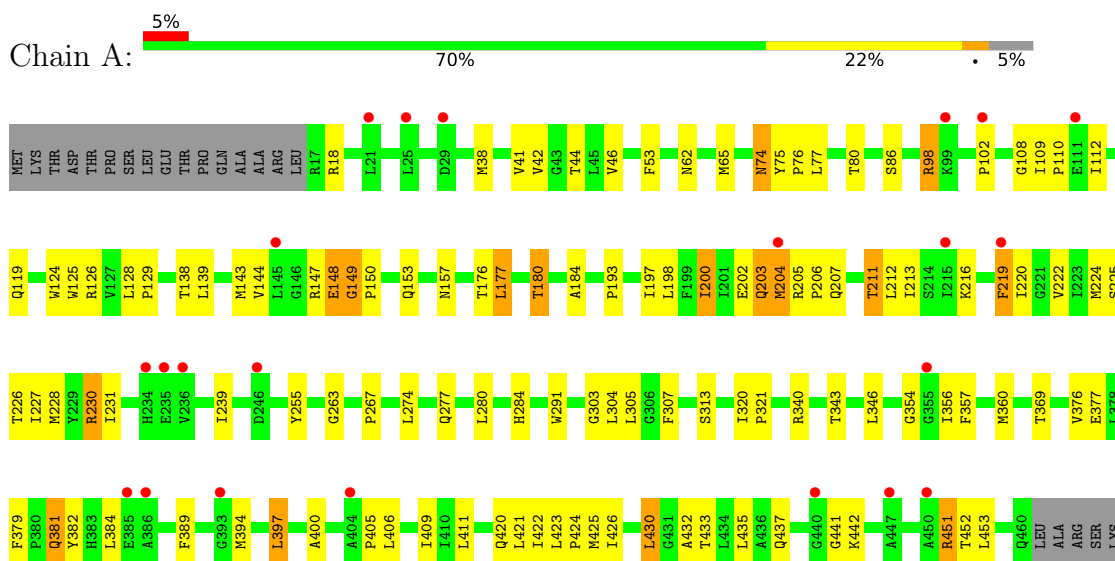
- Molecule 3 is a protein called Fab fragment, light chain.

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

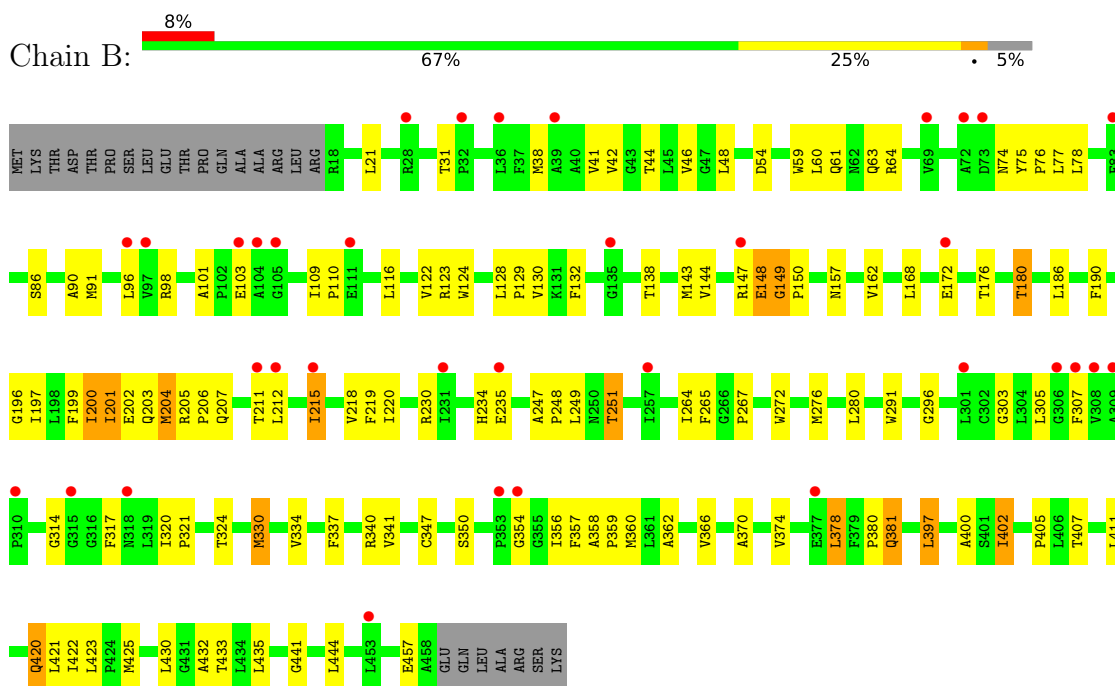
3 Residue-property plots i

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.

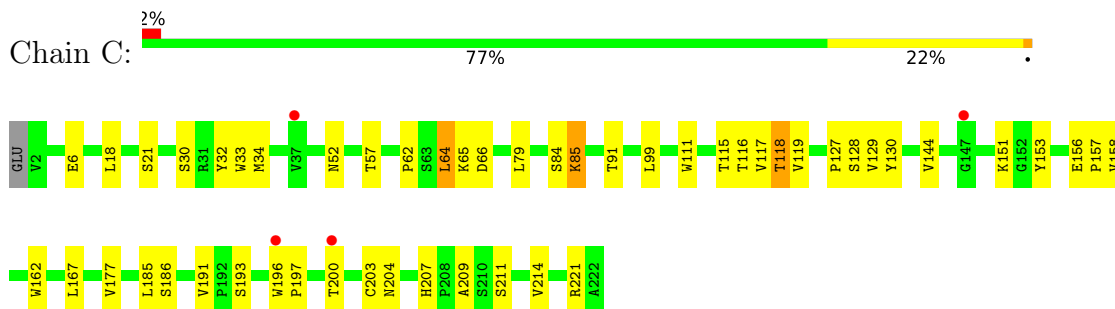
- Molecule 1: H(+)/Cl(-) exchange transporter clcA



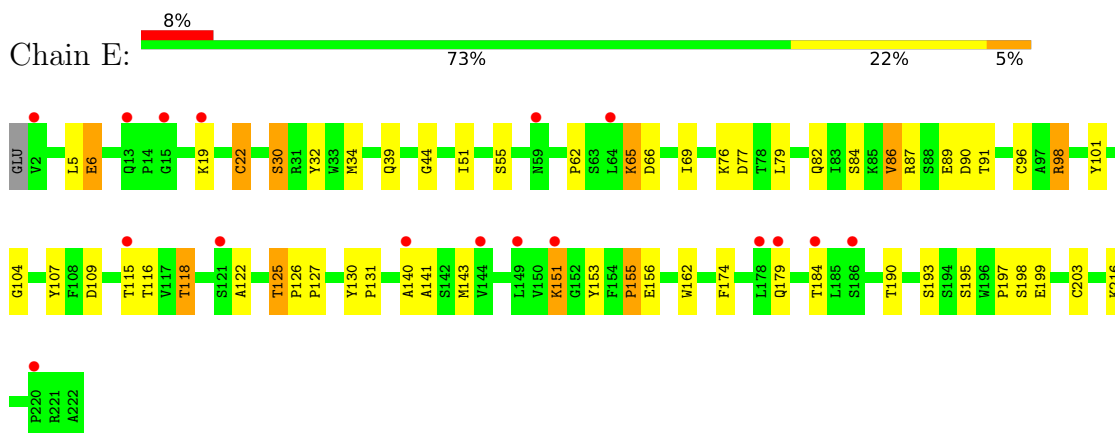
- Molecule 1: H(+)/Cl(-) exchange transporter clcA



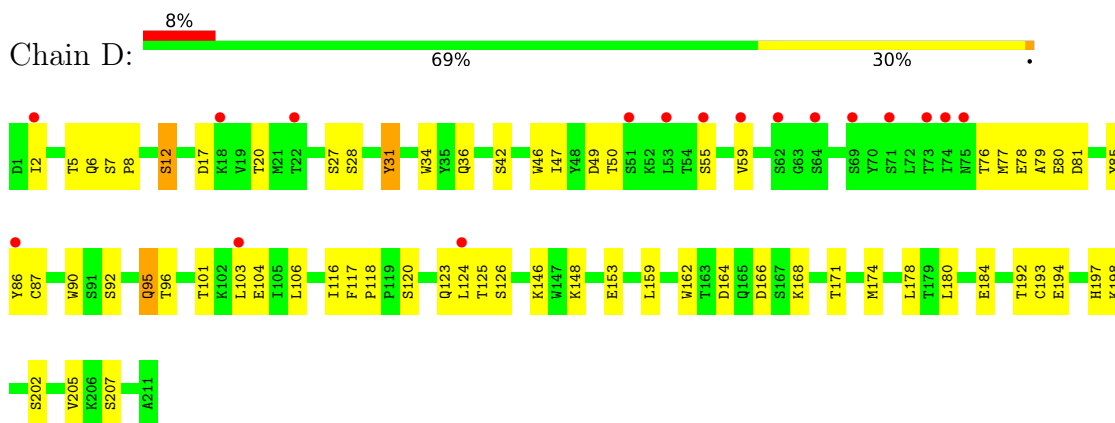
- Molecule 2: Fab fragment, heavy chain



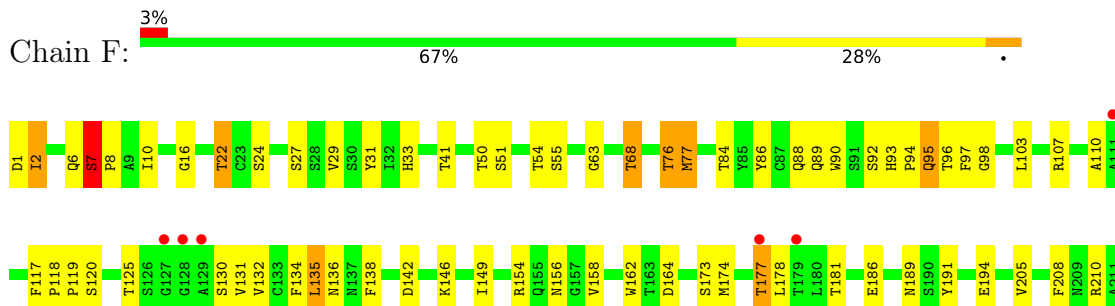
- Molecule 2: Fab fragment, heavy chain



- 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	232.27Å 98.23Å 170.36Å 90.00° 131.73° 90.00°	Depositor
Resolution (Å)	49.81 – 3.32 49.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.81-3.32) 89.7 (49.81-3.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.33Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.248 , 0.287 0.242 , 0.236	Depositor DCC
R_{free} test set	1946 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	94.2	Xtrriage
Anisotropy	0.272	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.47	0/3405	0.86	0/4621
1	B	0.52	0/3376	0.90	2/4583 (0.0%)
2	C	0.53	0/1721	0.81	0/2355
2	E	0.51	0/1721	0.82	0/2355
3	D	0.50	0/1660	0.82	2/2257 (0.1%)
3	F	0.48	0/1660	0.81	2/2257 (0.1%)
All	All	0.50	0/13543	0.85	6/18428 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	CA-C-N	-5.98	113.53	119.99
3	F	7	SER	C-N-CA	-5.98	113.53	119.99
1	B	247	ALA	CA-C-N	5.73	125.69	119.78
1	B	247	ALA	C-N-CA	5.73	125.69	119.78
3	D	202	SER	CA-C-N	5.05	124.81	119.76
3	D	202	SER	C-N-CA	5.05	124.81	119.76

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	3486	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3304	0	3459	78	0
2	C	1672	0	1654	25	0
2	E	1672	0	1654	26	0
3	D	1621	0	1546	39	0
3	F	1621	0	1546	45	0
All	All	13223	0	13345	271	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 10.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.21	1.18
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.30	1.13
3:F:7:SER:HB3	3:F:8:PRO:CD	1.86	1.05
3:D:95:GLN:CD	3:D:95:GLN:H	1.69	1.01
3:F:7:SER:HB2	3:F:22:THR:HB	1.45	0.97
1:A:381:GLN:H	1:A:381:GLN:HE21	1.04	0.96
1:B:381:GLN:H	1:B:381:GLN:HE21	1.25	0.85
3:F:7:SER:CB	3:F:8:PRO:HD3	2.07	0.85
1:B:148:GLU:CD	1:B:148:GLU:H	1.85	0.82
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.48	0.78
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.48	0.78
1:A:274:LEU:HA	1:A:277:GLN:HE21	1.49	0.77
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.64	0.77
3:D:95:GLN:CD	3:D:95:GLN:N	2.41	0.77
1:B:203:GLN:O	1:B:205:ARG:N	2.19	0.76
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.68	0.75
1:B:38:MET:O	1:B:42:VAL:HG23	1.87	0.74
1:A:203:GLN:O	1:A:205:ARG:N	2.20	0.73
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.71	0.72
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.71	0.72
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.55	0.70
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.92	0.69
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.76	0.68
3:F:7:SER:CB	3:F:22:THR:HB	2.21	0.68
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.76	0.67
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.77	0.66
1:A:148:GLU:CD	1:A:148:GLU:H	2.05	0.65
3:F:7:SER:HB2	3:F:22:THR:CB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:GLU:HA	2:E:22:CYS:HA	1.79	0.64
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.79	0.64
1:B:234:HIS:ND1	1:B:235:GLU:HG2	2.13	0.64
2:C:91:THR:HG23	2:C:118:THR:HA	1.81	0.63
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.64	0.62
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.64	0.62
1:B:202:GLU:OE2	1:B:405:PRO:HD2	1.99	0.62
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.65	0.62
1:A:200:ILE:HA	1:A:204:MET:HB2	1.83	0.61
1:A:38:MET:O	1:A:42:VAL:HG23	2.00	0.61
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.81	0.61
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.82	0.61
3:D:95:GLN:N	3:D:95:GLN:OE1	2.35	0.60
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.81	0.60
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.82	0.60
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.83	0.60
1:A:98:ARG:HH12	1:A:102:PRO:HB3	1.66	0.59
1:B:75:TYR:O	1:B:78:LEU:HG	2.01	0.59
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.38	0.59
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.67	0.59
2:C:52:ASN:ND2	2:C:57:THR:HB	2.17	0.59
2:E:174:PHE:HZ	3:F:136:ASN:HD21	1.50	0.58
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.85	0.58
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.39	0.58
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.67	0.58
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.85	0.58
2:E:39:GLN:HG3	2:E:44:GLY:O	2.04	0.58
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.39	0.58
3:F:95:GLN:N	3:F:95:GLN:OE1	2.37	0.58
1:A:381:GLN:HE21	1:A:381:GLN:N	1.88	0.57
1:B:176:THR:O	1:B:180:THR:HG23	2.04	0.57
2:C:33:TRP:CZ2	2:C:52:ASN:HB3	2.39	0.57
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.40	0.57
1:B:337:PHE:O	1:B:341:VAL:HG23	2.04	0.57
1:B:200:ILE:HA	1:B:204:MET:HB2	1.87	0.57
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.87	0.56
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.88	0.56
3:D:180:LEU:HD22	3:D:184:GLU:HG2	1.88	0.56
1:A:451:ARG:HH11	1:A:451:ARG:HB3	1.70	0.56
1:A:430:LEU:HD13	1:B:219:PHE:HB3	1.87	0.55
3:D:124:LEU:C	3:D:126:SER:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.41	0.55
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.41	0.55
3:F:110:ALA:O	3:F:138:PHE:HA	2.07	0.55
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.88	0.55
3:F:95:GLN:H	3:F:95:GLN:CD	2.15	0.55
2:C:30:SER:C	2:C:32:TYR:H	2.14	0.55
1:A:422:ILE:HA	1:A:425:MET:HE3	1.88	0.54
1:A:360:MET:HG2	1:A:397:LEU:HD12	1.90	0.54
1:A:193:PRO:HG3	1:A:226:THR:HG21	1.89	0.54
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.89	0.54
1:A:176:THR:O	1:A:180:THR:HG23	2.06	0.54
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.43	0.54
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.89	0.54
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.42	0.54
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.89	0.54
2:E:86:VAL:HG12	2:E:90:ASP:HB2	1.90	0.54
1:A:42:VAL:O	1:A:46:VAL:HG23	2.08	0.53
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.91	0.53
1:B:172:GLU:HB2	1:B:212:LEU:HD23	1.90	0.53
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.24	0.53
1:A:356:ILE:HG23	1:A:360:MET:CE	2.38	0.53
2:C:196:TRP:CG	2:C:197:PRO:HA	2.43	0.53
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.39	0.53
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.43	0.53
1:B:143:MET:HE2	1:B:347:CYS:SG	2.49	0.53
1:B:148:GLU:CD	1:B:148:GLU:N	2.61	0.53
1:A:144:VAL:HG21	1:A:343:THR:HB	1.90	0.53
3:D:197:HIS:CG	3:D:198:LYS:H	2.27	0.52
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.91	0.52
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.38	0.52
1:A:437:GLN:NE2	1:B:31:THR:H	2.07	0.52
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.92	0.52
1:A:108:GLY:O	1:A:112:ILE:HG12	2.10	0.51
1:A:227:ILE:O	1:A:231:ILE:HG12	2.10	0.51
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.93	0.51
2:C:33:TRP:HB2	2:C:99:LEU:HB2	1.93	0.51
1:B:60:LEU:O	1:B:64:ARG:HG3	2.11	0.50
2:C:84:SER:O	2:C:85:LYS:C	2.53	0.50
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.46	0.50
1:B:144:VAL:HG12	1:B:144:VAL:O	2.12	0.50
3:D:79:ALA:C	3:D:81:ASP:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:MET:HA	1:B:41:VAL:HG12	1.94	0.50
1:A:86:SER:OG	1:A:303:GLY:HA3	2.12	0.50
1:A:267:PRO:HB3	1:A:441:GLY:HA3	1.94	0.49
1:B:103:GLU:OE1	1:B:123:ARG:HB2	2.11	0.49
1:A:98:ARG:NH1	1:A:98:ARG:HA	2.27	0.49
1:B:86:SER:OG	1:B:303:GLY:HA3	2.12	0.49
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.59	0.49
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.95	0.49
1:B:272:TRP:O	1:B:276:MET:HB2	2.12	0.49
1:B:362:ALA:O	1:B:366:VAL:HG23	2.12	0.49
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.46	0.49
3:F:136:ASN:HD22	3:F:173:SER:HB3	1.77	0.49
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.43	0.49
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.93	0.49
3:F:54:THR:HG22	3:F:55:SER:N	2.28	0.49
1:A:421:LEU:O	1:A:425:MET:HG3	2.12	0.49
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.94	0.49
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.48	0.49
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.94	0.48
1:A:148:GLU:O	1:A:149:GLY:C	2.55	0.48
2:E:6:GLU:HB3	2:E:22:CYS:HB2	1.95	0.48
3:F:130:SER:HA	3:F:178:LEU:O	2.13	0.48
1:A:148:GLU:OE1	1:A:357:PHE:HB3	2.13	0.48
3:F:107:ARG:NH2	3:F:110:ALA:HB2	2.28	0.48
3:D:146:LYS:HE3	3:D:153:GLU:HG3	1.95	0.48
2:C:130:TYR:HB3	3:D:120:SER:OG	2.14	0.48
3:D:12:SER:HA	3:D:104:GLU:O	2.13	0.47
3:D:116:ILE:HD12	3:D:193:CYS:HB2	1.96	0.47
2:E:131:PRO:HD3	2:E:216:LYS:HG2	1.96	0.47
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.50	0.47
1:B:109:ILE:N	1:B:110:PRO:CD	2.78	0.47
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.48	0.47
3:F:93:HIS:CG	3:F:94:PRO:HA	2.50	0.47
1:A:274:LEU:HA	1:A:277:GLN:NE2	2.24	0.46
3:D:197:HIS:CG	3:D:198:LYS:N	2.83	0.46
1:A:38:MET:HB3	1:A:177:LEU:HD11	1.97	0.46
1:B:421:LEU:O	1:B:425:MET:HG3	2.15	0.46
2:E:143:MET:HE3	2:E:190:THR:HG22	1.96	0.46
1:B:54:ASP:OD1	1:B:147:ARG:NH2	2.47	0.46
3:D:7:SER:CB	3:D:8:PRO:HD3	2.44	0.46
1:A:357:PHE:HE2	1:A:411:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PRO:HB3	2:E:104:GLY:HA2	1.96	0.46
3:D:6:GLN:NE2	3:D:87:CYS:H	2.13	0.46
3:D:36:GLN:HG3	3:D:85:TYR:CE2	2.50	0.46
2:E:19:LYS:HG3	2:E:82:GLN:HG2	1.98	0.46
2:E:87:ARG:HE	2:E:89:GLU:CD	2.24	0.46
1:A:379:PHE:CB	1:A:382:TYR:CD1	2.99	0.46
2:C:167:LEU:HD21	2:C:191:VAL:HG11	1.97	0.46
3:F:189:ASN:HA	3:F:210:ARG:HD3	1.96	0.46
1:A:274:LEU:O	1:A:277:GLN:HB2	2.16	0.45
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.98	0.45
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.46	0.45
1:B:264:ILE:HG13	1:B:265:PHE:N	2.30	0.45
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.31	0.45
3:F:90:TRP:CH2	3:F:95:GLN:NE2	2.85	0.45
3:D:77:MET:HE3	3:D:78:GLU:O	2.16	0.45
1:A:384:LEU:HD22	1:A:389:PHE:HE1	1.82	0.45
3:F:2:ILE:HD12	3:F:27:SER:HB2	1.98	0.45
1:A:274:LEU:HD23	1:A:277:GLN:HE22	1.82	0.45
1:B:148:GLU:O	1:B:149:GLY:C	2.59	0.45
1:B:59:TRP:O	1:B:63:GLN:HG2	2.16	0.45
1:B:360:MET:HG2	1:B:397:LEU:HD12	1.98	0.45
2:C:177:VAL:HG21	3:D:159:LEU:HD13	1.98	0.45
3:D:168:LYS:HD3	3:D:168:LYS:HA	1.79	0.45
1:A:224:MET:O	1:A:228:MET:HG2	2.17	0.45
1:A:280:LEU:O	1:A:284:HIS:CD2	2.70	0.45
1:A:305:LEU:C	1:A:307:PHE:H	2.25	0.44
1:A:216:LYS:HE2	1:B:433:THR:HG22	1.98	0.44
1:B:215:ILE:H	1:B:215:ILE:HG13	1.48	0.44
1:B:249:LEU:C	1:B:251:THR:H	2.26	0.44
2:C:158:VAL:HG12	2:C:207:HIS:HB2	2.00	0.44
2:E:86:VAL:HG12	2:E:90:ASP:CB	2.48	0.44
2:E:130:TYR:HB3	3:F:120:SER:OG	2.18	0.44
1:A:203:GLN:HB3	1:A:204:MET:H	1.56	0.44
3:D:77:MET:HG2	3:D:78:GLU:H	1.83	0.44
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.99	0.44
3:D:192:THR:HA	3:D:207:SER:HB3	1.99	0.44
1:A:239:ILE:HD13	1:A:394:MET:HE1	2.00	0.43
1:B:305:LEU:C	1:B:307:PHE:H	2.27	0.43
3:F:149:ILE:HD11	3:F:178:LEU:HD21	1.99	0.43
2:E:197:PRO:C	2:E:199:GLU:H	2.27	0.43
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:191:TYR:HB2	3:F:208:PHE:CE2	2.53	0.43
1:A:340:ARG:HA	1:A:343:THR:OG1	2.19	0.43
1:B:280:LEU:HD13	1:B:350:SER:HB3	1.99	0.43
1:B:370:ALA:O	1:B:374:VAL:HG23	2.18	0.43
1:B:422:ILE:HD12	1:B:425:MET:HE3	1.99	0.43
2:C:6:GLU:HA	2:C:21:SER:O	2.18	0.43
1:A:109:ILE:N	1:A:110:PRO:CD	2.81	0.43
1:A:184:ALA:HB1	1:A:225:SER:HB3	2.00	0.43
1:A:197:ILE:HG13	1:A:222:VAL:HG21	2.01	0.43
1:A:313:SER:O	1:A:340:ARG:NH2	2.51	0.43
1:B:116:LEU:HD13	1:B:204:MET:O	2.19	0.43
2:E:91:THR:HG23	2:E:118:THR:HA	2.01	0.43
3:F:95:GLN:N	3:F:95:GLN:CD	2.75	0.43
1:A:379:PHE:CB	1:A:382:TYR:HD1	2.32	0.43
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.93	0.43
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.53	0.43
1:B:320:ILE:HB	1:B:321:PRO:HD3	2.00	0.43
2:C:18:LEU:HD11	2:C:117:VAL:HG22	2.01	0.43
3:F:51:SER:HB3	3:F:63:GLY:O	2.18	0.43
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.18	0.43
2:E:34:MET:HB3	2:E:79:LEU:HD22	2.01	0.43
1:B:360:MET:HE1	1:B:402:ILE:CG2	2.49	0.42
3:F:132:VAL:HG22	3:F:177:THR:HG23	2.01	0.42
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.01	0.42
3:F:29:VAL:HG11	3:F:89:GLN:HG2	2.02	0.42
1:A:211:THR:HB	1:A:213:ILE:HG13	2.01	0.42
1:B:201:ILE:O	1:B:201:ILE:HG13	2.17	0.42
3:D:77:MET:SD	3:D:103:LEU:HD21	2.60	0.42
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.49	0.42
1:A:202:GLU:OE2	1:A:405:PRO:HD2	2.19	0.42
2:E:151:LYS:HB2	2:E:184:THR:OG1	2.20	0.42
1:A:409:ILE:HD11	1:A:426:ILE:HA	2.02	0.42
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.46	0.42
1:A:220:ILE:HG12	1:B:430:LEU:HD21	2.01	0.42
1:B:356:ILE:O	1:B:356:ILE:HG12	2.19	0.42
2:C:144:VAL:HG12	2:C:191:VAL:O	2.20	0.42
1:B:90:ALA:HB3	1:B:296:GLY:HA2	2.00	0.41
1:B:330:MET:O	1:B:334:VAL:HG23	2.19	0.41
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.55	0.41
3:D:166:ASP:HB2	3:D:171:THR:O	2.20	0.41
2:E:125:THR:HA	2:E:126:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:THR:HB	1:B:218:VAL:HA	2.02	0.41
2:C:64:LEU:H	2:C:64:LEU:HG	1.52	0.41
2:E:155:PRO:HB2	2:E:156:GLU:H	1.72	0.41
3:F:24:SER:HA	3:F:68:THR:O	2.20	0.41
3:F:77:MET:HE2	3:F:103:LEU:HD11	2.01	0.41
2:C:127:PRO:HB3	2:C:153:TYR:HB3	2.02	0.41
2:C:221:ARG:HH22	3:D:120:SER:HA	1.86	0.41
3:F:31:TYR:HA	3:F:50:THR:OG1	2.19	0.41
3:F:89:GLN:C	3:F:89:GLN:CD	2.89	0.41
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.46	0.41
2:C:177:VAL:CG2	3:D:159:LEU:HD13	2.50	0.41
2:E:101:TYR:CD2	2:E:101:TYR:N	2.89	0.41
3:F:134:PHE:C	3:F:135:LEU:HD23	2.45	0.41
1:B:374:VAL:HG12	1:B:378:LEU:HD12	2.01	0.41
2:E:79:LEU:HD23	2:E:96:CYS:HB2	2.02	0.41
1:A:138:THR:O	1:A:143:MET:HB2	2.21	0.41
1:B:380:PRO:HG2	3:F:93:HIS:HB3	2.03	0.41
1:B:420:GLN:HE21	1:B:420:GLN:HB2	1.70	0.41
2:E:30:SER:C	2:E:32:TYR:H	2.29	0.41
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.02	0.41
3:D:77:MET:HG2	3:D:78:GLU:N	2.36	0.41
2:E:76:LYS:O	2:E:77:ASP:HB2	2.21	0.41
3:F:7:SER:CB	3:F:8:PRO:CD	2.71	0.41
1:B:314:GLY:O	1:B:340:ARG:NH2	2.54	0.41
2:C:111:TRP:CD1	2:C:111:TRP:N	2.89	0.41
3:D:17:ASP:H	3:D:77:MET:H	1.68	0.41
1:A:119:GLN:HG3	1:B:21:LEU:HD22	2.04	0.40
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.87	0.40
3:D:31:TYR:HA	3:D:50:THR:OG1	2.21	0.40
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.57	0.40
1:B:101:ALA:HB3	1:B:130:VAL:HG11	2.02	0.40
1:A:53:PHE:HE2	1:A:147:ARG:HG2	1.86	0.40
1:A:230:ARG:NH2	1:B:423:LEU:HB2	2.36	0.40
1:B:42:VAL:O	1:B:46:VAL:HG23	2.21	0.40
1:A:381:GLN:H	1:A:381:GLN:NE2	1.89	0.40
1:B:199:PHE:HB2	1:B:407:THR:HG21	2.02	0.40
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.57	0.40
3:F:158:VAL:HG22	3:F:178:LEU:HD13	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%)	402 (91%)	37 (8%)	3 (1%)	18	49
1	B	439/465 (94%)	400 (91%)	35 (8%)	4 (1%)	14	43
2	C	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	9	34
2	E	219/222 (99%)	192 (88%)	18 (8%)	9 (4%)	2	15
3	D	209/211 (99%)	184 (88%)	20 (10%)	5 (2%)	4	25
3	F	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	12	41
All	All	1737/1796 (97%)	1566 (90%)	145 (8%)	26 (2%)	8	33

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	MET
1	B	204	MET
3	F	7	SER
2	C	65	LYS
2	C	85	LYS
3	D	80	GLU
2	E	62	PRO
2	E	140	ALA
1	B	132	PHE
2	C	62	PRO
3	D	55	SER
2	E	141	ALA
2	E	65	LYS
2	E	122	ALA
2	E	195	SER
3	F	76	THR
1	B	206	PRO
3	D	31	TYR
3	D	76	THR
3	D	125	THR

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Mol	Chain	Res	Type
2	E	198	SER
1	A	206	PRO
1	B	149	GLY
1	A	149	GLY
2	E	51	ILE
2	E	155	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%)	303 (90%)	32 (10%)	8 29
1	B	332/353 (94%)	308 (93%)	24 (7%)	13 40
2	C	181/182 (100%)	165 (91%)	16 (9%)	9 33
2	E	181/182 (100%)	163 (90%)	18 (10%)	7 28
3	D	185/185 (100%)	172 (93%)	13 (7%)	14 41
3	F	185/185 (100%)	167 (90%)	18 (10%)	8 29
All	All	1399/1440 (97%)	1278 (91%)	121 (9%)	10 34

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	44	THR
1	A	62	ASN
1	A	65	MET
1	A	74	ASN
1	A	80	THR
1	A	98	ARG
1	A	139	LEU
1	A	148	GLU
1	A	177	LEU
1	A	180	THR
1	A	200	ILE

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Mol	Chain	Res	Type
1	A	203	GLN
1	A	207	GLN
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	230	ARG
1	A	304	LEU
1	A	346	LEU
1	A	369	THR
1	A	377	GLU
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
1	A	430	LEU
1	A	433	THR
1	A	442	LYS
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	44	THR
1	B	48	LEU
1	B	61	GLN
1	B	96	LEU
1	B	122	VAL
1	B	138	THR
1	B	148	GLU
1	B	180	THR
1	B	200	ILE
1	B	201	ILE
1	B	207	GLN
1	B	211	THR
1	B	215	ILE
1	B	230	ARG
1	B	251	THR
1	B	324	THR
1	B	330	MET
1	B	378	LEU
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN

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Mol	Chain	Res	Type
1	B	435	LEU
1	B	444	LEU
2	C	64	LEU
2	C	66	ASP
2	C	115	THR
2	C	116	THR
2	C	118	THR
2	C	119	VAL
2	C	128	SER
2	C	129	VAL
2	C	151	LYS
2	C	185	LEU
2	C	186	SER
2	C	193	SER
2	C	200	THR
2	C	204	ASN
2	C	211	SER
2	C	214	VAL
3	D	5	THR
3	D	12	SER
3	D	20	THR
3	D	28	SER
3	D	42	SER
3	D	46	TRP
3	D	59	VAL
3	D	92	SER
3	D	95	GLN
3	D	96	THR
3	D	101	THR
3	D	164	ASP
3	D	178	LEU
2	E	5	LEU
2	E	6	GLU
2	E	22	CYS
2	E	30	SER
2	E	55	SER
2	E	65	LYS
2	E	66	ASP
2	E	69	ILE
2	E	84	SER
2	E	86	VAL
2	E	98	ARG

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Mol	Chain	Res	Type
2	E	115	THR
2	E	116	THR
2	E	118	THR
2	E	125	THR
2	E	151	LYS
2	E	179	GLN
2	E	193	SER
3	F	1	ASP
3	F	2	ILE
3	F	7	SER
3	F	10	ILE
3	F	22	THR
3	F	41	THR
3	F	68	THR
3	F	77	MET
3	F	84	THR
3	F	92	SER
3	F	95	GLN
3	F	96	THR
3	F	125	THR
3	F	135	LEU
3	F	142	ASP
3	F	164	ASP
3	F	177	THR
3	F	181	THR

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	24	GLN
1	A	61	GLN
1	A	62	ASN
1	A	119	GLN
1	A	157	ASN
1	A	203	GLN
1	A	207	GLN
1	A	270	ASN
1	A	277	GLN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	62	ASN

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Mol	Chain	Res	Type
1	B	74	ASN
1	B	157	ASN
1	B	270	ASN
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	420	GLN
3	D	6	GLN
3	D	93	HIS
3	D	136	ASN
3	D	137	ASN
2	E	179	GLN
3	F	6	GLN
3	F	75	ASN
3	F	136	ASN
3	F	137	ASN
3	F	156	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

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	444/465 (95%)	0.48	22 (4%) 34 23	73, 95, 127, 145	0
1	B	441/465 (94%)	0.64	35 (7%) 18 14	72, 100, 133, 150	0
2	C	221/222 (99%)	0.39	4 (1%) 67 49	67, 84, 101, 111	0
2	E	221/222 (99%)	0.41	17 (7%) 19 14	68, 88, 103, 110	0
3	D	211/211 (100%)	0.68	17 (8%) 18 13	84, 101, 113, 115	0
3	F	211/211 (100%)	0.21	6 (2%) 55 36	61, 81, 114, 121	0
All	All	1749/1796 (97%)	0.49	101 (5%) 29 19	61, 93, 122, 150	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	128	GLY	5.9
3	F	127	GLY	5.7
1	B	307	PHE	5.6
1	A	29	ASP	5.6
2	E	59	ASN	4.9
1	B	72	ALA	4.8
1	B	308	VAL	4.7
1	B	105	GLY	4.7
1	B	104	ALA	4.4
3	D	73	THR	4.1
3	F	129	ALA	4.1
2	C	37	VAL	4.0
1	A	235	GLU	3.9
3	D	53	LEU	3.8
1	B	353	PRO	3.7
2	E	13	GLN	3.7
1	B	306	GLY	3.6
1	A	219	PHE	3.5
3	F	177	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	215	ILE	3.5
1	B	377	GLU	3.4
1	A	355	GLY	3.4
1	B	135	GLY	3.3
2	E	179	GLN	3.3
1	B	212	LEU	3.3
1	B	97	VAL	3.3
3	D	18	LYS	3.2
1	B	36	LEU	3.2
1	B	96	LEU	3.1
3	D	62	SER	3.1
1	B	73	ASP	3.1
1	B	32	PRO	3.1
2	E	140	ALA	3.0
3	D	22	THR	3.0
1	B	83	PHE	3.0
1	B	215	ILE	2.9
1	A	450	ALA	2.9
1	B	211	THR	2.8
2	C	147	GLY	2.8
1	B	310	PRO	2.8
1	B	172	GLU	2.8
3	F	179	THR	2.8
2	E	178	LEU	2.8
2	E	64	LEU	2.7
2	E	186	SER	2.7
1	A	246	ASP	2.7
1	B	354	GLY	2.7
3	D	51	SER	2.7
1	A	447	ALA	2.7
1	A	236	VAL	2.7
2	E	220	PRO	2.7
2	C	200	THR	2.7
2	E	144	VAL	2.6
1	B	39	ALA	2.6
3	D	59	VAL	2.6
3	D	124	LEU	2.6
3	D	55	SER	2.6
3	D	71	SER	2.6
3	D	69	SER	2.5
1	A	393	GLY	2.5
1	A	145	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	28	ARG	2.5
3	F	111	ALA	2.4
1	A	234	HIS	2.4
3	D	75	ASN	2.4
1	B	235	GLU	2.4
2	E	184	THR	2.4
1	B	309	ALA	2.4
1	A	21	LEU	2.4
2	E	115	THR	2.3
3	D	2	ILE	2.3
1	A	25	LEU	2.3
1	B	301	LEU	2.3
3	D	103	LEU	2.3
1	B	111	GLU	2.3
1	A	386	ALA	2.3
1	A	440	GLY	2.3
1	B	315	GLY	2.3
1	A	102	PRO	2.3
2	E	15	GLY	2.3
1	A	385	GLU	2.2
1	A	99	LYS	2.2
2	E	19	LYS	2.2
2	E	121	SER	2.2
1	B	318	ASN	2.2
1	B	231	ILE	2.2
3	D	74	ILE	2.1
2	E	151	LYS	2.1
1	A	404	ALA	2.1
2	E	149	LEU	2.1
1	A	111	GLU	2.1
3	D	64	SER	2.1
2	C	196	TRP	2.1
1	A	204	MET	2.1
3	D	86	TYR	2.0
1	B	103	GLU	2.0
1	B	69	VAL	2.0
1	B	147	ARG	2.0
2	E	2	VAL	2.0
1	B	453	LEU	2.0
1	B	257	ILE	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.