Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 04:43 AM EDT

PDB ID	:	2FED
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 (i) 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 (1)) were used in the production of this report:

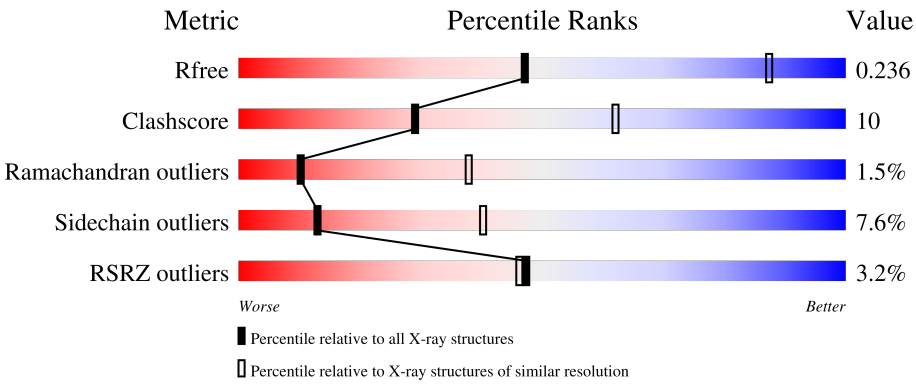
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 <=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	2% 71% 21% • 5%
1	B	465	3% 69% 24% • 5%
2	C	222	3% 77% 21% •
2	E	222	3% 75% 21% •
3	D	211	6% 70% 28% •

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Mol	Chain	Length	Quality of chain
3	F	211	4% 69% 28%

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.

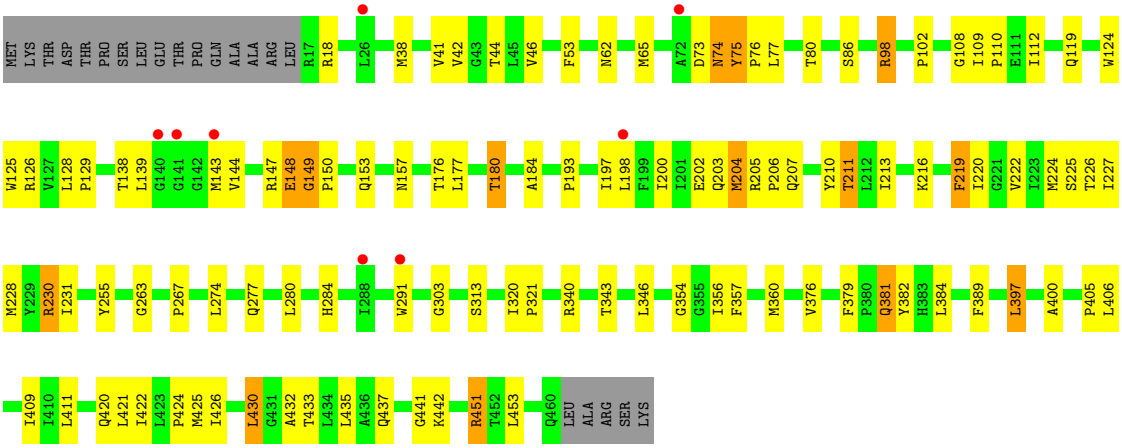
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	211	1621	1008	271	334	8	0	0	0
3	F	211	1621	1008	271	334	8	0	0	0

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.

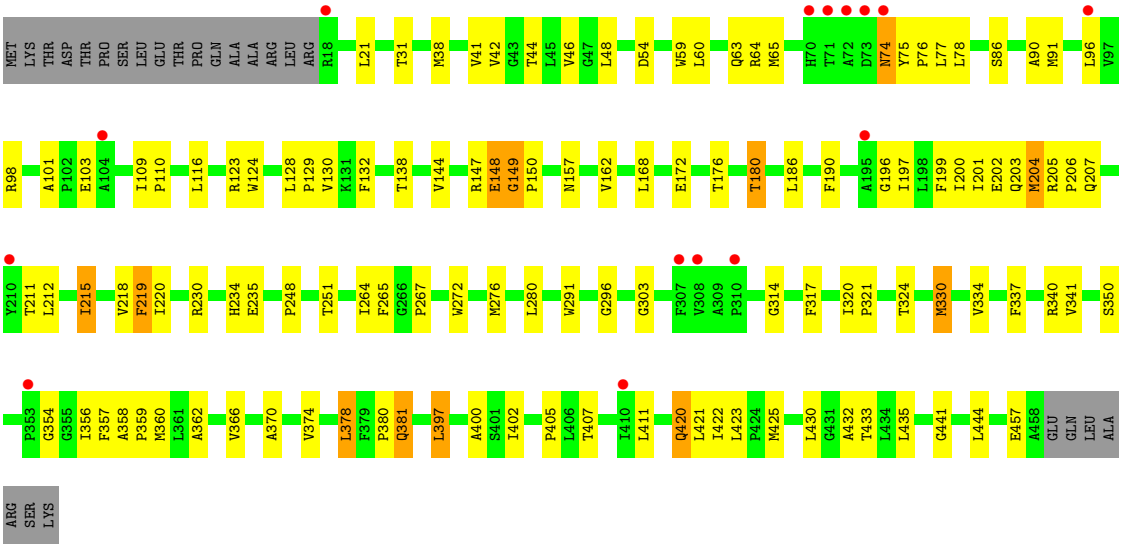
• Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain A:



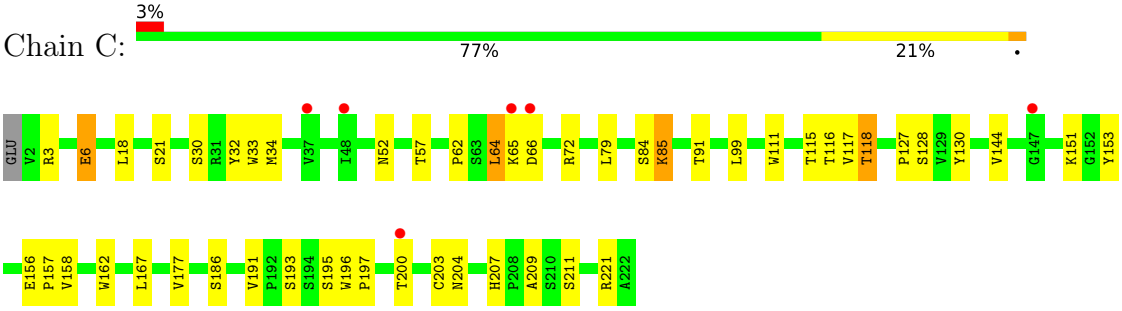
• Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain B:



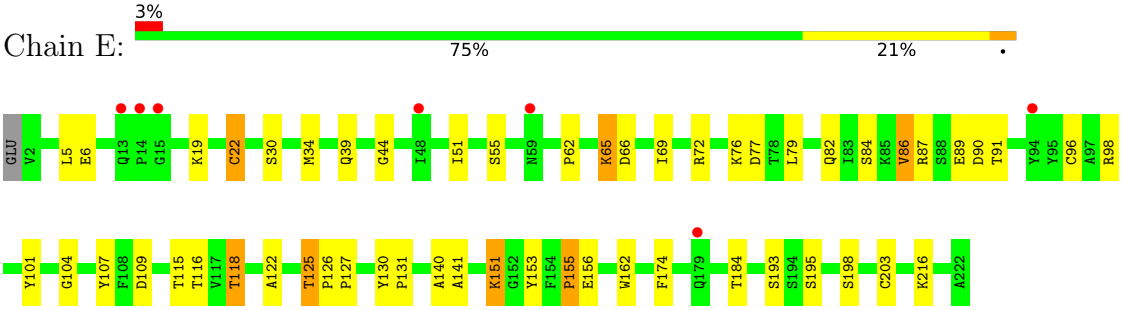
• Molecule 2: Fab fragment, heavy chain

Chain C:



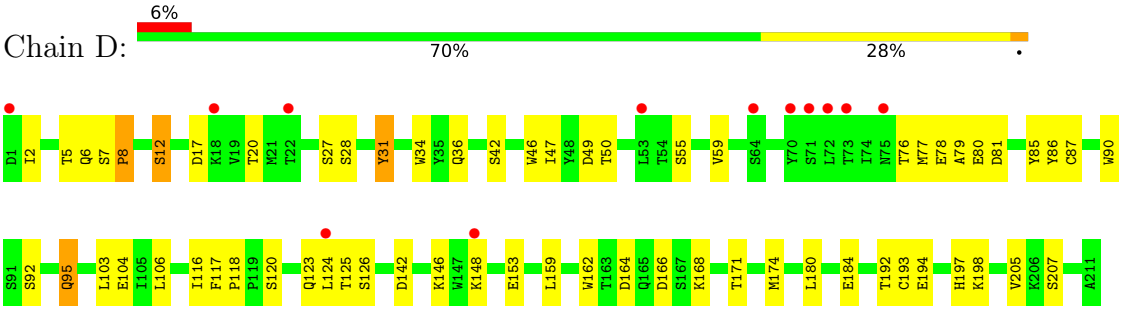
• Molecule 2: Fab fragment, heavy chain

Chain E:



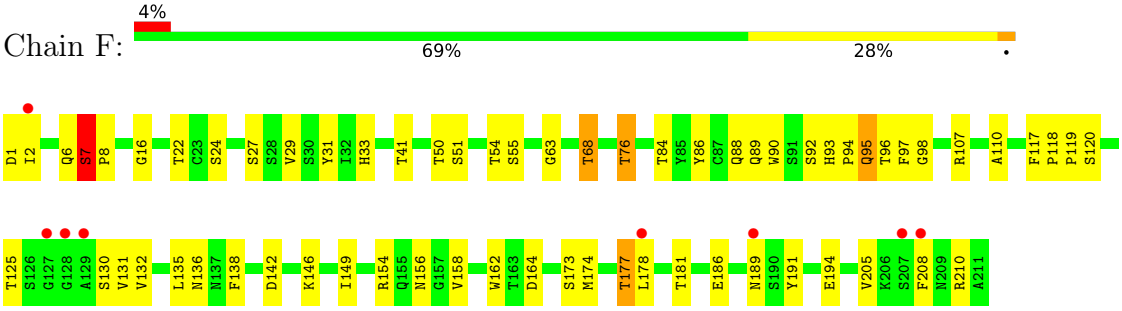
• Molecule 3: Fab fragment, light chain

Chain D:



• Molecule 3: Fab fragment, light chain

Chain F:



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 49.80 – 3.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.81-3.32) 89.7 (49.80-3.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.33Å)	Xtriage
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 (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	94.2	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
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

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/3405	0.52	0/4621
1	B	0.40	0/3376	0.53	0/4583
2	C	0.41	0/1721	0.58	0/2355
2	E	0.40	0/1721	0.58	0/2355
3	D	0.39	0/1660	0.54	0/2257
3	F	0.37	0/1660	0.56	0/2257
All	All	0.39	0/13543	0.55	0/18428

There are no bond length outliers.

There are no bond angle outliers.

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	76	0
1	B	3304	0	3459	73	0
2	C	1672	0	1654	25	0
2	E	1672	0	1654	23	0
3	D	1621	0	1546	38	0
3	F	1621	0	1546	41	0
All	All	13223	0	13345	255	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 (255) 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: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
3:D:95:GLN:CD	3:D:95:GLN:H	1.69	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
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:B:148:GLU:CD	1:B:148:GLU:H	1.85	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
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
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:D:95:GLN:CD	3:D:95:GLN:N	2.41	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:422:ILE:HA	1:A:425:MET:HE3	1.79	0.65
3:F:7:SER:HB2	3:F:22:THR:CB	2.25	0.65
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
1:A:148:GLU:CD	1:A:148:GLU:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.90	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: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
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.46	0.50
3:D:124:LEU:C	3:D:126:SER:H	2.14	0.50
1:B:144:VAL:HG12	1:B:144:VAL:O	2.12	0.50
3:F:95:GLN:H	3:F:95:GLN:CD	2.15	0.50
2:C:30:SER:C	2:C:32:TYR:H	2.14	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:148:GLU:CD	1:B:148:GLU:N	2.61	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
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
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
1:A:379:PHE:CB	1:A:382:TYR:CD1	2.99	0.46
2:C:84:SER:O	2:C:85:LYS:C	2.53	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:79:ALA:C	3:D:81:ASP:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:422:ILE:HD12	1:B:425:MET:HE3	1.98	0.45
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
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:148:GLU:O	1:A:149:GLY:C	2.55	0.43
3:F:149:ILE:HD11	3:F:178:LEU:HD21	1.99	0.43
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.85	0.43
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG12	1:B:356:ILE:O	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
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
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
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
1:B:374:VAL:HG12	1:B:378:LEU:HD12	2.01	0.41
2:E:87:ARG:HE	2:E:89:GLU:CD	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:GLU:O	1:B:149:GLY:C	2.59	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%)	22	55
1	B	439/465 (94%)	400 (91%)	35 (8%)	4 (1%)	17	49
2	C	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	11	39
2	E	219/222 (99%)	192 (88%)	18 (8%)	9 (4%)	3	18
3	D	209/211 (99%)	184 (88%)	20 (10%)	5 (2%)	6	29
3	F	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	15	47
All	All	1737/1796 (97%)	1566 (90%)	145 (8%)	26 (2%)	10	38

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	MET
1	B	204	MET

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Mol	Chain	Res	Type
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
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%)	309 (92%)	26 (8%)	12	39
1	B	332/353 (94%)	309 (93%)	23 (7%)	15	45
2	C	181/182 (100%)	165 (91%)	16 (9%)	10	34
2	E	181/182 (100%)	165 (91%)	16 (9%)	10	34
3	D	185/185 (100%)	173 (94%)	12 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	185/185 (100%)	171 (92%)	14 (8%)	13	40
All	All	1399/1440 (97%)	1292 (92%)	107 (8%)	13	40

All (107) 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	73	ASP
1	A	74	ASN
1	A	75	TYR
1	A	80	THR
1	A	98	ARG
1	A	139	LEU
1	A	148	GLU
1	A	180	THR
1	A	207	GLN
1	A	210	TYR
1	A	211	THR
1	A	219	PHE
1	A	230	ARG
1	A	346	LEU
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	430	LEU
1	A	433	THR
1	A	442	LYS
1	A	451	ARG
1	A	453	LEU
1	B	44	THR
1	B	48	LEU
1	B	65	MET
1	B	74	ASN
1	B	96	LEU
1	B	138	THR
1	B	148	GLU
1	B	180	THR
1	B	207	GLN
1	B	211	THR

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Mol	Chain	Res	Type
1	B	215	ILE
1	B	219	PHE
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
1	B	435	LEU
1	B	444	LEU
2	C	3	ARG
2	C	6	GLU
2	C	64	LEU
2	C	66	ASP
2	C	72	ARG
2	C	115	THR
2	C	116	THR
2	C	118	THR
2	C	128	SER
2	C	151	LYS
2	C	186	SER
2	C	193	SER
2	C	195	SER
2	C	200	THR
2	C	204	ASN
2	C	211	SER
3	D	5	THR
3	D	8	PRO
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	142	ASP
3	D	164	ASP
2	E	5	LEU

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Mol	Chain	Res	Type
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	72	ARG
2	E	84	SER
2	E	86	VAL
2	E	115	THR
2	E	116	THR
2	E	118	THR
2	E	125	THR
2	E	151	LYS
2	E	193	SER
3	F	1	ASP
3	F	7	SER
3	F	41	THR
3	F	68	THR
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	62	ASN
1	A	74	ASN
1	A	153	GLN
1	A	157	ASN
1	A	270	ASN
1	A	277	GLN
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN

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Mol	Chain	Res	Type
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	157	ASN
1	B	270	ASN
1	B	277	GLN
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	420	GLN
1	B	437	GLN
3	D	6	GLN
3	D	36	GLN
3	D	93	HIS
3	D	136	ASN
3	D	137	ASN
2	E	179	GLN
3	F	6	GLN
3	F	136	ASN
3	F	137	ASN
3	F	155	GLN

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 monosaccharides 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%)	0.30	8 (1%)	68	67	73, 95, 127, 145	0
1	B	441/465 (94%)	0.29	15 (3%)	45	43	72, 100, 133, 150	0
2	C	221/222 (99%)	0.18	6 (2%)	54	53	67, 84, 101, 111	0
2	E	221/222 (99%)	0.11	7 (3%)	47	46	68, 88, 103, 110	0
3	D	211/211 (100%)	0.32	12 (5%)	23	24	84, 101, 113, 115	0
3	F	211/211 (100%)	0.36	8 (3%)	40	39	61, 81, 114, 121	0
All	All	1749/1796 (97%)	0.27	56 (3%)	47	46	61, 93, 122, 150	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	6.1
1	B	72	ALA	5.4
1	B	307	PHE	4.8
1	B	70	HIS	3.6
3	D	18	LYS	3.5
1	B	74	ASN	3.4
2	C	65	LYS	3.3
3	F	128	GLY	3.2
2	E	15	GLY	3.2
3	F	129	ALA	3.2
1	A	26	LEU	3.1
2	E	59	ASN	3.1
1	B	71	THR	3.0
2	C	147	GLY	3.0
2	C	66	ASP	3.0
3	D	64	SER	2.8
3	D	71	SER	2.8
1	B	353	PRO	2.8
1	A	141	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	195	ALA	2.6
2	E	13	GLN	2.6
3	D	1	ASP	2.6
1	A	288	ILE	2.6
2	E	14	PRO	2.5
1	B	104	ALA	2.5
1	A	291	TRP	2.5
3	D	75	ASN	2.5
1	A	143	MET	2.4
2	C	200	THR	2.4
1	B	96	LEU	2.4
3	F	208	PHE	2.4
3	D	53	LEU	2.4
3	F	2	ILE	2.4
2	C	48	ILE	2.4
1	B	18	ARG	2.3
1	B	210	TYR	2.3
3	F	207	SER	2.3
2	E	94	TYR	2.3
3	F	189	ASN	2.3
3	D	73	THR	2.3
2	C	37	VAL	2.2
3	D	72	LEU	2.2
3	F	127	GLY	2.2
3	D	70	TYR	2.2
3	D	22	THR	2.2
1	A	72	ALA	2.1
1	B	308	VAL	2.1
1	A	140	GLY	2.1
1	B	410	ILE	2.1
3	F	178	LEU	2.0
1	B	310	PRO	2.0
3	D	148	LYS	2.0
2	E	179	GLN	2.0
2	E	48	ILE	2.0
3	D	124	LEU	2.0
1	A	198	LEU	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 monosaccharides 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.