



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:51 PM UTC

PDB ID : 4FG6 / pdb_00004fg6
Title : Structure of EcCLC E148A mutant in Glutamate
Authors : Feng, L.; MacKinnon, R.
Deposited on : 2012-06-04
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

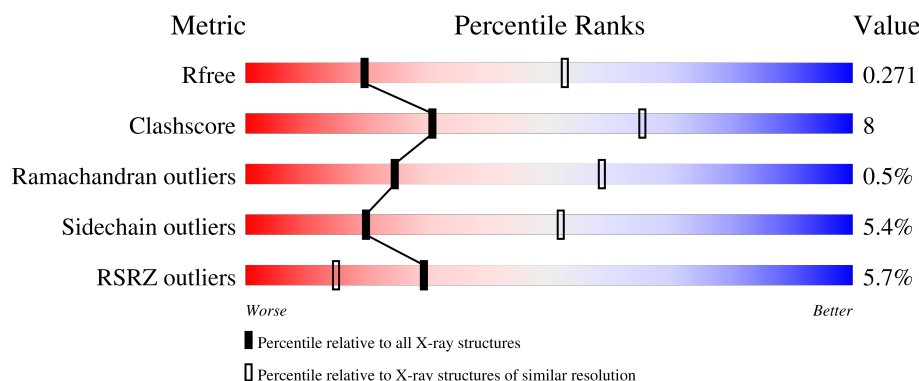
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	5% 76% 21%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13158 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
			3314	2180	555	559	20			
1	B	441	Total	C	N	O	S	0	0	0
			3285	2161	551	553	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	GLU	conflict	UNP P37019
B	148	ALA	GLU	conflict	UNP P37019

- Molecule 2 is a protein called Fab fragment (Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1658	1069	270	313	6			
2	E	221	Total	C	N	O	S	0	0	0
			1662	1071	270	315	6			

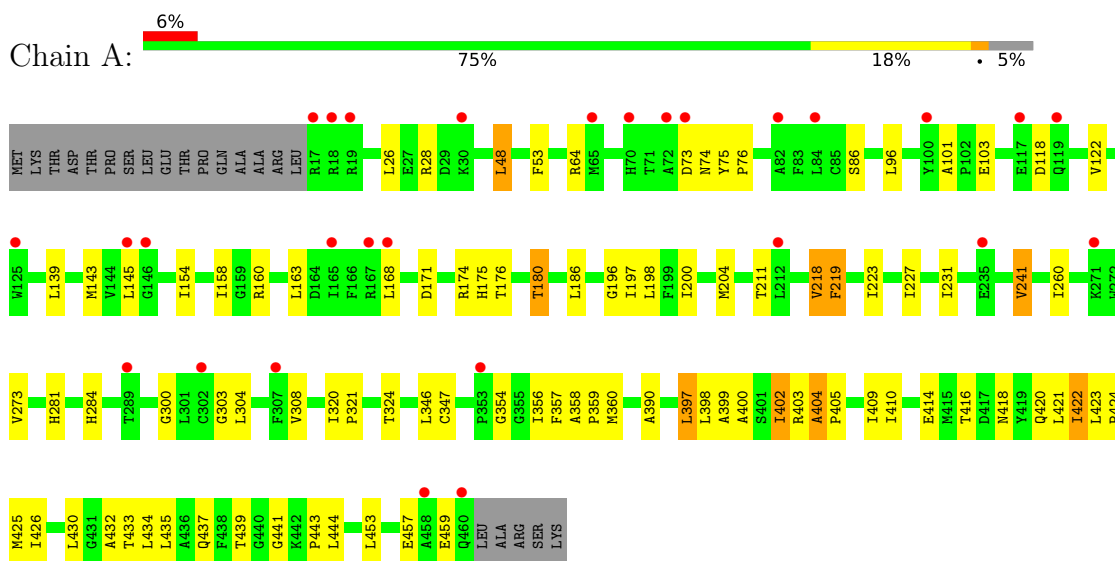
- Molecule 3 is a protein called Fab fragment (Light chain).

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
			1618	1007	271	332	8			

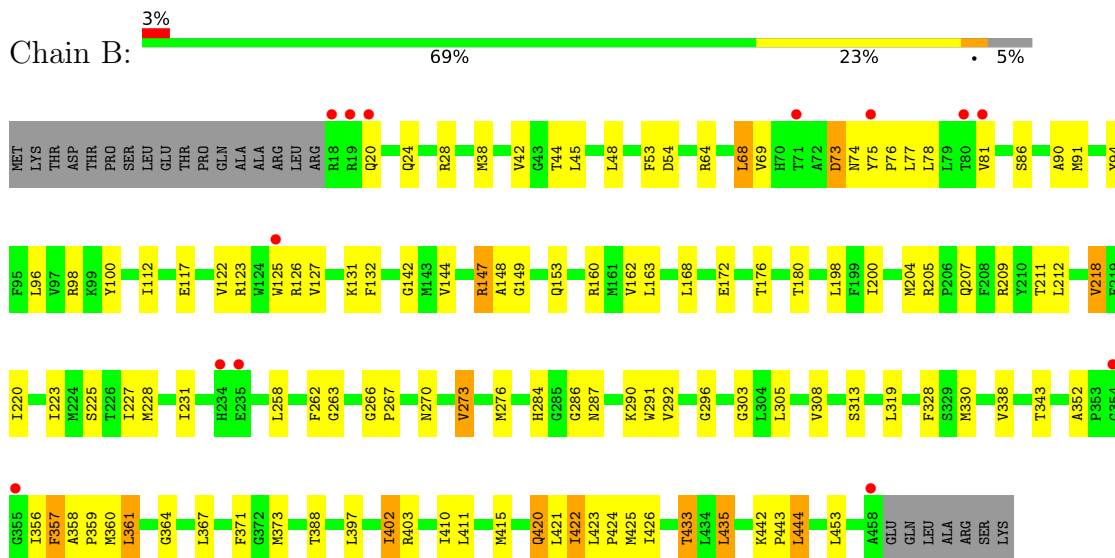
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

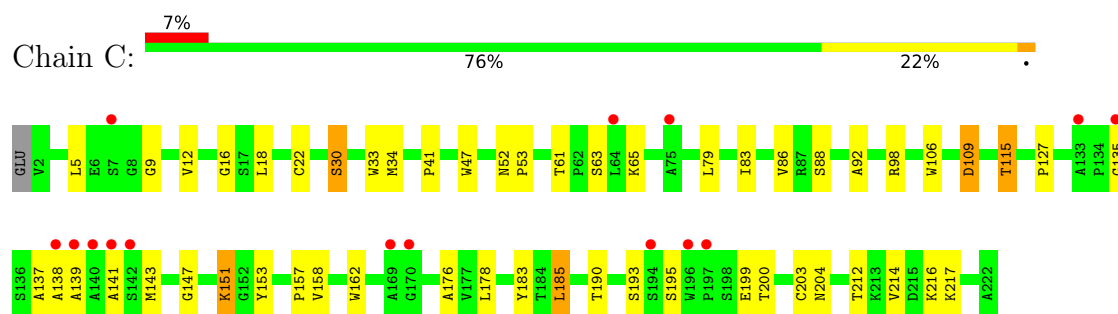
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



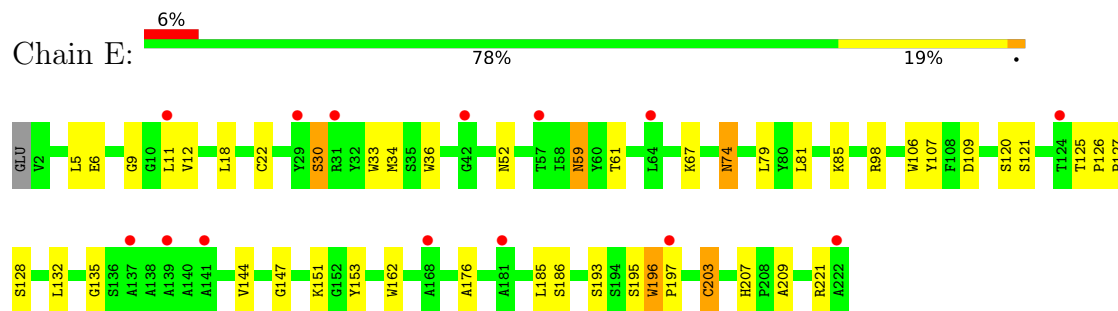
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



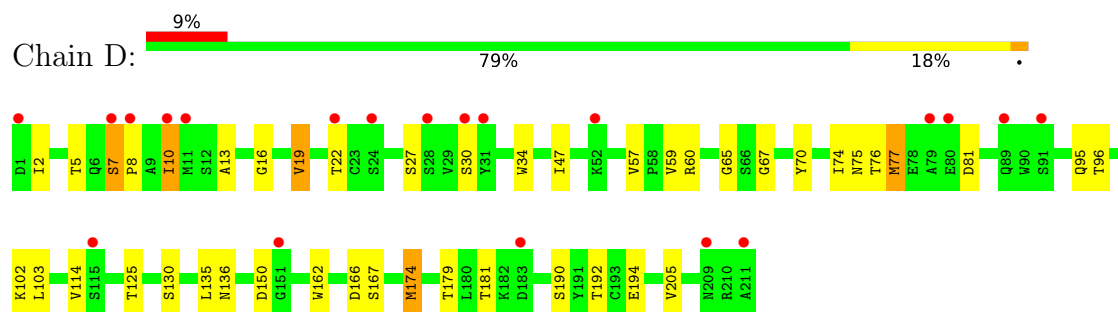
- Molecule 2: Fab fragment (Heavy chain)



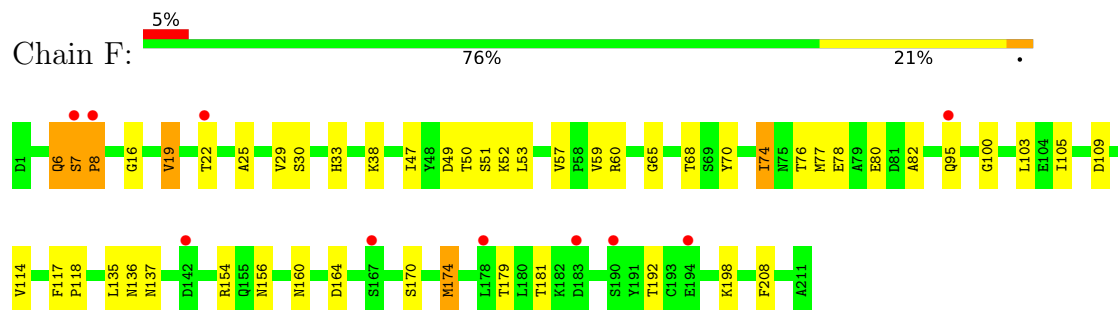
- Molecule 2: Fab fragment (Heavy chain)



- Molecule 3: Fab fragment (Light chain)



- Molecule 3: Fab fragment (Light chain)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.46Å 121.28Å 151.70Å 90.00° 128.08° 90.00°	Depositor
Resolution (Å)	49.55 – 3.02 49.55 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.55-3.02) 98.8 (49.55-3.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.237 , 0.274 0.233 , 0.271	Depositor DCC
R_{free} test set	3061 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13158	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.49	0/3385	0.99	7/4596 (0.2%)
1	B	0.53	0/3355	1.02	6/4556 (0.1%)
2	C	0.53	0/1707	1.05	10/2339 (0.4%)
2	E	0.50	0/1711	0.97	7/2344 (0.3%)
3	D	0.42	0/1660	0.91	5/2257 (0.2%)
3	F	0.49	0/1657	0.94	8/2253 (0.4%)
All	All	0.50	0/13475	0.99	43/18345 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	30	SER	N-CA-C	8.87	121.75	111.11
3	D	7	SER	CA-C-N	-7.02	111.06	119.84
3	D	7	SER	C-N-CA	-7.02	111.06	119.84
3	F	7	SER	CA-C-N	-6.81	111.33	119.84
3	F	7	SER	C-N-CA	-6.81	111.33	119.84
2	C	195	SER	N-CA-C	6.30	118.22	111.36
3	F	136	ASN	N-CA-C	6.11	120.22	109.96
2	E	195	SER	N-CA-C	6.01	117.83	111.28
1	B	361	LEU	N-CA-C	-6.00	104.66	111.14
2	C	65	LYS	CB-CA-C	-5.98	109.66	116.54
3	F	137	ASN	N-CA-C	5.97	119.34	111.28
1	A	101	ALA	CA-C-N	5.94	126.36	119.47
1	A	101	ALA	C-N-CA	5.94	126.36	119.47
3	F	117	PHE	CA-C-N	5.74	126.30	120.38
3	F	117	PHE	C-N-CA	5.74	126.30	120.38
2	C	106	TRP	N-CA-C	5.73	117.69	110.24
2	E	106	TRP	N-CA-C	5.71	117.66	110.24
2	E	196	TRP	CA-C-N	-5.70	112.64	118.85
2	E	196	TRP	C-N-CA	-5.70	112.64	118.85
3	D	136	ASN	N-CA-C	5.69	119.52	109.96
1	A	218	VAL	N-CA-C	-5.63	105.01	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	147	GLY	N-CA-C	5.62	118.95	110.75
3	F	57	VAL	CA-C-N	5.61	125.63	119.90
3	F	57	VAL	C-N-CA	5.61	125.63	119.90
2	C	88	SER	N-CA-C	5.54	118.04	111.33
2	E	30	SER	N-CA-C	-5.50	102.61	110.59
1	B	388	THR	N-CA-C	-5.48	106.10	112.89
1	B	127	VAL	N-CA-C	5.47	115.67	110.42
2	C	212	THR	N-CA-C	5.46	118.15	109.24
1	B	422	ILE	N-CA-C	5.41	116.04	110.36
1	B	218	VAL	N-CA-C	-5.37	105.27	110.42
1	A	422	ILE	N-CA-C	5.36	115.99	110.36
2	E	151	LYS	N-CA-C	5.36	117.34	109.24
2	C	151	LYS	N-CA-C	5.36	118.31	109.85
1	A	404	ALA	CA-C-N	5.26	124.71	119.24
1	A	404	ALA	C-N-CA	5.26	124.71	119.24
2	C	135	GLY	N-CA-C	5.17	118.50	112.50
1	A	439	THR	N-CA-C	-5.17	105.65	112.94
1	B	338	VAL	N-CA-C	5.12	115.73	110.36
2	E	61	THR	N-CA-C	-5.06	102.80	110.39
3	D	57	VAL	CA-C-N	5.06	125.05	119.89
3	D	57	VAL	C-N-CA	5.06	125.05	119.89
2	C	65	LYS	N-CA-C	5.05	115.98	108.31

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	3314	0	3463	57	0
1	B	3285	0	3440	77	0
2	C	1658	0	1628	24	0
2	E	1662	0	1632	22	0
3	D	1621	0	1546	22	0
3	F	1618	0	1544	29	0
All	All	13158	0	13253	220	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 8.

All (220) 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:223:ILE:HD11	1:B:426:ILE:HG22	1.63	0.81
1:A:403:ARG:HH22	1:A:437:GLN:HB2	1.50	0.76
1:B:131:LYS:NZ	1:B:153:GLN:OE1	2.21	0.74
2:C:137:ALA:HA	2:C:138:ALA:HB3	1.69	0.73
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.20	0.73
1:B:422:ILE:HA	1:B:425:MET:HE2	1.69	0.72
1:B:180:THR:HG22	1:B:218:VAL:HA	1.71	0.72
3:F:95:GLN:OE1	3:F:95:GLN:N	2.20	0.72
3:D:95:GLN:OE1	3:D:95:GLN:N	2.23	0.71
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.74	0.69
1:B:44:THR:HG23	1:B:228:MET:HE3	1.74	0.69
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.75	0.67
1:B:284:HIS:HD2	1:B:286:GLY:H	1.41	0.67
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.78	0.66
3:D:19:VAL:HG13	3:D:74:ILE:HB	1.77	0.66
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.77	0.65
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.79	0.65
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.79	0.64
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.79	0.64
2:E:162:TRP:CZ3	2:E:203:CYS:HB2	2.33	0.63
2:C:141:ALA:O	2:C:193:SER:HB2	1.99	0.63
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.80	0.62
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.80	0.62
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.81	0.61
1:B:73:ASP:OD2	1:B:73:ASP:N	2.32	0.61
1:B:273:VAL:HG11	1:B:444:LEU:HD11	1.83	0.61
1:A:28:ARG:HD3	1:B:443:PRO:HG2	1.81	0.61
3:D:19:VAL:HG11	3:D:77:MET:HE2	1.84	0.60
2:E:74:ASN:OD1	2:E:74:ASN:N	2.35	0.60
2:C:162:TRP:CZ3	2:C:203:CYS:HB2	2.37	0.60
3:D:60:ARG:NH1	3:D:81:ASP:OD1	2.34	0.59
3:F:77:MET:SD	3:F:103:LEU:HD21	2.42	0.59
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.84	0.59
1:B:176:THR:O	1:B:180:THR:HG23	2.03	0.58
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.84	0.58
3:F:38:LYS:NZ	3:F:80:GLU:O	2.35	0.58
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.86	0.58
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.85	0.58
2:C:143:MET:HE3	2:C:190:THR:HG22	1.87	0.57
3:F:6:GLN:HG3	3:F:100:GLY:H	1.68	0.57
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.40	0.56
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.85	0.56
1:B:200:ILE:HA	1:B:204:MET:HB2	1.87	0.56
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.39	0.56
3:D:13:ALA:HB3	3:D:77:MET:HE3	1.87	0.56
1:B:227:ILE:O	1:B:231:ILE:HG13	2.06	0.56
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.88	0.55
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.87	0.55
1:A:403:ARG:NH2	1:A:433:THR:O	2.39	0.55
2:E:11:LEU:HD11	2:E:120:SER:HB3	1.88	0.55
2:C:9:GLY:H	2:C:115:THR:HG21	1.70	0.55
1:A:64:ARG:NH1	1:A:86:SER:OG	2.40	0.55
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.88	0.54
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.88	0.54
1:A:416:THR:O	1:A:418:ASN:ND2	2.37	0.54
3:F:60:ARG:NH2	3:F:80:GLU:OE2	2.41	0.54
2:E:6:GLU:OE1	2:E:6:GLU:N	2.39	0.54
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.73	0.54
1:A:73:ASP:OD2	1:A:74:ASN:N	2.39	0.54
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.90	0.53
3:F:30:SER:HA	3:F:70:TYR:OH	2.07	0.53
2:E:176:ALA:HB2	2:E:185:LEU:HD23	1.90	0.53
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.44	0.53
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.90	0.53
1:B:284:HIS:CD2	1:B:286:GLY:H	2.25	0.53
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.90	0.53
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.90	0.53
1:A:422:ILE:HA	1:A:425:MET:HE3	1.90	0.52
1:A:402:ILE:HD11	1:A:404:ALA:HB3	1.90	0.51
1:B:361:LEU:HD13	1:B:415:MET:HE1	1.91	0.51
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.91	0.51
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.91	0.51
1:B:112:ILE:HD11	1:B:153:GLN:HG3	1.93	0.51
1:A:421:LEU:O	1:A:425:MET:HG3	2.10	0.51
1:B:53:PHE:HD1	1:B:132:PHE:CD1	2.29	0.51
2:E:6:GLU:HA	2:E:22:CYS:HA	1.92	0.50
1:A:176:THR:O	1:A:180:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:HD2	1:B:433:THR:HG23	1.93	0.50
2:E:67:LYS:NZ	2:E:85:LYS:O	2.44	0.50
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.77	0.50
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.27	0.50
3:F:49:ASP:OD2	3:F:52:LYS:NZ	2.45	0.50
1:B:180:THR:HG22	1:B:218:VAL:CA	2.42	0.49
2:C:30:SER:O	2:C:53:PRO:HB3	2.12	0.49
1:A:281:HIS:HA	1:A:284:HIS:NE2	2.27	0.49
1:A:398:LEU:O	1:A:402:ILE:HG12	2.11	0.49
1:B:357:PHE:HE1	1:B:402:ILE:HD13	1.76	0.49
3:F:109:ASP:OD2	3:F:198:LYS:NZ	2.45	0.49
1:B:411:LEU:HG	1:B:415:MET:HE2	1.94	0.49
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.95	0.48
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.48	0.48
2:C:16:GLY:O	2:C:86:VAL:HG22	2.13	0.48
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.95	0.48
1:B:420:GLN:H	1:B:420:GLN:HG3	1.33	0.48
2:C:61:THR:O	2:C:63:SER:N	2.41	0.48
1:A:180:THR:HB	1:A:218:VAL:HA	1.95	0.48
2:C:137:ALA:HB1	2:C:139:ALA:H	1.78	0.48
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.94	0.48
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.49	0.48
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.49	0.48
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.96	0.48
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.77	0.48
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.95	0.48
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.97	0.47
3:D:77:MET:HE1	3:D:103:LEU:HD11	1.96	0.47
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.97	0.47
3:D:130:SER:OG	3:D:179:THR:HG22	2.14	0.47
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.96	0.47
3:D:60:ARG:HB2	3:D:75:ASN:O	2.14	0.47
2:E:36:TRP:NE1	2:E:81:LEU:HB2	2.30	0.47
1:A:403:ARG:O	1:A:405:PRO:HD3	2.15	0.47
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.39	0.47
1:B:421:LEU:O	1:B:425:MET:HG3	2.14	0.47
3:F:95:GLN:H	3:F:95:GLN:CD	2.17	0.47
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.50	0.46
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.98	0.46
3:F:29:VAL:HG23	3:F:70:TYR:HE1	1.80	0.46
1:A:74:ASN:OD1	1:A:76:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:C	1:A:405:PRO:HD3	2.39	0.46
1:B:270:ASN:CG	1:B:444:LEU:HG	2.41	0.46
3:D:30:SER:HA	3:D:70:TYR:OH	2.15	0.46
1:B:90:ALA:O	1:B:94:TYR:HD1	1.99	0.46
1:A:154:ILE:O	1:A:158:ILE:HG13	2.16	0.46
2:C:137:ALA:HB1	2:C:139:ALA:N	2.29	0.46
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.98	0.46
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.97	0.46
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.98	0.46
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.51	0.45
1:A:430:LEU:HG	1:A:434:LEU:HD23	1.98	0.45
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.98	0.45
2:C:41:PRO:HD3	2:C:92:ALA:HA	1.97	0.45
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.52	0.45
1:B:24:GLN:O	1:B:28:ARG:N	2.50	0.45
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.52	0.45
3:F:7:SER:CB	3:F:22:THR:HB	2.47	0.45
3:F:160:ASN:HB3	3:F:174:MET:HE2	1.99	0.45
1:B:54:ASP:OD1	1:B:147:ARG:NH2	2.50	0.45
3:F:25:ALA:O	3:F:68:THR:OG1	2.33	0.45
1:A:145:LEU:HB3	1:A:354:GLY:HA3	1.99	0.45
2:C:12:VAL:HG11	2:C:18:LEU:HB3	1.99	0.44
1:A:443:PRO:HG2	1:B:28:ARG:HD3	1.99	0.44
1:B:38:MET:O	1:B:42:VAL:HG23	2.17	0.44
2:E:132:LEU:HB2	2:E:147:GLY:O	2.17	0.44
1:A:405:PRO:O	1:A:409:ILE:HG12	2.17	0.44
1:A:171:ASP:HA	1:A:174:ARG:NH1	2.32	0.44
1:B:20:GLN:O	1:B:24:GLN:HG3	2.18	0.44
3:F:49:ASP:O	3:F:50:THR:HB	2.16	0.44
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.00	0.44
1:B:270:ASN:OD1	1:B:444:LEU:HG	2.18	0.44
1:B:86:SER:OG	1:B:303:GLY:HA3	2.17	0.44
1:B:263:GLY:HA3	1:B:435:LEU:HB2	1.99	0.44
1:A:86:SER:OG	1:A:303:GLY:HA3	2.18	0.43
3:F:77:MET:HG2	3:F:78:GLU:N	2.32	0.43
2:C:200:THR:HG23	2:C:217:LYS:HG3	1.99	0.43
1:A:118:ASP:OD1	1:A:174:ARG:NH2	2.50	0.43
1:A:324:THR:HG23	1:A:390:ALA:HB3	2.00	0.43
1:B:262:PHE:HZ	1:B:364:GLY:HA2	1.83	0.43
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.54	0.43
1:B:172:GLU:HG3	1:B:212:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.53	0.43
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.86	0.43
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.99	0.43
1:A:399:ALA:O	1:A:403:ARG:HA	2.19	0.43
1:A:410:ILE:O	1:A:414:GLU:HG3	2.18	0.43
1:B:328:PHE:O	1:B:373:MET:HE1	2.19	0.43
3:D:150:ASP:HA	3:D:190:SER:HB3	2.01	0.43
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.99	0.43
1:B:357:PHE:CE1	1:B:402:ILE:HD13	2.53	0.43
3:F:19:VAL:HG13	3:F:74:ILE:HB	2.00	0.43
1:B:42:VAL:CG2	1:B:162:VAL:HG21	2.48	0.43
1:B:91:MET:HG2	1:B:292:VAL:O	2.18	0.43
2:C:18:LEU:HD21	2:C:83:ILE:HD12	2.01	0.43
2:E:59:ASN:OD1	2:E:59:ASN:N	2.51	0.43
3:F:114:VAL:HG22	3:F:135:LEU:HD22	2.00	0.43
3:D:10:ILE:HG23	3:D:102:LYS:HB3	2.01	0.43
1:A:457:GLU:C	1:A:459:GLU:H	2.26	0.42
1:B:68:LEU:HD13	1:B:78:LEU:HD22	2.00	0.42
3:D:34:TRP:N	3:D:47:ILE:O	2.45	0.42
3:F:7:SER:HB2	3:F:22:THR:HB	2.01	0.42
1:B:142:GLY:O	1:B:313:SER:OG	2.38	0.42
1:B:421:LEU:O	1:B:424:PRO:HD2	2.19	0.42
1:B:266:GLY:N	1:B:267:PRO:HD2	2.33	0.42
3:F:29:VAL:HG23	3:F:70:TYR:CE1	2.54	0.42
1:A:320:ILE:HB	1:A:321:PRO:HD3	2.02	0.42
1:B:78:LEU:HA	1:B:78:LEU:HD23	1.85	0.42
1:B:287:ASN:OD1	1:B:290:LYS:N	2.43	0.42
1:B:64:ARG:NH1	1:B:86:SER:OG	2.53	0.42
2:E:207:HIS:NE2	2:E:209:ALA:HB3	2.34	0.42
3:F:47:ILE:HG12	3:F:53:LEU:HD23	2.00	0.42
1:A:143:MET:HE2	1:A:347:CYS:SG	2.60	0.42
2:E:34:MET:HB3	2:E:79:LEU:HD22	2.02	0.42
1:B:144:VAL:HG21	1:B:343:THR:HB	2.01	0.42
1:A:358:ALA:HB3	1:A:359:PRO:HD3	2.03	0.41
1:B:53:PHE:HD1	1:B:132:PHE:HD1	1.69	0.41
3:D:16:GLY:HA2	3:D:76:THR:CG2	2.49	0.41
3:D:166:ASP:OD1	3:D:167:SER:N	2.53	0.41
3:F:16:GLY:HA2	3:F:76:THR:CG2	2.50	0.41
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.02	0.41
2:E:33:TRP:CH2	2:E:52:ASN:HB3	2.55	0.41
2:E:144:VAL:HG12	2:E:193:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.56	0.41
1:A:174:ARG:NH2	1:A:175:HIS:HE1	2.19	0.41
1:B:100:TYR:O	1:B:126:ARG:NH1	2.53	0.41
1:B:262:PHE:CZ	1:B:364:GLY:HA2	2.55	0.41
1:B:305:LEU:HA	1:B:308:VAL:HG22	2.01	0.41
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.89	0.41
2:E:125:THR:HA	2:E:126:PRO:HD2	1.93	0.41
2:C:216:LYS:HD2	2:C:216:LYS:HA	1.90	0.41
1:B:75:TYR:HB3	1:B:76:PRO:HD3	2.03	0.40
1:B:160:ARG:HD2	1:B:160:ARG:HA	1.84	0.40
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.56	0.40
3:F:60:ARG:H	3:F:60:ARG:HG2	1.66	0.40
1:A:26:LEU:O	1:B:442:LYS:NZ	2.46	0.40
1:A:304:LEU:O	1:A:308:VAL:HG22	2.21	0.40
1:A:53:PHE:CE2	1:A:139:LEU:HD12	2.56	0.40
1:A:227:ILE:O	1:A:231:ILE:HG12	2.21	0.40
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.88	0.40
3:D:7:SER:HB3	3:D:22:THR:HB	2.03	0.40
2:E:196:TRP:HB3	2:E:197: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%)	415 (94%)	26 (6%)	1 (0%)	43 75
1	B	439/465 (94%)	408 (93%)	29 (7%)	2 (0%)	24 59
2	C	219/222 (99%)	205 (94%)	12 (6%)	2 (1%)	14 46
2	E	219/222 (99%)	202 (92%)	16 (7%)	1 (0%)	24 59
3	D	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	12 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	209/211 (99%)	195 (93%)	13 (6%)	1 (0%)	24 59
All	All	1737/1796 (97%)	1616 (93%)	112 (6%)	9 (0%)	24 59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	GLY
3	D	67	GLY
3	D	8	PRO
3	F	8	PRO
1	B	148	ALA
2	C	109	ASP
1	B	149	GLY
2	E	9	GLY
2	C	157	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	331/352 (94%)	316 (96%)	15 (4%)	24 57
1	B	328/352 (93%)	305 (93%)	23 (7%)	14 42
2	C	178/182 (98%)	170 (96%)	8 (4%)	24 57
2	E	179/182 (98%)	171 (96%)	8 (4%)	24 57
3	D	185/185 (100%)	175 (95%)	10 (5%)	20 52
3	F	184/185 (100%)	173 (94%)	11 (6%)	17 48
All	All	1385/1438 (96%)	1310 (95%)	75 (5%)	20 52

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	180	THR
1	A	211	THR
1	A	219	PHE
1	A	241	VAL
1	A	273	VAL
1	A	346	LEU
1	A	357	PHE
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	444	LEU
1	A	453	LEU
1	B	45	LEU
1	B	48	LEU
1	B	68	LEU
1	B	69	VAL
1	B	73	ASP
1	B	96	LEU
1	B	147	ARG
1	B	205	ARG
1	B	211	THR
1	B	225	SER
1	B	273	VAL
1	B	276	MET
1	B	319	LEU
1	B	330	MET
1	B	357	PHE
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	423	LEU
1	B	433	THR
1	B	435	LEU
1	B	444	LEU
1	B	453	LEU
2	C	5	LEU
2	C	115	THR
2	C	151	LYS
2	C	158	VAL
2	C	185	LEU
2	C	199	GLU

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Mol	Chain	Res	Type
2	C	204	ASN
2	C	214	VAL
3	D	5	THR
3	D	10	ILE
3	D	19	VAL
3	D	59	VAL
3	D	77	MET
3	D	96	THR
3	D	125	THR
3	D	174	MET
3	D	181	THR
3	D	192	THR
2	E	5	LEU
2	E	30	SER
2	E	59	ASN
2	E	74	ASN
2	E	121	SER
2	E	128	SER
2	E	186	SER
2	E	203	CYS
3	F	6	GLN
3	F	19	VAL
3	F	51	SER
3	F	59	VAL
3	F	74	ILE
3	F	164	ASP
3	F	170	SER
3	F	174	MET
3	F	179	THR
3	F	181	THR
3	F	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	B	207	GLN
1	B	284	HIS
3	F	137	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 ⓘ

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%)	0.72	28 (6%)	26	13	77, 98, 120, 142	0
1	B	441/465 (94%)	0.58	13 (2%)	53	31	73, 93, 125, 149	0
2	C	221/222 (99%)	0.66	15 (6%)	23	12	69, 88, 122, 153	0
2	E	221/222 (99%)	0.73	14 (6%)	26	13	67, 90, 121, 141	0
3	D	211/211 (100%)	0.93	20 (9%)	14	7	80, 107, 122, 135	0
3	F	211/211 (100%)	0.71	10 (4%)	36	19	70, 89, 124, 136	0
All	All	1749/1796 (97%)	0.70	100 (5%)	29	15	67, 94, 123, 153	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	140	ALA	4.8
1	B	458	ALA	4.3
1	B	18	ARG	4.1
2	C	139	ALA	4.0
1	B	354	GLY	4.0
1	A	302	CYS	3.9
2	E	181	ALA	3.9
3	D	211	ALA	3.7
3	D	209	ASN	3.7
2	E	64	LEU	3.6
1	B	20	GLN	3.6
1	A	460	GLN	3.5
3	D	7	SER	3.5
3	F	22	THR	3.5
1	A	458	ALA	3.4
2	E	124	THR	3.4
3	D	79	ALA	3.3
1	B	235	GLU	3.2
1	A	212	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	ASP	3.1
2	C	135	GLY	3.1
2	C	133	ALA	3.1
2	C	138	ALA	3.0
3	D	11	MET	3.0
3	D	28	SER	3.0
1	A	165	ILE	3.0
2	C	64	LEU	2.9
1	A	72	ALA	2.8
2	C	141	ALA	2.8
2	C	197	PRO	2.8
2	E	139	ALA	2.8
2	C	142	SER	2.7
1	A	82	ALA	2.7
3	D	22	THR	2.7
3	F	7	SER	2.7
3	F	190	SER	2.7
2	C	75	ALA	2.7
3	F	183	ASP	2.7
1	B	234	HIS	2.6
2	E	197	PRO	2.6
1	B	19	ARG	2.5
1	A	70	HIS	2.5
2	C	170	GLY	2.5
2	E	42	GLY	2.5
1	A	289	THR	2.4
2	C	196	TRP	2.4
3	D	8	PRO	2.4
2	E	29	TYR	2.4
2	E	57	THR	2.4
1	B	355	GLY	2.4
3	D	151	GLY	2.4
3	D	24	SER	2.4
2	E	141	ALA	2.3
1	B	125	TRP	2.3
2	C	169	ALA	2.3
3	F	167	SER	2.3
3	D	183	ASP	2.3
3	D	1	ASP	2.3
3	D	80	GLU	2.3
1	A	168	LEU	2.3
1	A	100	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	65	MET	2.2
1	B	80	THR	2.2
1	A	271	LYS	2.2
3	D	30	SER	2.2
3	D	91	SER	2.2
1	A	235	GLU	2.2
3	F	8	PRO	2.2
2	E	11	LEU	2.2
3	F	142	ASP	2.2
2	E	222	ALA	2.2
1	A	30	LYS	2.2
3	D	89	GLN	2.2
3	F	194	GLU	2.2
1	A	146	GLY	2.2
1	A	125	TRP	2.2
3	D	10	ILE	2.2
3	D	115	SER	2.2
1	A	84	LEU	2.2
1	A	18	ARG	2.2
1	A	17	ARG	2.1
1	A	145	LEU	2.1
2	E	31	ARG	2.1
1	A	117	GLU	2.1
2	C	7	SER	2.1
1	A	119	GLN	2.1
3	F	95	GLN	2.1
1	A	307	PHE	2.1
1	B	81	VAL	2.0
1	A	167	ARG	2.0
2	E	137	ALA	2.0
3	D	52	LYS	2.0
1	A	19	ARG	2.0
3	F	178	LEU	2.0
2	C	194	SER	2.0
1	B	71	THR	2.0
2	E	168	ALA	2.0
1	B	75	TYR	2.0
3	D	31	TYR	2.0
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.