



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 02:03 am GMT

PDB ID : 2XNY
Title : A fragment of streptococcal M1 protein in complex with human fibrinogen
Authors : Macheboeuf, P.; Y Fu, C.; Zinkernagel, A.S.; Johnson, J.E.; Nizet, V.; Ghosh, P.
Deposited on : 2010-08-06
Resolution : 7.50 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

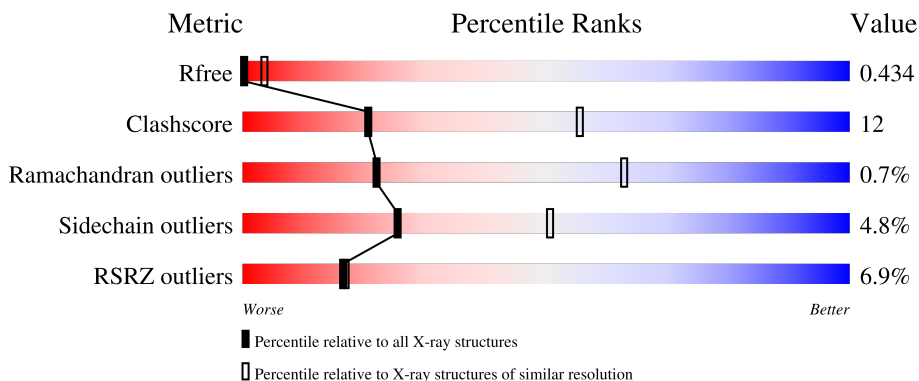
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 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.



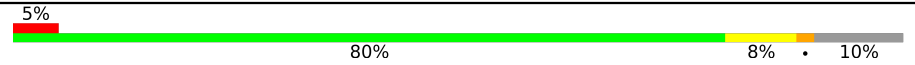


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	87	
1	D	87	
2	B	328	
2	E	328	
3	C	319	

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Mol	Chain	Length	Quality of chain
3	F	319	
4	M	102	
4	N	102	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10956 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 FIBRINOGEN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	57	Total 463	C 283	N 88	O 89	S 3	0	0	0
1	D	57	Total 463	C 283	N 88	O 89	S 3	0	0	0

- Molecule 2 is a protein called FIBRINOGEN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	298	Total 2392	C 1494	N 422	O 454	S 22	0	0	0
2	E	298	Total 2392	C 1494	N 422	O 454	S 22	0	0	0

- Molecule 3 is a protein called FIBRINOGEN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	288	Total 2311	C 1467	N 390	O 443	S 11	0	0	0
3	F	288	Total 2311	C 1467	N 390	O 443	S 11	0	0	0

- Molecule 4 is a protein called M PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	M	37	Total 315	C 192	N 58	O 65	0	0	0
4	N	36	Total 309	C 189	N 55	O 65	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	40	MET	-	expression tag	UNP Q48WD8
M	41	VAL	-	expression tag	UNP Q48WD8
M	136	HIS	-	expression tag	UNP Q48WD8
M	137	HIS	-	expression tag	UNP Q48WD8
M	138	HIS	-	expression tag	UNP Q48WD8
M	139	HIS	-	expression tag	UNP Q48WD8
M	140	HIS	-	expression tag	UNP Q48WD8
M	141	HIS	-	expression tag	UNP Q48WD8
N	40	MET	-	expression tag	UNP Q48WD8
N	41	VAL	-	expression tag	UNP Q48WD8
N	136	HIS	-	expression tag	UNP Q48WD8
N	137	HIS	-	expression tag	UNP Q48WD8
N	138	HIS	-	expression tag	UNP Q48WD8
N	139	HIS	-	expression tag	UNP Q48WD8
N	140	HIS	-	expression tag	UNP Q48WD8
N	141	HIS	-	expression tag	UNP Q48WD8

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.

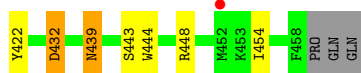
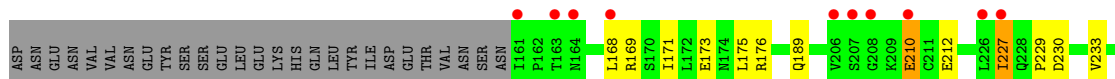
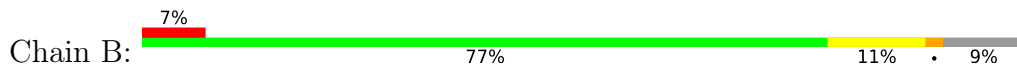
- Molecule 1: FIBRINOGEN ALPHA CHAIN



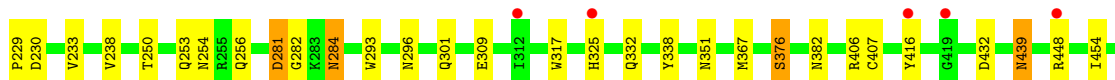
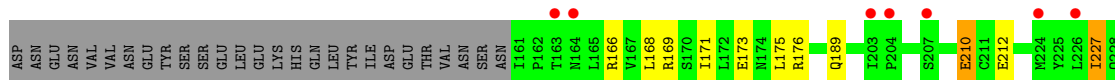
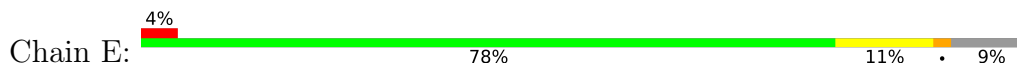
- Molecule 1: FIBRINOGEN ALPHA CHAIN



- Molecule 2: FIBRINOGEN BETA CHAIN



- Molecule 2: FIBRINOGEN BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.69Å 165.69Å 289.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	142.86 – 7.50 47.83 – 6.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (142.86-7.50) 43.9 (47.83-6.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 6.15Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.424 , 0.408 0.423 , 0.434	Depositor DCC
R_{free} test set	247 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtrriage
Anisotropy	0.564	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	10956	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.05% 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	0.32	0/463	0.52	0/617
1	D	0.32	0/463	0.52	0/617
2	B	0.42	0/2453	0.55	1/3312 (0.0%)
2	E	0.42	0/2453	0.55	1/3312 (0.0%)
3	C	0.50	0/2375	0.58	0/3211
3	F	0.50	0/2375	0.58	0/3211
4	M	1.86	8/317 (2.5%)	1.35	6/421 (1.4%)
4	N	1.63	3/311 (1.0%)	1.31	5/414 (1.2%)
All	All	0.60	11/11210 (0.1%)	0.63	13/15115 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	N	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	124	GLU	CD-OE2	12.07	1.39	1.25
4	M	118	ASP	CG-OD1	11.15	1.51	1.25
4	M	132	ARG	CZ-NH1	9.32	1.45	1.33
4	M	107	ASP	CG-OD2	8.91	1.45	1.25
4	M	127	SER	CB-OG	8.71	1.53	1.42
4	M	124	GLU	CD-OE1	7.27	1.33	1.25
4	N	125	SER	CB-OG	7.21	1.51	1.42
4	M	118	ASP	CG-OD2	6.31	1.39	1.25
4	N	107	ASP	CG-OD2	6.30	1.39	1.25
4	N	120	ASP	C-O	6.28	1.35	1.23
4	M	107	ASP	CG-OD1	6.04	1.39	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	132	ARG	NE-CZ-NH2	-9.71	115.44	120.30
4	N	120	ASP	CB-CG-OD1	8.35	125.82	118.30
4	M	118	ASP	CB-CG-OD2	-7.96	111.14	118.30
4	M	107	ASP	CB-CG-OD1	-6.89	112.09	118.30
4	M	107	ASP	CB-CG-OD2	-6.86	112.13	118.30
4	M	107	ASP	OD1-CG-OD2	6.29	135.25	123.30
4	N	120	ASP	O-C-N	6.12	132.50	122.70
4	N	107	ASP	C-N-CA	6.10	136.95	121.70
4	N	133	LEU	CA-CB-CG	6.10	129.32	115.30
4	M	132	ARG	NE-CZ-NH1	5.70	123.15	120.30
4	N	120	ASP	CB-CG-OD2	-5.43	113.41	118.30
2	B	432	ASP	CB-CG-OD2	5.17	122.95	118.30
2	E	432	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	N	124	GLU	Peptide

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	463	0	482	9	0
1	D	463	0	482	9	0
2	B	2392	0	2260	39	3
2	E	2392	0	2257	79	3
3	C	2311	0	2163	46	5
3	F	2311	0	2161	58	0
4	M	315	0	310	112	0
4	N	309	0	301	43	0
All	All	10956	0	10416	263	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (263) 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:110:LEU:CD2	4:M:115:LEU:CD2	1.93	1.45
2:E:166:ARG:HB3	4:M:123:LYS:CE	1.53	1.36
2:E:166:ARG:CB	4:M:123:LYS:HZ1	1.39	1.36
2:E:166:ARG:CB	4:M:123:LYS:NZ	1.86	1.35
2:E:173:GLU:OE2	4:M:116:GLN:HA	1.19	1.35
3:C:110:LEU:HD11	4:M:114:GLU:OE2	1.23	1.32
2:E:166:ARG:HB3	4:M:123:LYS:NZ	0.99	1.30
2:E:173:GLU:CD	4:M:116:GLN:HA	1.49	1.30
3:F:110:LEU:CD2	4:M:115:LEU:HD21	1.56	1.30
3:C:108:ARG:HH12	4:M:117:GLN:CB	1.45	1.30
2:E:173:GLU:OE2	4:M:116:GLN:CA	1.79	1.29
3:C:108:ARG:NH1	4:M:117:GLN:HG3	1.47	1.26
2:E:169:ARG:HB3	4:M:119:TYR:CE2	1.64	1.26
2:E:169:ARG:CB	4:M:119:TYR:CE2	2.05	1.25
3:F:110:LEU:HD21	4:M:115:LEU:CD2	1.56	1.21
2:E:173:GLU:OE2	4:M:115:LEU:O	1.57	1.21
2:B:432:ASP:OD2	2:B:443:SER:HB3	1.37	1.21
3:C:108:ARG:HH12	4:M:117:GLN:CG	1.53	1.19
4:M:115:LEU:O	4:M:119:TYR:HB3	1.43	1.17
3:C:108:ARG:CZ	4:M:117:GLN:HG3	1.74	1.17
2:E:173:GLU:OE2	4:M:115:LEU:C	1.84	1.14
2:E:169:ARG:HD2	4:N:118:ASP:OD2	1.47	1.12
3:F:110:LEU:CD2	4:M:115:LEU:HD22	1.75	1.12
2:B:432:ASP:OD2	2:B:443:SER:CB	1.98	1.12
2:B:422:TYR:OH	2:B:432:ASP:OD1	1.65	1.12
3:C:108:ARG:HH22	4:M:117:GLN:CD	1.54	1.10
3:F:110:LEU:HD22	4:M:115:LEU:HD22	1.32	1.10
4:M:112:LEU:HD22	4:N:111:LYS:HD3	1.11	1.09
2:B:432:ASP:CG	2:B:443:SER:O	1.90	1.08
3:C:108:ARG:NH1	4:M:117:GLN:CG	2.14	1.08
2:B:432:ASP:OD1	2:B:443:SER:O	1.70	1.07
2:E:169:ARG:CD	4:N:118:ASP:OD2	2.03	1.06
4:M:114:GLU:HB2	4:N:115:LEU:HD11	1.35	1.05
2:E:173:GLU:HG2	4:M:116:GLN:HG2	1.35	1.05
3:C:110:LEU:HD11	4:M:114:GLU:CD	1.76	1.04
2:B:432:ASP:OD2	2:B:443:SER:CA	2.07	1.01
2:E:173:GLU:OE2	4:M:116:GLN:N	1.92	1.01
2:E:166:ARG:C	4:M:123:LYS:HE3	1.80	1.01
2:E:169:ARG:HB3	4:M:119:TYR:HE2	0.92	1.00
3:C:110:LEU:CD1	4:M:114:GLU:OE2	2.10	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:110:LEU:HD23	4:M:115:LEU:CD1	1.92	0.99
3:F:110:LEU:HD21	4:N:114:GLU:HB3	1.43	0.99
2:E:166:ARG:CG	4:M:123:LYS:HZ1	1.76	0.98
3:F:110:LEU:HD22	4:M:115:LEU:CD2	1.80	0.98
2:E:169:ARG:CZ	4:N:118:ASP:HB3	1.94	0.98
3:F:110:LEU:HD23	4:M:115:LEU:HD13	1.46	0.98
2:B:432:ASP:OD2	2:B:443:SER:O	1.81	0.97
2:E:169:ARG:NE	4:N:118:ASP:OD2	1.97	0.96
3:C:108:ARG:NH1	4:M:117:GLN:CB	2.27	0.95
3:F:110:LEU:CD2	4:M:115:LEU:CD1	2.44	0.95
4:M:115:LEU:HD21	4:N:114:GLU:HB3	1.48	0.94
4:M:114:GLU:O	4:N:115:LEU:HD21	1.68	0.94
4:M:126:THR:O	4:M:128:TRP:N	2.02	0.93
3:F:110:LEU:HD21	4:M:115:LEU:HD21	0.93	0.93
2:E:169:ARG:NH1	4:M:119:TYR:O	1.95	0.92
2:E:166:ARG:CB	4:M:123:LYS:CE	2.38	0.92
4:M:112:LEU:CD2	4:N:111:LYS:HD3	1.99	0.90
3:C:108:ARG:HH12	4:M:117:GLN:HB3	1.34	0.90
2:E:166:ARG:HB3	4:M:123:LYS:HZ2	1.33	0.89
3:F:112:GLU:OE2	4:M:112:LEU:HD11	1.74	0.88
3:C:108:ARG:NH2	4:M:117:GLN:HG3	1.89	0.87
2:E:169:ARG:NH2	4:N:118:ASP:HB3	1.88	0.87
2:B:169:ARG:HH22	4:N:119:TYR:CB	1.86	0.87
2:E:176:ARG:NH1	4:M:112:LEU:O	2.09	0.86
2:B:173:GLU:OE1	4:N:119:TYR:CE1	2.29	0.86
2:B:169:ARG:NH2	4:N:119:TYR:CG	2.39	0.84
2:B:432:ASP:OD2	2:B:443:SER:C	2.15	0.83
2:E:166:ARG:CA	4:M:123:LYS:HE3	2.10	0.82
3:C:264:MET:HE1	3:C:389:PHE:CD2	2.15	0.81
2:E:166:ARG:HB3	4:M:123:LYS:HE3	1.61	0.81
2:E:169:ARG:NE	4:N:118:ASP:CG	2.34	0.81
4:M:127:SER:HA	4:M:130:ARG:HD2	1.62	0.81
3:F:307:HIS:HE1	3:F:341:ALA:H	1.29	0.80
3:C:307:HIS:HE1	3:C:341:ALA:H	1.29	0.80
3:F:112:GLU:OE2	4:M:112:LEU:CD1	2.30	0.79
4:M:114:GLU:CB	4:N:115:LEU:HD11	2.13	0.78
4:M:119:TYR:HB2	4:N:118:ASP:HB3	1.62	0.78
3:F:110:LEU:HD21	4:M:115:LEU:CG	2.13	0.78
4:M:109:GLU:HA	4:M:112:LEU:HG	1.66	0.77
3:F:110:LEU:CD2	4:N:114:GLU:HB3	2.12	0.76
2:E:169:ARG:O	4:M:119:TYR:CE1	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:CD	4:M:123:LYS:HZ1	1.97	0.76
4:M:112:LEU:HD22	4:N:111:LYS:CD	2.06	0.76
3:C:108:ARG:NH2	4:M:117:GLN:CG	2.49	0.76
3:C:108:ARG:HH22	4:M:117:GLN:CG	1.99	0.75
3:F:110:LEU:CD2	4:M:115:LEU:CG	2.65	0.75
3:F:110:LEU:HD21	4:M:115:LEU:CD1	2.17	0.73
3:F:108:ARG:HD3	4:N:114:GLU:HG3	1.71	0.73
3:F:110:LEU:CD2	4:M:115:LEU:HD11	2.17	0.73
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.53	0.73
2:E:166:ARG:CB	4:M:123:LYS:HE3	2.13	0.72
3:C:108:ARG:NH2	4:M:117:GLN:CD	2.38	0.72
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.53	0.72
2:E:169:ARG:NE	4:N:118:ASP:CB	2.54	0.71
3:C:249:GLU:HG3	3:C:383:THR:HB	1.72	0.70
2:E:166:ARG:CB	4:M:123:LYS:HZ2	1.91	0.70
2:E:173:GLU:HB2	4:M:119:TYR:HE1	1.55	0.70
3:F:249:GLU:HG3	3:F:383:THR:HB	1.72	0.70
2:B:176:ARG:HH22	4:N:112:LEU:HB3	1.56	0.70
2:E:169:ARG:HG2	4:M:119:TYR:CZ	2.02	0.69
3:F:264:MET:HE1	3:F:389:PHE:CD2	2.28	0.69
3:F:110:LEU:HD21	4:N:114:GLU:CB	2.20	0.69
2:B:173:GLU:OE1	4:N:119:TYR:CD1	2.46	0.69
1:A:169:LEU:H	2:B:189:GLN:HE22	1.41	0.68
2:E:173:GLU:CD	4:M:116:GLN:CA	2.41	0.68
1:D:169:LEU:H	2:E:189:GLN:HE22	1.41	0.67
3:F:108:ARG:HB3	4:N:114:GLU:CD	2.14	0.67
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.42	0.67
4:M:126:THR:C	4:M:128:TRP:H	1.95	0.67
3:F:110:LEU:N	4:N:114:GLU:OE1	2.28	0.66
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.42	0.66
2:B:376:SER:HB3	2:B:382:ASN:H	1.62	0.65
3:C:169:ILE:HD11	3:C:178:PHE:CE2	2.32	0.65
2:E:173:GLU:HG2	4:M:116:GLN:CG	2.20	0.65
3:F:110:LEU:CA	4:N:114:GLU:OE1	2.45	0.65
4:M:122:ALA:O	4:M:126:THR:OG1	2.15	0.65
3:F:169:ILE:HD11	3:F:178:PHE:CE2	2.32	0.65
2:E:166:ARG:HD2	4:M:123:LYS:HZ1	1.62	0.64
2:E:376:SER:HB3	2:E:382:ASN:H	1.62	0.64
4:M:109:GLU:O	4:M:113:LYS:N	2.29	0.64
2:E:169:ARG:NE	4:N:118:ASP:HB3	2.12	0.64
2:B:169:ARG:HH22	4:N:119:TYR:HB2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:112:LEU:N	4:M:112:LEU:HD23	2.13	0.63
4:M:114:GLU:C	4:N:115:LEU:HD21	2.19	0.63
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.81	0.63
2:E:176:ARG:CZ	4:M:113:LYS:HA	2.29	0.63
2:B:439:ASN:H	2:B:439:ASN:HD22	1.47	0.62
2:E:169:ARG:CD	4:N:118:ASP:CG	2.66	0.62
3:F:108:ARG:HB3	4:N:114:GLU:CG	2.29	0.62
3:F:307:HIS:CE1	3:F:341:ALA:H	2.14	0.62
2:E:367:MET:HB2	2:E:406:ARG:HB2	1.81	0.62
2:E:166:ARG:CA	4:M:123:LYS:CE	2.77	0.62
2:E:166:ARG:HB3	4:M:123:LYS:HZ1	0.82	0.62
2:E:166:ARG:O	4:M:123:LYS:HE3	1.99	0.62
2:E:439:ASN:HD22	2:E:439:ASN:H	1.47	0.61
3:C:307:HIS:CE1	3:C:341:ALA:H	2.14	0.61
3:F:110:LEU:HD21	4:M:115:LEU:HD11	1.78	0.61
2:E:176:ARG:NH2	4:M:113:LYS:HA	2.17	0.60
2:E:169:ARG:HG2	4:M:119:TYR:CE1	2.37	0.60
3:F:264:MET:CE	3:F:389:PHE:CD2	2.85	0.60
3:C:264:MET:CE	3:C:389:PHE:CD2	2.85	0.59
3:C:110:LEU:HD11	4:M:114:GLU:OE1	2.01	0.59
4:N:106:LYS:O	4:N:106:LYS:HG3	2.04	0.58
3:F:307:HIS:HD2	3:F:335:TRP:O	1.87	0.57
3:C:108:ARG:NH1	4:M:117:GLN:HB3	2.09	0.57
3:F:110:LEU:CD2	4:N:114:GLU:CB	2.82	0.57
1:A:147:MET:HG3	2:B:175:LEU:HD22	1.87	0.57
3:C:307:HIS:HD2	3:C:335:TRP:O	1.87	0.57
2:E:309:GLU:OE1	2:E:325:HIS:HE1	1.87	0.57
2:B:432:ASP:OD2	2:B:443:SER:HA	2.04	0.56
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.19	0.56
1:D:147:MET:HG3	2:E:175:LEU:HD22	1.87	0.56
2:E:173:GLU:CG	4:M:119:TYR:CE1	2.88	0.56
3:F:151:LYS:HB3	3:F:239:GLN:NE2	2.19	0.56
4:M:98:LYS:O	4:M:102:GLU:HB2	2.06	0.56
2:B:309:GLU:OE1	2:B:325:HIS:HE1	1.88	0.56
1:D:169:LEU:H	2:E:189:GLN:NE2	2.03	0.56
4:M:126:THR:C	4:M:128:TRP:N	2.58	0.55
1:D:144:LEU:HD12	2:E:175:LEU:HD21	1.90	0.54
1:A:144:LEU:HD12	2:B:175:LEU:HD21	1.89	0.54
4:M:115:LEU:O	4:M:119:TYR:CB	2.36	0.54
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.56	0.54
2:E:173:GLU:CD	4:M:115:LEU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:ASP:OD1	2:E:282:GLY:N	2.38	0.53
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.56	0.53
1:A:169:LEU:H	2:B:189:GLN:NE2	2.03	0.53
3:C:249:GLU:CG	3:C:383:THR:HB	2.39	0.53
3:F:189:ASN:ND2	3:F:391:ARG:HE	2.06	0.53
3:F:249:GLU:CG	3:F:383:THR:HB	2.39	0.53
3:C:229:GLY:O	3:C:233:ILE:HG12	2.08	0.53
3:C:194:PHE:CG	3:C:233:ILE:HD12	2.43	0.53
2:E:169:ARG:HG2	4:M:119:TYR:CD1	2.39	0.52
3:F:194:PHE:CG	3:F:233:ILE:HD12	2.43	0.52
3:F:229:GLY:O	3:F:233:ILE:HG12	2.09	0.52
3:F:112:GLU:OE2	4:M:112:LEU:HD13	2.08	0.52
3:C:194:PHE:HB2	3:C:233:ILE:CD1	2.40	0.52
2:E:166:ARG:HD2	4:M:123:LYS:NZ	2.25	0.52
1:A:152:VAL:O	1:A:156:ILE:HG12	2.10	0.52
4:M:109:GLU:O	4:M:113:LYS:HB2	2.09	0.52
4:M:128:TRP:C	4:M:130:ARG:H	2.12	0.52
3:C:189:ASN:ND2	3:C:391:ARG:HE	2.06	0.51
3:F:194:PHE:HB2	3:F:233:ILE:CD1	2.40	0.51
1:D:152:VAL:O	1:D:156:ILE:HG12	2.10	0.51
2:E:439:ASN:HD22	2:E:439:ASN:N	2.09	0.51
2:B:281:ASP:OD1	2:B:282:GLY:N	2.38	0.51
3:F:264:MET:HE2	3:F:264:MET:H	1.77	0.50
3:F:390:ASN:C	3:F:390:ASN:HD22	2.15	0.50
4:M:119:TYR:HA	4:N:118:ASP:O	2.11	0.50
3:F:113:ILE:HD11	4:M:115:LEU:HD13	1.95	0.49
3:C:390:ASN:HD22	3:C:390:ASN:C	2.15	0.49
2:B:439:ASN:HD22	2:B:439:ASN:N	2.09	0.49
3:C:323:GLU:H	3:C:323:GLU:CD	2.17	0.48
2:E:176:ARG:NH2	4:M:113:LYS:CA	2.77	0.48
3:F:323:GLU:H	3:F:323:GLU:CD	2.17	0.48
1:D:178:TYR:O	1:D:182:GLN:HB2	2.13	0.48
2:E:169:ARG:HE	4:N:118:ASP:CB	2.27	0.48
4:M:110:THR:HA	4:M:113:LYS:HB2	1.95	0.48
2:E:173:GLU:CB	4:M:119:TYR:HE1	2.26	0.48
1:A:178:TYR:O	1:A:182:GLN:HB2	2.13	0.47
1:D:156:ILE:HD12	2:E:416:TYR:O	2.14	0.47
2:E:176:ARG:HH22	4:M:112:LEU:C	2.17	0.47
4:M:106:LYS:C	4:M:108:LEU:H	2.17	0.47
1:A:156:ILE:HD12	2:B:416:TYR:O	2.14	0.47
2:E:238:VAL:HG21	2:E:250:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:VAL:HG21	2:B:250:THR:CG2	2.45	0.47
1:A:139:ASN:N	1:A:139:ASN:HD22	2.13	0.46
4:M:122:ALA:C	4:M:126:THR:OG1	2.55	0.46
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.16	0.46
2:E:176:ARG:HH22	4:M:113:LYS:N	2.13	0.46
2:B:317:TRP:CE3	2:B:448:ARG:HD2	2.51	0.45
1:D:139:ASN:N	1:D:139:ASN:HD22	2.13	0.45
1:A:139:ASN:HD22	1:A:139:ASN:H	1.65	0.45
2:E:284:ASN:C	2:E:284:ASN:HD22	2.20	0.45
2:E:317:TRP:CE3	2:E:448:ARG:HD2	2.51	0.45
1:D:139:ASN:HD22	1:D:139:ASN:H	1.65	0.45
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.16	0.45
3:C:108:ARG:NH1	4:M:117:GLN:HB2	2.24	0.45
3:C:365:ASN:HD22	3:C:365:ASN:H	1.64	0.45
3:F:365:ASN:HD22	3:F:365:ASN:H	1.64	0.45
3:F:108:ARG:HB3	4:N:114:GLU:OE2	2.16	0.45
3:C:189:ASN:ND2	3:C:391:ARG:HH21	2.15	0.44
4:N:108:LEU:HA	4:N:111:LYS:HB2	1.99	0.44
2:B:284:ASN:C	2:B:284:ASN:HD22	2.20	0.44
2:E:227:ILE:HG12	2:E:229:PRO:HD3	1.99	0.44
4:N:110:THR:HA	4:N:113:LYS:HE3	1.99	0.44
2:B:227:ILE:HG12	2:B:229:PRO:HD3	1.99	0.44
3:C:390:ASN:HD22	3:C:391:ARG:N	2.15	0.44
3:F:148:ILE:HD12	3:F:148:ILE:H	1.82	0.44
3:F:189:ASN:ND2	3:F:391:ARG:HH21	2.15	0.44
3:C:148:ILE:H	3:C:148:ILE:HD12	1.82	0.44
3:F:390:ASN:HD22	3:F:391:ARG:N	2.15	0.44
3:C:264:MET:HE1	3:C:389:PHE:HD2	1.78	0.43
3:F:110:LEU:HD23	4:M:115:LEU:CD2	2.24	0.43
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.17	0.43
4:M:109:GLU:C	4:M:111:LYS:H	2.21	0.43
3:F:264:MET:HE2	3:F:264:MET:N	2.34	0.43
2:E:230:ASP:HB3	2:E:233:VAL:HG23	2.00	0.42
2:B:230:ASP:HB3	2:B:233:VAL:HG23	2.00	0.42
2:E:166:ARG:HB2	4:M:123:LYS:HZ2	1.80	0.42
4:N:115:LEU:HD23	4:N:115:LEU:HA	1.82	0.42
2:B:254:ASN:HD21	2:B:256:GLN:NE2	2.17	0.42
3:C:198:LEU:CD2	3:C:381:LYS:HD3	2.50	0.42
2:B:332:GLN:O	2:B:338:TYR:HA	2.20	0.41
2:B:389:ASP:HA	2:B:390:PRO:HD3	1.92	0.41
3:F:198:LEU:CD2	3:F:381:LYS:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:112:GLU:HB3	4:N:111:LYS:HE2	1.42	0.41
4:M:129:ASP:OD1	4:N:129:ASP:HA	2.20	0.41
3:F:325:ASN:HD22	3:F:325:ASN:C	2.24	0.41
3:C:183:GLU:HB3	3:C:191:TRP:HB2	2.03	0.41
3:F:323:GLU:CD	3:F:323:GLU:N	2.74	0.41
3:C:323:GLU:CD	3:C:323:GLU:N	2.74	0.41
3:C:325:ASN:ND2	3:C:328:GLU:H	2.19	0.41
2:B:238:VAL:HG21	2:B:250:THR:HG23	2.03	0.41
3:C:307:HIS:CE1	3:C:342:GLY:H	2.39	0.41
2:B:168:LEU:HA	2:B:171:ILE:HG22	2.03	0.41
2:E:238:VAL:HG21	2:E:250:THR:HG23	2.03	0.40
2:E:332:GLN:O	2:E:338:TYR:HA	2.20	0.40
2:E:168:LEU:HA	2:E:171:ILE:HG22	2.03	0.40
2:E:406:ARG:N	2:E:407:CYS:HA	2.36	0.40
3:F:307:HIS:CE1	3:F:342:GLY:H	2.39	0.40
4:N:110:THR:HG22	4:N:113:LYS:NZ	2.36	0.40
2:B:439:ASN:N	2:B:439:ASN:ND2	2.69	0.40
3:C:325:ASN:C	3:C:325:ASN:HD22	2.24	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:GLU:OE2	3:C:328:GLU:OE2[4_556]	1.59	0.61
3:C:328:GLU:OE1	3:C:328:GLU:OE2[4_556]	1.63	0.57
2:B:444:TRP:NE1	2:E:458:PHE:CA[5_445]	1.66	0.54
2:B:444:TRP:CZ2	2:E:458:PHE:O[5_445]	1.68	0.52
3:C:328:GLU:CD	3:C:328:GLU:OE2[4_556]	1.78	0.42
3:C:328:GLU:CD	3:C:328:GLU:CD[4_556]	2.02	0.18
3:C:328:GLU:CD	3:C:328:GLU:OE1[4_556]	2.13	0.07
2:B:444:TRP:CE2	2:E:458:PHE:O[5_445]	2.16	0.04

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	55/87 (63%)	49 (89%)	6 (11%)	0	100	100
1	D	55/87 (63%)	49 (89%)	6 (11%)	0	100	100
2	B	296/328 (90%)	281 (95%)	14 (5%)	1 (0%)	41	77
2	E	296/328 (90%)	281 (95%)	14 (5%)	1 (0%)	41	77
3	C	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	22	63
3	F	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	22	63
4	M	35/102 (34%)	20 (57%)	12 (34%)	3 (9%)	1	11
4	N	34/102 (33%)	24 (71%)	9 (26%)	1 (3%)	4	29
All	All	1343/1672 (80%)	1248 (93%)	85 (6%)	10 (1%)	22	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	127	SER
4	M	99	GLN
4	M	107	ASP
3	C	110	LEU
3	C	111	GLN
3	F	110	LEU
3	F	111	GLN
2	B	281	ASP
2	E	281	ASP
4	N	107	ASP

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	52/82 (63%)	50 (96%)	2 (4%)	33	57
1	D	52/82 (63%)	50 (96%)	2 (4%)	33	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	256/286 (90%)	247 (96%)	9 (4%)	36	59
2	E	256/286 (90%)	247 (96%)	9 (4%)	36	59
3	C	242/267 (91%)	235 (97%)	7 (3%)	42	64
3	F	242/267 (91%)	235 (97%)	7 (3%)	42	64
4	M	34/89 (38%)	24 (71%)	10 (29%)	0	2
4	N	34/89 (38%)	24 (71%)	10 (29%)	0	2
All	All	1168/1448 (81%)	1112 (95%)	56 (5%)	25	50

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	158	ILE
2	B	210	GLU
2	B	227	ILE
2	B	253	GLN
2	B	284	ASN
2	B	301	GLN
2	B	351	ASN
2	B	376	SER
2	B	439	ASN
2	B	454	ILE
3	C	169	ILE
3	C	244	TYR
3	C	317	ASN
3	C	325	ASN
3	C	337	ASN
3	C	365	ASN
3	C	390	ASN
1	D	139	ASN
1	D	158	ILE
2	E	210	GLU
2	E	227	ILE
2	E	253	GLN
2	E	284	ASN
2	E	301	GLN
2	E	351	ASN
2	E	376	SER
2	E	439	ASN
2	E	454	ILE

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Mol	Chain	Res	Type
3	F	169	ILE
3	F	244	TYR
3	F	317	ASN
3	F	325	ASN
3	F	337	ASN
3	F	365	ASN
3	F	390	ASN
4	M	96	LYS
4	M	99	GLN
4	M	101	LEU
4	M	112	LEU
4	M	115	LEU
4	M	119	TYR
4	M	121	LEU
4	M	126	THR
4	M	127	SER
4	M	129	ASP
4	N	104	GLN
4	N	108	LEU
4	N	109	GLU
4	N	114	GLU
4	N	119	TYR
4	N	121	LEU
4	N	125	SER
4	N	126	THR
4	N	132	ARG
4	N	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	164	ASN
2	B	180	GLN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN

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Mol	Chain	Res	Type
2	B	421	GLN
2	B	439	ASN
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	136	GLN
3	C	189	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	337	ASN
3	C	365	ASN
3	C	390	ASN
1	D	182	GLN
2	E	164	ASN
2	E	180	GLN
2	E	189	GLN
2	E	253	GLN
2	E	256	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	339	GLN
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN
3	F	136	GLN
3	F	189	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	337	ASN
3	F	365	ASN

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Mol	Chain	Res	Type
3	F	390	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 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

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	57/87 (65%)	0.58	4 (7%) 16 17	34, 65, 96, 97	0
1	D	57/87 (65%)	0.66	5 (8%) 10 12	34, 65, 96, 97	0
2	B	298/328 (90%)	0.36	23 (7%) 13 15	17, 32, 76, 102	0
2	E	298/328 (90%)	0.08	12 (4%) 38 34	17, 32, 76, 102	0
3	C	288/319 (90%)	0.31	23 (7%) 12 14	13, 20, 64, 100	0
3	F	288/319 (90%)	0.38	16 (5%) 24 24	13, 20, 64, 100	0
4	M	37/102 (36%)	0.80	6 (16%) 1 4	24, 37, 82, 116	0
4	N	36/102 (35%)	0.88	5 (13%) 2 6	21, 32, 70, 86	0
All	All	1359/1672 (81%)	0.34	94 (6%) 16 17	13, 28, 84, 116	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	207	SER	7.6
2	B	400	GLY	5.4
4	N	106	LYS	4.9
2	B	206	VAL	4.8
2	E	203	ILE	4.1
2	B	226	LEU	4.0
3	F	179	LEU	4.0
3	C	360	PRO	3.9
3	C	177	GLN	3.8
3	C	305	THR	3.8
2	B	325	HIS	3.8
3	C	361	ASN	3.7
3	C	105	SER	3.7
2	B	401	GLY	3.5
3	C	392	LEU	3.5
3	F	265	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	164	ASN	3.4
3	C	340	HIS	3.4
4	N	125	SER	3.4
1	D	185	LEU	3.3
3	C	179	LEU	3.3
2	B	161	ILE	3.3
2	E	448	ARG	3.2
2	B	237	ARG	3.2
2	B	395	SER	3.2
2	B	168	LEU	3.2
2	E	419	GLY	3.2
3	F	266	LYS	3.2
3	C	351	GLY	3.1
4	M	130	ARG	3.1
3	C	307	HIS	3.1
3	F	297	ASP	3.1
2	B	251	VAL	3.1
2	B	396	LYS	3.1
4	M	105	ARG	3.0
1	A	134	GLN	3.0
1	D	173	VAL	2.9
2	B	208	GLY	2.9
1	D	188	VAL	2.9
2	B	452	MET	2.9
3	F	105	SER	2.8
4	N	105	ARG	2.8
2	E	325	HIS	2.8
1	A	185	LEU	2.8
3	C	341	ALA	2.8
2	B	252	ILE	2.7
2	E	164	ASN	2.7
2	B	399	GLY	2.7
3	F	298	ASP	2.7
3	F	392	LEU	2.7
3	C	297	ASP	2.7
2	E	204	PRO	2.6
3	F	267	VAL	2.6
4	N	131	GLN	2.6
3	F	284	GLY	2.6
1	D	189	ILE	2.6
3	F	379	MET	2.6
3	C	176	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	293	PHE	2.5
2	B	163	THR	2.5
2	E	224	MET	2.5
3	C	339	CYS	2.5
2	B	210	GLU	2.5
3	F	341	ALA	2.5
2	B	273	PHE	2.4
2	E	207	SER	2.4
4	M	131	GLN	2.4
3	C	168	PHE	2.4
4	M	97	ALA	2.4
2	E	416	TYR	2.4
4	M	111	LYS	2.4
3	C	353	THR	2.4
2	E	312	ILE	2.4
1	A	141	ARG	2.3
2	E	226	LEU	2.3
3	F	362	GLY	2.3
3	F	180	VAL	2.2
4	M	129	ASP	2.2
2	E	163	THR	2.2
4	N	111	LYS	2.2
2	B	357	ALA	2.2
2	B	227	ILE	2.2
3	F	369	TRP	2.1
3	F	136	GLN	2.1
1	D	134	GLN	2.1
3	C	308	ASN	2.1
3	C	292	GLY	2.1
1	A	190	ALA	2.1
3	C	338	LYS	2.0
2	B	404	TYR	2.0
3	C	121	ILE	2.0
3	C	306	SER	2.0
3	F	276	LEU	2.0
3	C	324	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.