



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:46 PM EDT

PDB ID : 2XNY / pdb_00002xny
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 : 4-5-2 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

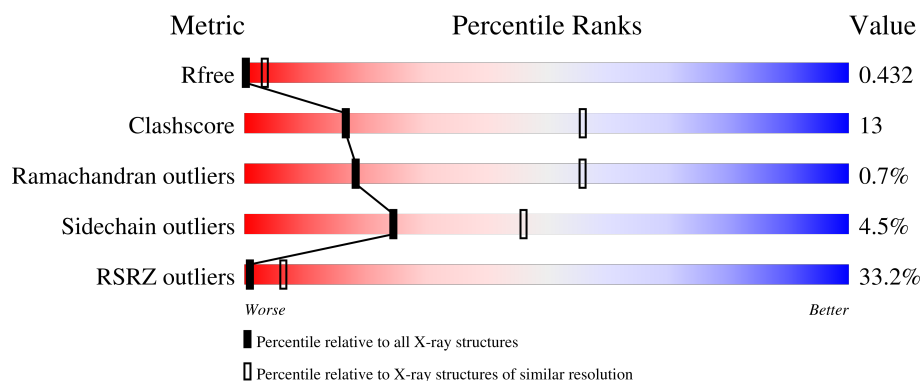
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	319	28% 80% 9% 10%
4	M	102	24% 7% 20% 8% 64%
4	N	102	22% 9% 20% 7% 65%

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
1	A	57	Total	C	N	O	S	0	0	0
			463	283	88	89	3			
1	D	57	Total	C	N	O	S	0	0	0
			463	283	88	89	3			

- Molecule 2 is a protein called FIBRINOGEN BETA CHAIN.

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

- Molecule 3 is a protein called FIBRINOGEN GAMMA CHAIN.

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

- Molecule 4 is a protein called M PROTEIN.

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

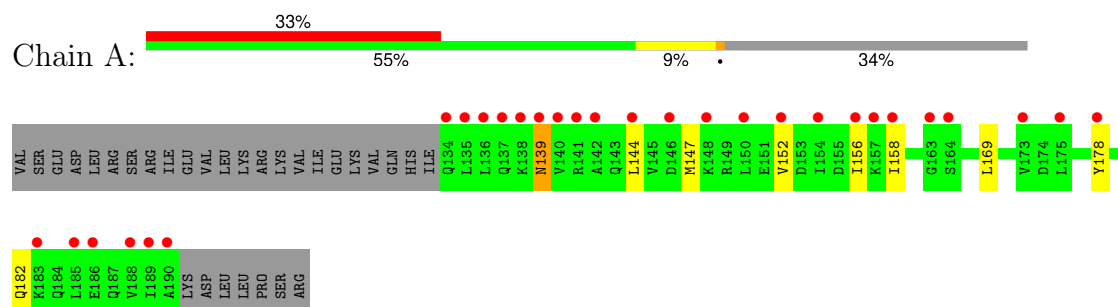
There are 16 discrepancies between the modelled and reference sequences:

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

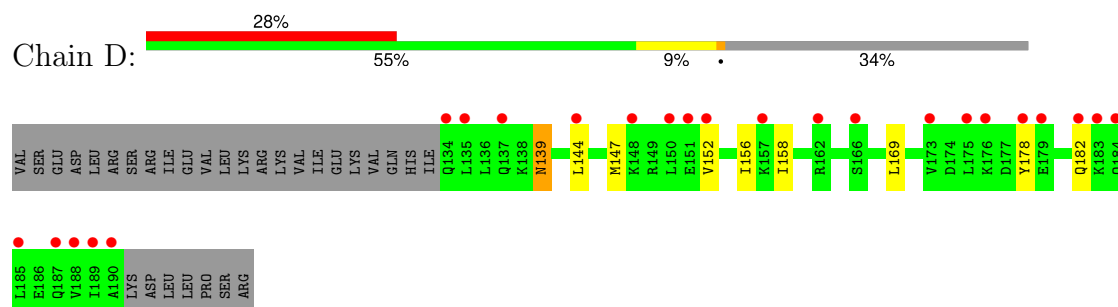
3 Residue-property plots [i](#)

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.

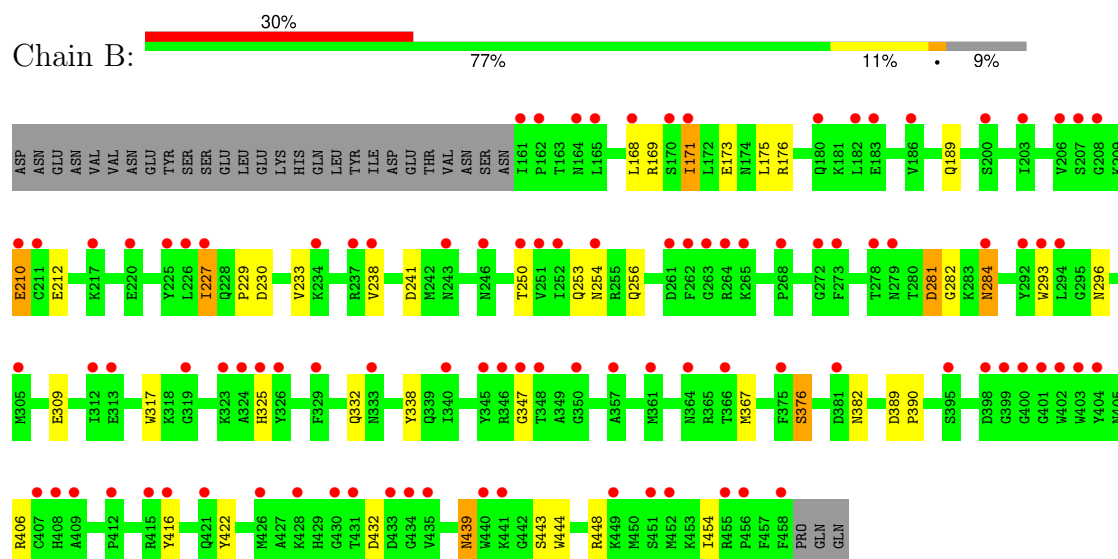
• Molecule 1: FIBRINOGEN ALPHA CHAIN



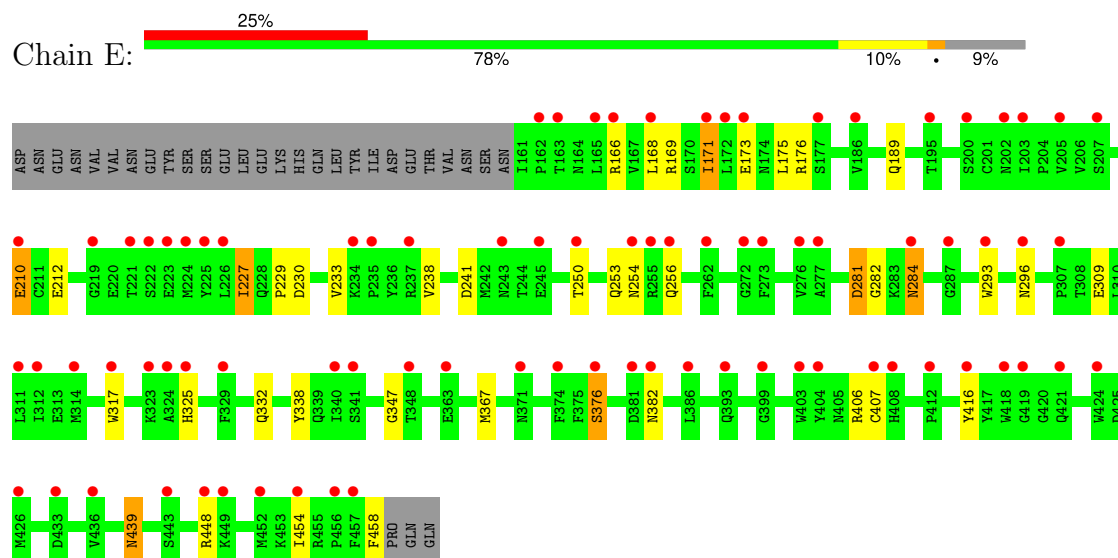
• Molecule 1: FIBRINOGEN ALPHA CHAIN



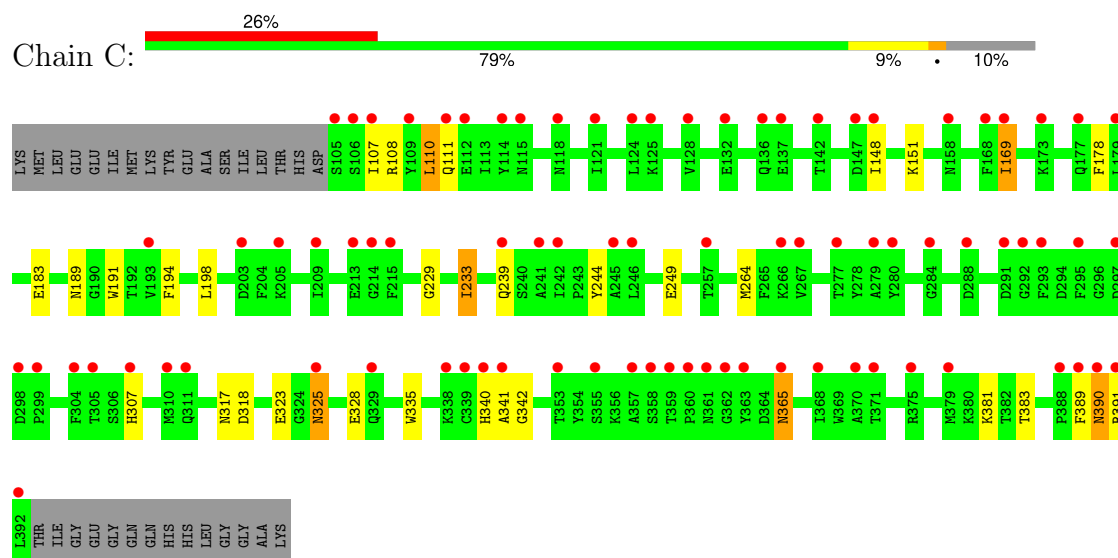
• Molecule 2: FIBRINOGEN BETA CHAIN



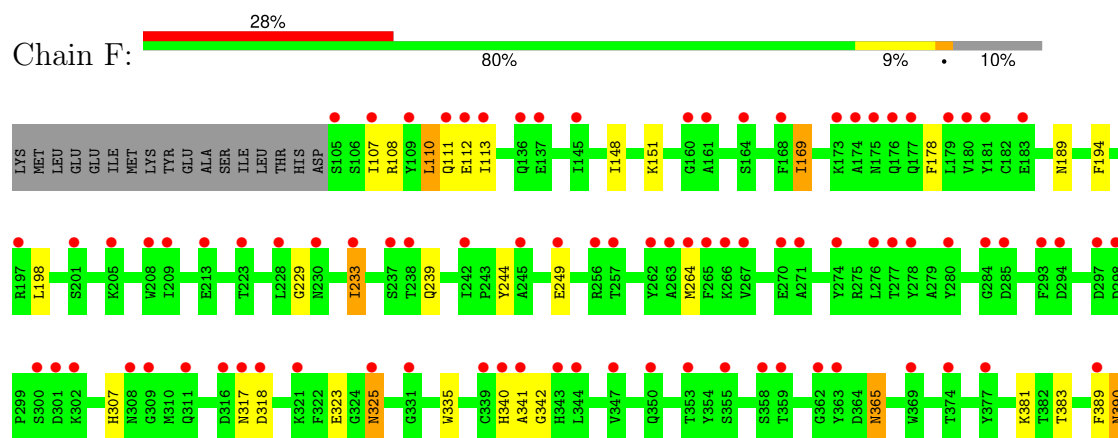
• Molecule 2: FIBRINOGEN BETA CHAIN



• Molecule 3: FIBRINOGEN GAMMA CHAIN



• Molecule 3: FIBRINOGEN GAMMA 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 – 7.50 142.86 – 7.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (142.86-7.50) 67.1 (142.86-7.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.424 , 0.408 0.423 , 0.432	Depositor DCC
R_{free} test set	247 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 141.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	10956	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage'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

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	0.45	0/463	0.82	0/617
1	D	0.44	0/463	0.82	0/617
2	B	0.53	0/2453	0.76	1/3312 (0.0%)
2	E	0.52	0/2453	0.76	1/3312 (0.0%)
3	C	0.58	0/2375	0.79	2/3211 (0.1%)
3	F	0.57	0/2375	0.79	2/3211 (0.1%)
4	M	2.01	9/317 (2.8%)	1.36	4/421 (1.0%)
4	N	2.00	12/311 (3.9%)	1.61	5/414 (1.2%)
All	All	0.71	21/11210 (0.2%)	0.83	15/15115 (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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	118	ASP	CG-OD1	13.50	1.51	1.25
4	M	107	ASP	CG-OD2	10.79	1.45	1.25
4	M	132	ARG	CZ-NH1	8.87	1.45	1.32
4	M	118	ASP	CG-OD2	7.64	1.39	1.25
4	N	107	ASP	CG-OD2	7.63	1.39	1.25
4	N	120	ASP	CA-C	7.38	1.63	1.52
4	N	120	ASP	C-O	7.36	1.35	1.23
4	M	107	ASP	CG-OD1	7.31	1.39	1.25
4	M	124	GLU	CD-OE2	7.14	1.39	1.25
4	N	110	THR	CA-CB	6.53	1.64	1.53
4	N	122	ALA	C-O	5.93	1.32	1.24
4	N	118	ASP	C-O	5.84	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	126	THR	CA-CB	5.77	1.62	1.53
4	N	107	ASP	CG-OD1	5.75	1.36	1.25
4	M	127	SER	CB-OG	5.71	1.53	1.42
4	N	126	THR	N-CA	5.51	1.53	1.46
4	N	133	LEU	N-CA	5.37	1.53	1.46
4	N	131	GLN	CD-OE1	5.34	1.33	1.23
4	M	110	THR	CA-CB	5.31	1.62	1.53
4	M	123	LYS	C-O	5.14	1.30	1.24
4	N	131	GLN	CD-NE2	5.00	1.43	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	107	ASP	CA-C-N	8.47	136.95	121.70
4	N	107	ASP	C-N-CA	8.47	136.95	121.70
4	M	125	SER	N-CA-C	-7.35	103.45	113.30
4	N	120	ASP	O-C-N	7.15	132.50	121.63
4	N	105	ARG	N-CA-C	-6.75	105.17	113.41
4	N	123	LYS	N-CA-C	-6.00	105.78	114.12
4	M	100	ALA	N-CA-C	-5.83	103.64	112.04
3	F	233	ILE	CB-CA-C	-5.80	104.32	112.14
3	C	233	ILE	CB-CA-C	-5.72	104.42	112.14
4	M	111	LYS	N-CA-C	-5.62	107.07	114.04
3	F	340	HIS	N-CA-C	5.23	116.80	108.79
3	C	340	HIS	N-CA-C	5.22	116.77	108.79
4	M	107	ASP	OD1-CG-OD2	5.15	135.25	122.90
2	E	347	GLY	N-CA-C	5.06	116.86	110.38
2	B	347	GLY	N-CA-C	5.06	116.86	110.38

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

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	41	3
2	E	2392	0	2257	81	3
3	C	2311	0	2163	48	5
3	F	2311	0	2161	59	0
4	M	315	0	310	114	0
4	N	309	0	301	45	0
All	All	10956	0	10416	273	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 13.

All (273) 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:173:GLU:CD	4:M:116:GLN:HA	1.49	1.35
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
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
2:E:173:GLU:OE2	4:M:115:LEU:C	1.84	1.18
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
3:C:108:ARG:HH22	4:M:117:GLN:CD	1.54	1.15
2:B:432:ASP:CG	2:B:443:SER:O	1.90	1.13
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:TYR:OH	2:B:432:ASP:OD1	1.65	1.12
3:F:110:LEU:HD22	4:M:115:LEU:HD22	1.32	1.10
3:C:110:LEU:HD11	4:M:114:GLU:CD	1.76	1.09
4:M:112:LEU:HD22	4:N:111:LYS:HD3	1.11	1.09
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
2:E:166:ARG:C	4:M:123:LYS:HE3	1.80	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: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
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: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:B:432:ASP:OD2	2:B:443:SER:C	2.15	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:E:169:ARG:NE	4:N:118:ASP:CG	2.34	0.85
2:B:169:ARG:NH2	4:N:119:TYR:CG	2.39	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:CA	4:M:123:LYS:HE3	2.10	0.82
2:E:166:ARG:HB3	4:M:123:LYS:HE3	1.61	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
2:E:169:ARG:NH1	4:M:119:TYR:O	1.95	0.77
4:M:109:GLU:HA	4:M:112:LEU:HG	1.66	0.77
3:C:108:ARG:NH2	4:M:117:GLN:CD	2.38	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
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
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.53	0.72
3:F:108:ARG:HB3	4:N:114:GLU:CD	2.14	0.72
4:M:126:THR:C	4:M:128:TRP:H	1.95	0.71
2:E:169:ARG:NE	4:N:118:ASP:CB	2.54	0.71
2:E:173:GLU:CD	4:M:116:GLN:CA	2.41	0.70
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: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
4:M:114:GLU:C	4:N:115:LEU:HD21	2.19	0.68
1:D:169:LEU:H	2:E:189:GLN:HE22	1.41	0.67
2:E:169:ARG:CD	4:N:118:ASP:CG	2.66	0.67
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:CB	4:M:123:LYS:HE3	2.13	0.66
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
3:C:264:MET:HE1	3:C:389:PHE:CD2	2.31	0.66
3:F:264:MET:HE1	3:F:389:PHE:CD2	2.31	0.65
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
4:M:112:LEU:N	4:M:112:LEU:HD23	2.13	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
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:173:GLU:CD	4:M:115:LEU:O	2.42	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
4:M:126:THR:C	4:M:128:TRP:N	2.58	0.59
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:128:TRP:C	4:M:130:ARG:H	2.12	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
4:N:106:LYS:O	4:N:106:LYS:HG3	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
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
2:E:169:ARG:HD2	4:N:118:ASP:CG	2.28	0.55
3:F:390:ASN:C	3:F:390:ASN:HD22	2.15	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
3:C:390:ASN:HD22	3:C:390:ASN:C	2.15	0.54
3:F:264:MET:HE2	3:F:264:MET:H	1.73	0.54
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.56	0.54
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:C:323:GLU:H	3:C:323:GLU:CD	2.17	0.53
3:F:249:GLU:CG	3:F:383:THR:HB	2.39	0.53
3:F:323:GLU:H	3:F:323:GLU:CD	2.17	0.53
2:E:173:GLU:CG	4:M:119:TYR:CE1	2.88	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:264:MET:HE2	3:C:264:MET:H	1.73	0.52
3:C:194:PHE:HB2	3:C:233:ILE:CD1	2.40	0.52
4:M:106:LYS:C	4:M:108:LEU:H	2.17	0.52
2:E:176:ARG:HH22	4:M:112:LEU:C	2.17	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
3:C:189:ASN:ND2	3:C:391:ARG:HE	2.06	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:284:ASN:C	2:E:284:ASN:HD22	2.20	0.50
4:M:122:ALA:C	4:M:126:THR:OG1	2.55	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
2:B:284:ASN:C	2:B:284:ASN:HD22	2.20	0.49
2:B:439:ASN:HD22	2:B:439:ASN:N	2.09	0.49
4:M:109:GLU:C	4:M:111:LYS:H	2.21	0.49
2:E:176:ARG:NH2	4:M:113:LYS:CA	2.77	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
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
2:B:238:VAL:HG21	2:B:250:THR:CG2	2.45	0.47
3:F:264:MET:HE2	3:F:264:MET:N	2.30	0.47
1:A:139:ASN:N	1:A:139:ASN:HD22	2.13	0.46
3:F:325:ASN:HD22	3:F:325:ASN:C	2.24	0.46
3:F:323:GLU:CD	3:F:323:GLU:N	2.74	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
3:C:323:GLU:CD	3:C:323:GLU:N	2.74	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: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:C:264:MET:HE2	3:C:264:MET:N	2.30	0.45
3:F:108:ARG:HB3	4:N:114:GLU:OE2	2.16	0.45
3:C:325:ASN:C	3:C:325:ASN:HD22	2.24	0.45
3:C:189:ASN:ND2	3:C:391:ARG:HH21	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:108:LEU:HA	4:N:111:LYS:HB2	1.99	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: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:98:LYS:C	4:M:102:GLU:HB2	2.44	0.43
2:E:230:ASP:HB3	2:E:233:VAL:HG23	2.00	0.42
4:M:113:LYS:HA	4:M:116:GLN:CD	2.45	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
3:C:318:ASP:OD1	3:C:318:ASP:C	2.63	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
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:C:183:GLU:HB3	3:C:191:TRP:HB2	2.03	0.41
2:E:241:ASP:OD1	2:E:241:ASP:C	2.64	0.41
2:B:432:ASP:CG	2:B:443:SER:HB3	2.30	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
4:N:128:TRP:O	4:N:129:ASP:C	2.62	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
3:F:318:ASP:C	3:F:318:ASP:OD1	2.63	0.40
2:B:241:ASP:OD1	2:B:241:ASP:C	2.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:N	2:B:439:ASN:ND2	2.69	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	36	72
2	E	296/328 (90%)	281 (95%)	14 (5%)	1 (0%)	36	72
3	C	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	18	56
3	F	286/319 (90%)	272 (95%)	12 (4%)	2 (1%)	18	56
4	M	35/102 (34%)	20 (57%)	12 (34%)	3 (9%)	0	9
4	N	34/102 (33%)	24 (71%)	9 (26%)	1 (3%)	3	23
All	All	1343/1672 (80%)	1248 (93%)	85 (6%)	10 (1%)	18	56

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 ⓘ

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%)	29	50
1	D	52/82 (63%)	50 (96%)	2 (4%)	29	50
2	B	256/286 (90%)	248 (97%)	8 (3%)	35	56
2	E	256/286 (90%)	248 (97%)	8 (3%)	35	56
3	C	242/267 (91%)	235 (97%)	7 (3%)	37	58
3	F	242/267 (91%)	235 (97%)	7 (3%)	37	58
4	M	34/89 (38%)	25 (74%)	9 (26%)	0	3
4	N	34/89 (38%)	24 (71%)	10 (29%)	0	2
All	All	1168/1448 (81%)	1115 (96%)	53 (4%)	24	46

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	158	ILE
2	B	171	ILE
2	B	210	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	227	ILE
2	B	253	GLN
2	B	284	ASN
2	B	376	SER
2	B	439	ASN
2	B	454	ILE
3	C	107	ILE
3	C	169	ILE
3	C	244	TYR
3	C	317	ASN
3	C	325	ASN
3	C	365	ASN
3	C	390	ASN
1	D	139	ASN
1	D	158	ILE
2	E	171	ILE
2	E	210	GLU
2	E	227	ILE
2	E	253	GLN
2	E	284	ASN
2	E	376	SER
2	E	439	ASN
2	E	454	ILE
3	F	107	ILE
3	F	169	ILE
3	F	244	TYR
3	F	317	ASN
3	F	325	ASN
3	F	365	ASN
3	F	390	ASN
4	M	99	GLN
4	M	101	LEU
4	M	110	THR
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	N	102	GLU
4	N	104	GLN
4	N	108	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	109	GLU
4	N	114	GLU
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 (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	184	GLN
2	B	164	ASN
2	B	189	GLN
2	B	202	ASN
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
2	B	382	ASN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	115	ASN
3	C	118	ASN
3	C	123	ASN
3	C	146	HIS
3	C	177	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	139	ASN
1	D	184	GLN
2	E	164	ASN
2	E	189	GLN
2	E	202	ASN
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	115	ASN
3	F	118	ASN
3	F	123	ASN
3	F	136	GLN
3	F	177	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
3	F	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	57/87 (65%)	2.15	29 (50%) 0 3	34, 65, 96, 97	0
1	D	57/87 (65%)	2.13	24 (42%) 0 4	34, 65, 96, 97	0
2	B	298/328 (90%)	1.63	98 (32%) 1 6	17, 32, 76, 102	0
2	E	298/328 (90%)	1.52	83 (27%) 1 8	17, 32, 76, 102	0
3	C	288/319 (90%)	1.51	83 (28%) 1 7	13, 20, 64, 100	0
3	F	288/319 (90%)	1.58	88 (30%) 1 7	13, 20, 64, 100	0
4	M	37/102 (36%)	2.90	24 (64%) 0 2	24, 37, 82, 116	0
4	N	36/102 (35%)	2.62	22 (61%) 0 2	21, 32, 70, 86	0
All	All	1359/1672 (81%)	1.67	451 (33%) 1 6	13, 28, 84, 116	0

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	419	GLY	20.6
2	B	273	PHE	15.1
1	D	185	LEU	13.1
2	B	207	SER	11.3
1	A	185	LEU	10.6
3	F	179	LEU	10.4
3	C	340	HIS	9.9
3	C	361	ASN	9.8
2	B	400	GLY	9.6
2	E	203	ILE	8.9
3	F	389	PHE	8.7
2	B	168	LEU	8.7
3	C	360	PRO	8.6
2	B	348	THR	8.5
3	C	305	THR	8.5
3	F	265	PHE	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	176	LYS	7.7
2	E	448	ARG	7.7
4	M	115	LEU	7.7
3	F	284	GLY	7.6
2	E	226	LEU	7.4
4	M	130	ARG	7.3
2	E	163	THR	7.2
2	E	323	LYS	7.1
1	A	137	GLN	7.0
4	N	100	ALA	6.9
3	F	237	SER	6.8
1	D	173	VAL	6.8
4	N	125	SER	6.8
4	N	105	ARG	6.8
4	M	96	LYS	6.8
2	E	287	GLY	6.7
4	N	108	LEU	6.7
4	M	97	ALA	6.5
2	B	433	ASP	6.5
3	F	344	LEU	6.5
3	C	341	ALA	6.5
2	E	262	PHE	6.3
2	B	404	TYR	6.1
2	B	399	GLY	6.1
2	E	221	THR	6.1
2	E	433	ASP	6.0
1	D	188	VAL	5.8
4	M	121	LEU	5.7
2	E	207	SER	5.7
2	B	206	VAL	5.7
1	A	134	GLN	5.6
3	C	137	GLU	5.6
2	E	223	GLU	5.6
3	C	307	HIS	5.5
2	E	325	HIS	5.5
2	B	210	GLU	5.4
3	F	298	ASP	5.4
2	B	319	GLY	5.4
2	B	452	MET	5.3
3	C	365	ASN	5.3
2	E	371	ASN	5.2
3	C	339	CYS	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	389	PHE	5.0
3	F	112	GLU	4.9
3	F	213	GLU	4.9
3	C	242	ILE	4.9
2	B	262	PHE	4.9
2	E	416	TYR	4.8
2	B	200	SER	4.8
2	B	227	ILE	4.8
3	C	353	THR	4.8
2	B	408	HIS	4.8
2	B	364	ASN	4.7
1	A	152	VAL	4.7
3	F	105	SER	4.7
2	B	415	ARG	4.7
1	D	152	VAL	4.6
3	F	274	TYR	4.6
2	E	399	GLY	4.6
2	B	347	GLY	4.6
2	E	237	ARG	4.6
1	A	140	VAL	4.6
4	N	106	LYS	4.6
3	F	173	LYS	4.5
4	M	101	LEU	4.5
3	C	112	GLU	4.5
4	M	112	LEU	4.5
3	F	209	ILE	4.5
2	B	251	VAL	4.5
3	F	174	ALA	4.5
2	B	237	ARG	4.4
3	F	107	ILE	4.4
4	M	129	ASP	4.4
1	A	190	ALA	4.4
1	D	134	GLN	4.4
2	B	180	GLN	4.4
2	E	255	ARG	4.4
2	E	272	GLY	4.4
3	F	392	LEU	4.4
2	E	273	PHE	4.3
3	C	136	GLN	4.3
1	A	141	ARG	4.3
3	F	267	VAL	4.3
2	B	357	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	270	GLU	4.2
2	B	254	ASN	4.2
4	M	111	LYS	4.2
4	M	110	THR	4.2
2	B	272	GLY	4.2
3	C	107	ILE	4.1
2	B	458	PHE	4.1
3	C	292	GLY	4.1
4	M	105	ARG	4.1
3	C	358	SER	4.1
4	M	118	ASP	4.1
2	B	243	ASN	4.1
1	D	189	ILE	4.1
2	B	226	LEU	4.0
2	E	254	ASN	4.0
2	B	292	TYR	4.0
2	B	203	ILE	4.0
2	E	186	VAL	4.0
2	B	345	TYR	4.0
3	F	180	VAL	4.0
2	E	421	GLN	3.9
4	N	111	LYS	3.9
2	B	346	ARG	3.9
4	M	100	ALA	3.9
1	A	144	LEU	3.9
3	C	148	ILE	3.9
4	N	128	TRP	3.9
2	E	312	ILE	3.9
3	C	177	GLN	3.9
1	A	183	LYS	3.9
1	A	163	GLY	3.9
3	C	132	GLU	3.9
1	D	187	GLN	3.8
3	F	309	GLY	3.8
2	E	443	SER	3.8
2	B	325	HIS	3.8
2	B	246	ASN	3.8
4	M	131	GLN	3.8
4	N	126	THR	3.8
2	E	311	LEU	3.8
1	D	178	TYR	3.8
1	D	144	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	3.7
4	N	129	ASP	3.7
3	F	308	ASN	3.7
3	C	105	SER	3.7
3	F	358	SER	3.6
2	E	340	ILE	3.6
2	B	403	TRP	3.6
2	E	329	PHE	3.6
2	E	205	VAL	3.6
3	F	111	GLN	3.6
3	F	277	THR	3.6
3	C	168	PHE	3.6
3	C	128	VAL	3.5
3	C	310	MET	3.5
3	F	353	THR	3.5
2	E	341	SER	3.5
3	F	276	LEU	3.5
3	C	391	ARG	3.5
3	C	266	LYS	3.5
3	C	239	GLN	3.5
3	F	249	GLU	3.5
3	C	304	PHE	3.5
4	M	127	SER	3.5
3	F	176	GLN	3.5
4	N	107	ASP	3.5
3	F	347	VAL	3.5
2	B	186	VAL	3.4
2	E	452	MET	3.4
3	C	111	GLN	3.4
3	F	177	GLN	3.4
2	E	457	PHE	3.4
3	F	297	ASP	3.4
3	F	223	THR	3.4
2	E	403	TRP	3.3
2	B	238	VAL	3.3
2	B	208	GLY	3.3
3	C	390	ASN	3.3
2	E	162	PRO	3.3
3	F	233	ILE	3.3
2	B	456	PRO	3.3
3	C	291	ASP	3.3
2	E	250	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	164	ASN	3.3
3	C	213	GLU	3.3
2	B	430	GLY	3.3
2	B	183	GLU	3.3
2	E	222	SER	3.3
2	B	252	ILE	3.3
2	B	421	GLN	3.3
4	N	101	LEU	3.3
2	E	200	SER	3.3
3	F	109	TYR	3.3
2	B	284	ASN	3.2
3	F	137	GLU	3.2
3	C	359	THR	3.2
1	D	137	GLN	3.2
2	B	402	TRP	3.2
2	B	440	TRP	3.2
3	C	297	ASP	3.2
2	B	294	LEU	3.2
1	A	142	ALA	3.2
3	C	338	LYS	3.2
2	E	412	PRO	3.2
2	E	177	SER	3.1
3	C	295	PHE	3.1
2	B	171	ILE	3.1
3	F	263	ALA	3.1
2	E	386	LEU	3.1
2	E	276	VAL	3.1
3	C	267	VAL	3.1
2	B	366	THR	3.1
3	C	214	GLY	3.1
1	A	154	ILE	3.1
3	C	109	TYR	3.0
3	C	205	LYS	3.0
2	B	412	PRO	3.0
3	F	160	GLY	3.0
3	C	329	GLN	3.0
3	F	293	PHE	3.0
3	C	392	LEU	3.0
1	A	157	LYS	3.0
2	E	293	TRP	3.0
2	B	278	THR	3.0
2	E	426	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	359	THR	3.0
3	F	266	LYS	3.0
2	B	279	ASN	3.0
2	B	333	ASN	3.0
1	D	190	ALA	3.0
1	D	184	GLN	3.0
2	B	165	LEU	2.9
3	C	284	GLY	2.9
2	E	307	PRO	2.9
3	C	173	LYS	2.9
2	E	376	SER	2.9
3	F	175	ASN	2.9
4	N	114	GLU	2.9
3	C	279	ALA	2.9
2	E	173	GLU	2.9
2	B	225	TYR	2.9
2	E	172	LEU	2.9
2	E	195	THR	2.9
1	D	151	GLU	2.9
4	N	123	LYS	2.9
1	A	178	TYR	2.9
3	C	368	ILE	2.9
3	C	147	ASP	2.9
3	C	121	ILE	2.9
2	E	224	MET	2.9
3	F	316	ASP	2.9
2	B	401	GLY	2.9
2	B	381	ASP	2.8
3	F	183	GLU	2.8
3	F	311	GLN	2.8
3	C	158	ASN	2.8
1	D	179	GLU	2.8
2	B	312	ILE	2.8
2	B	416	TYR	2.8
3	C	114	TYR	2.8
4	N	112	LEU	2.8
3	C	142	THR	2.8
3	C	379	MET	2.8
3	F	318	ASP	2.8
3	F	331	GLY	2.8
2	B	409	ALA	2.8
2	B	329	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	210	GLU	2.8
2	E	317	TRP	2.8
3	F	355	SER	2.8
3	F	339	CYS	2.8
2	B	264	ARG	2.8
3	F	280	TYR	2.8
4	N	104	GLN	2.8
2	B	211	CYS	2.7
3	F	362	GLY	2.7
1	A	150	LEU	2.7
2	E	324	ALA	2.7
4	M	99	GLN	2.7
3	C	106	SER	2.7
3	F	168	PHE	2.7
3	F	301	ASP	2.7
3	C	325	ASN	2.7
2	B	182	LEU	2.7
3	F	136	GLN	2.7
2	B	250	THR	2.7
3	C	288	ASP	2.7
4	N	102	GLU	2.7
3	C	193	VAL	2.7
3	F	208	TRP	2.7
1	A	189	ILE	2.7
2	B	455	ARG	2.7
4	N	103	ASP	2.7
2	B	263	GLY	2.7
2	B	161	ILE	2.7
4	N	131	GLN	2.7
2	B	395	SER	2.7
3	F	377	TYR	2.7
3	F	317	ASN	2.7
4	M	117	GLN	2.7
2	E	418	TRP	2.6
3	C	298	ASP	2.6
1	A	139	ASN	2.6
1	A	164	SER	2.6
3	C	169	ILE	2.6
2	E	314	MET	2.6
3	C	203	ASP	2.6
3	F	343	HIS	2.6
3	F	325	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	145	ILE	2.6
2	E	168	LEU	2.6
3	C	124	LEU	2.6
3	F	197	ARG	2.6
3	F	294	ASP	2.6
3	F	245	ALA	2.6
2	E	404	TYR	2.6
3	F	340	HIS	2.6
2	B	326	TYR	2.6
3	C	311	GLN	2.6
2	B	265	LYS	2.5
1	A	146	ASP	2.5
1	A	175	LEU	2.5
2	B	340	ILE	2.5
1	D	182	GLN	2.5
2	B	305	MET	2.5
3	F	363	TYR	2.5
2	B	268	PRO	2.5
3	C	357	ALA	2.5
2	B	398	ASP	2.5
3	C	362	GLY	2.5
4	N	133	LEU	2.5
2	B	407	CYS	2.5
2	B	324	ALA	2.5
3	C	241	ALA	2.5
1	A	138	LYS	2.5
1	D	157	LYS	2.5
2	B	217	LYS	2.5
1	D	135	LEU	2.5
2	E	393	GLN	2.5
4	M	102	GLU	2.5
2	E	235	PRO	2.5
2	E	202	ASN	2.5
2	E	408	HIS	2.5
3	F	228	LEU	2.4
3	F	300	SER	2.4
2	B	293	TRP	2.4
2	E	382	ASN	2.4
2	E	374	PHE	2.4
3	F	374	THR	2.4
1	A	188	VAL	2.4
2	B	361	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	299	PRO	2.4
1	A	135	LEU	2.4
3	F	341	ALA	2.4
2	E	219	GLY	2.4
2	B	431	THR	2.4
3	C	277	THR	2.4
4	M	104	GLN	2.4
2	B	170	SER	2.4
3	C	215	PHE	2.3
1	A	156	ILE	2.3
3	F	113	ILE	2.3
2	E	363	GLU	2.3
2	B	451	SER	2.3
2	B	313	GLU	2.3
3	F	230	ASN	2.3
4	M	116	GLN	2.3
3	C	257	THR	2.3
3	F	205	LYS	2.3
3	F	302	LYS	2.3
3	C	293	PHE	2.3
3	F	285	ASP	2.3
3	F	256	ARG	2.3
4	N	134	GLU	2.3
2	E	296	ASN	2.3
1	A	173	VAL	2.3
2	B	261	ASP	2.3
3	F	161	ALA	2.3
4	M	108	LEU	2.3
2	E	245	GLU	2.3
3	C	115	ASN	2.3
3	F	164	SER	2.3
2	B	428	LYS	2.3
2	B	375	PHE	2.2
2	E	171	ILE	2.2
1	A	158	ILE	2.2
3	F	262	TYR	2.2
2	B	449	LYS	2.2
1	D	166	SER	2.2
3	C	370	ALA	2.2
3	C	209	ILE	2.2
2	B	234	LYS	2.2
2	E	424	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	2.2
2	E	407	CYS	2.2
3	F	278	TYR	2.2
3	F	321	LYS	2.2
1	D	175	LEU	2.2
3	F	369	TRP	2.2
2	E	284	ASN	2.2
2	E	348	THR	2.2
1	D	162	ARG	2.2
2	E	381	ASP	2.2
1	D	148	LYS	2.2
2	B	323	LYS	2.2
2	B	441	LYS	2.2
3	F	201	SER	2.2
4	N	127	SER	2.2
2	E	454	ILE	2.1
3	F	242	ILE	2.1
3	C	371	THR	2.1
3	F	257	THR	2.1
3	F	264	MET	2.1
2	E	456	PRO	2.1
1	D	150	LEU	2.1
3	C	363	TYR	2.1
3	F	271	ALA	2.1
1	D	183	LYS	2.1
3	C	388	PRO	2.1
2	E	436	VAL	2.1
2	B	426	MET	2.1
3	F	238	THR	2.1
3	C	246	LEU	2.1
3	C	280	TYR	2.1
2	B	350	GLY	2.1
2	B	434	GLY	2.1
4	M	106	LYS	2.1
2	E	256	GLN	2.1
2	E	165	LEU	2.1
3	C	125	LYS	2.1
2	E	243	ASN	2.1
3	C	355	SER	2.1
4	M	125	SER	2.1
3	C	179	LEU	2.0
2	E	225	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	245	ALA	2.0
3	C	118	ASN	2.0
3	F	350	GLN	2.0
2	E	166	ARG	2.0
2	E	277	ALA	2.0
1	A	186	GLU	2.0
3	C	375	ARG	2.0
2	E	449	LYS	2.0
3	F	181	TYR	2.0
4	N	122	ALA	2.0
2	B	162	PRO	2.0
2	B	435	VAL	2.0
2	B	220	GLU	2.0
2	E	234	LYS	2.0
4	M	126	THR	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.