



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 12:30 AM EDT

PDB ID : 4JFB
Title : Crystal structure of OmpF in C2 with tNCS
Authors : Wiseman, B.; Kilburg, A.; Chaptal, V.; Reyes-Meija, G.C.; Sarwan, J.; Falson, P.; Jault, J.M.
Deposited on : unknown
Resolution : 3.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

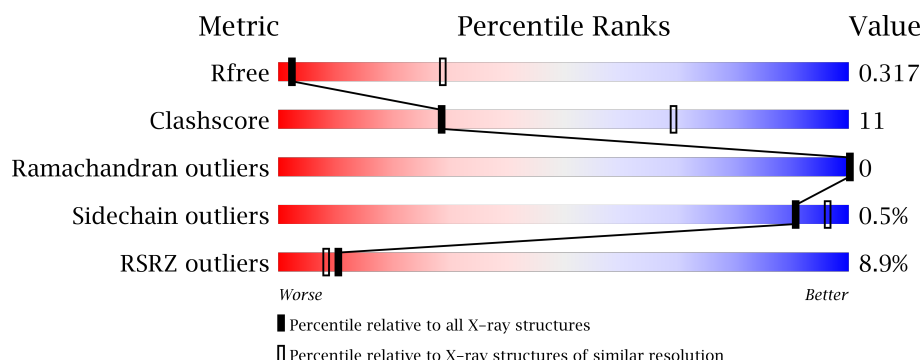
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	340	<div> <div>2%</div> <div>79%</div> <div>21%</div> </div>
1	B	340	<div> <div>4%</div> <div>78%</div> <div>22%</div> </div>
1	C	340	<div> <div>5%</div> <div>74%</div> <div>26%</div> </div>
1	D	340	<div> <div>12%</div> <div>76%</div> <div>23%</div> </div>
1	E	340	<div> <div>19%</div> <div>75%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	340	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '10%', a green segment in the middle labeled '73%', and a yellow segment at the end labeled '27%'.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15765 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.

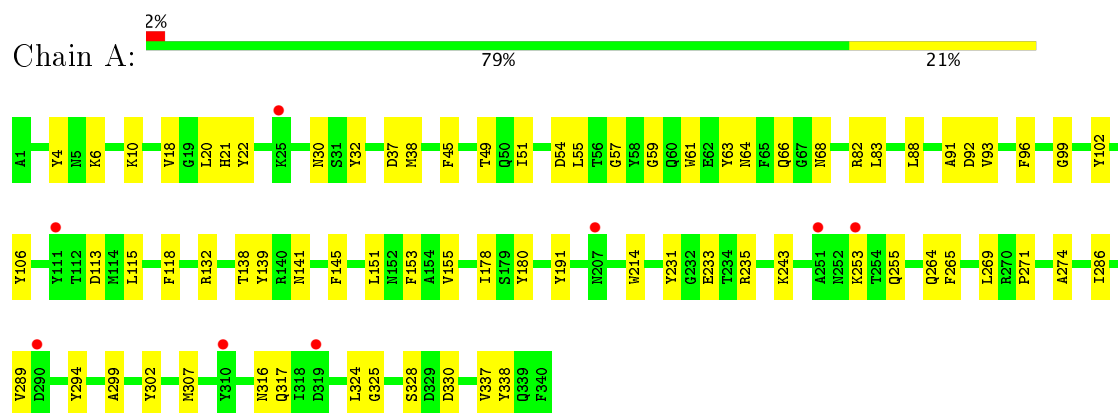
- Molecule 1 is a protein called Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	1	0
			2630	1656	438	533	3			
1	F	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

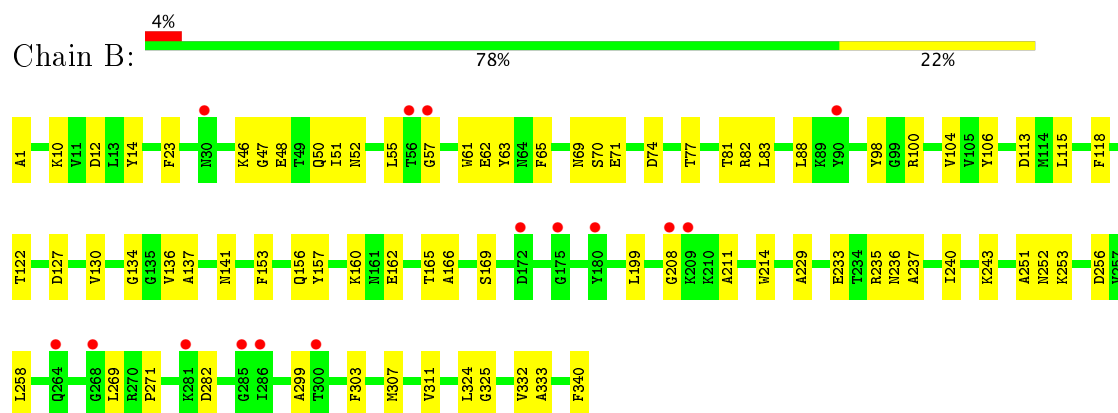
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

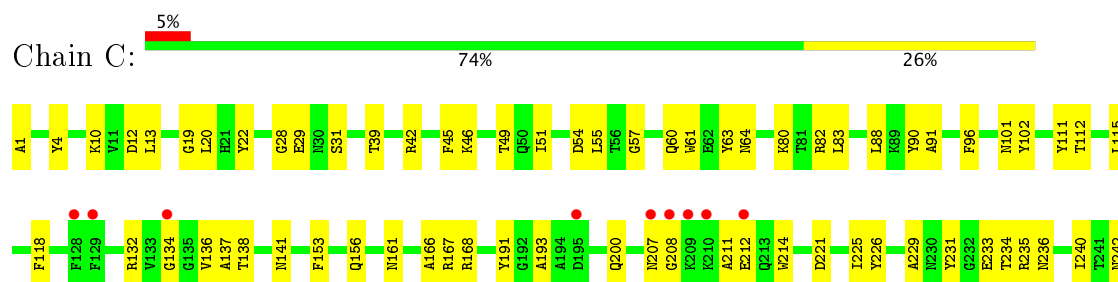
• Molecule 1: Outer membrane protein F

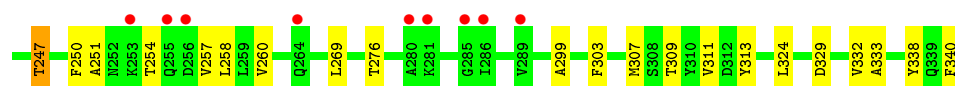


• Molecule 1: Outer membrane protein F

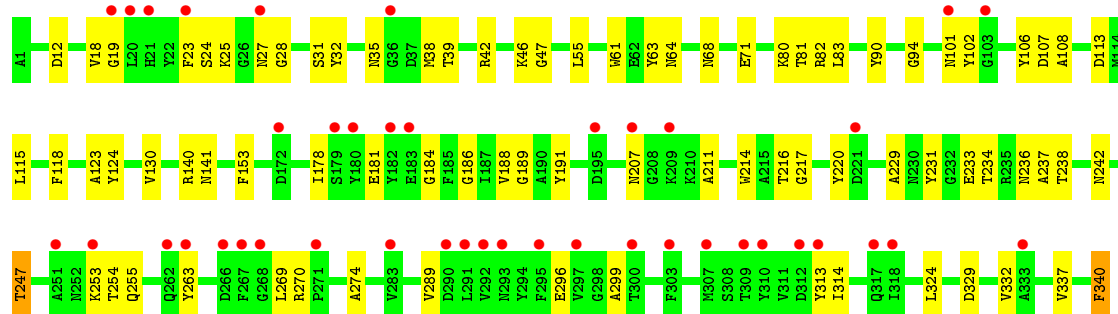
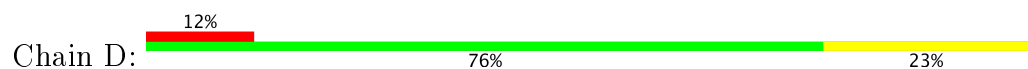


• Molecule 1: Outer membrane protein F

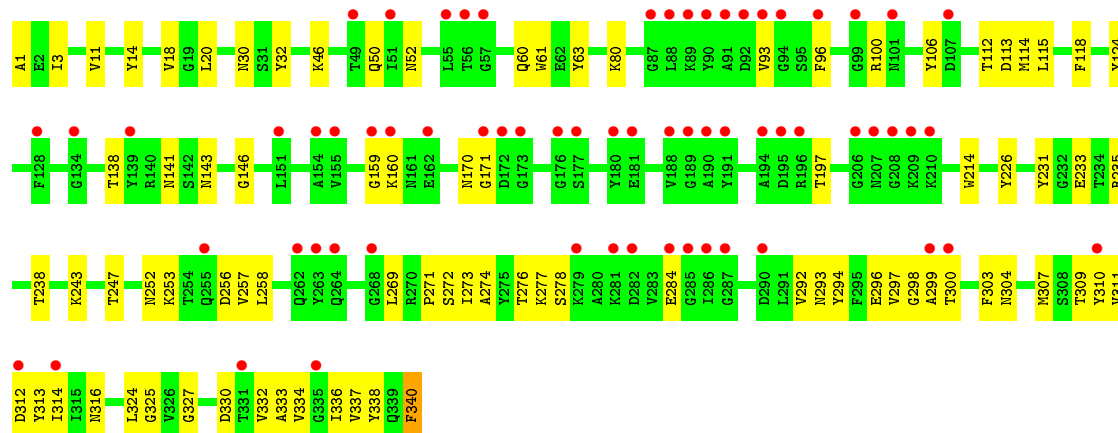
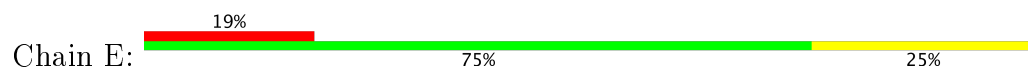




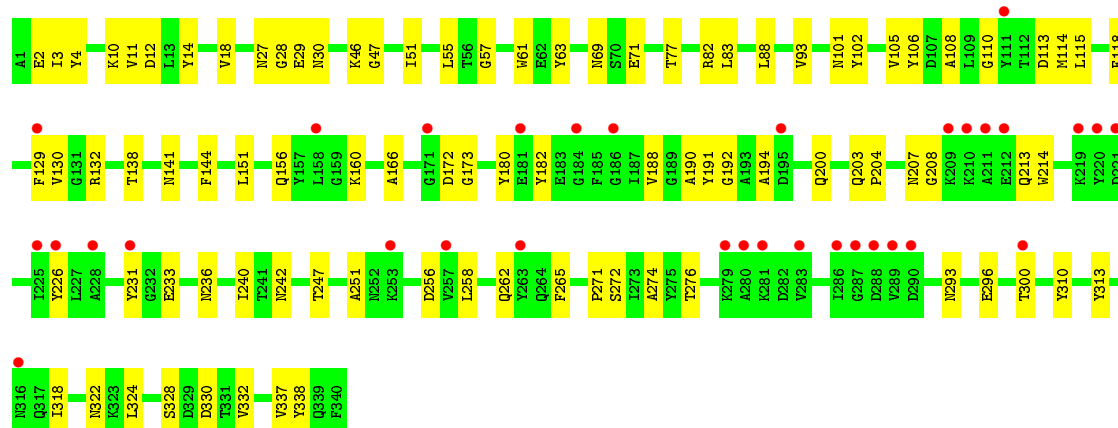
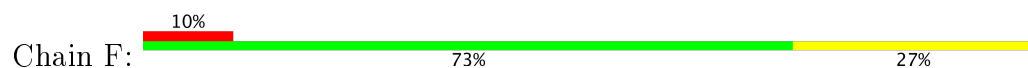
• Molecule 1: Outer membrane protein F



• Molecule 1: Outer membrane protein F



• Molecule 1: Outer membrane protein F



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.91Å 110.88Å 226.14Å 90.00° 104.46° 90.00°	Depositor
Resolution (Å)	68.57 – 3.80 78.39 – 3.80	Depositor EDS
% Data completeness (in resolution range)	83.3 (68.57-3.80) 83.6 (78.39-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.262 , 0.314 0.258 , 0.317	Depositor DCC
R_{free} test set	1582 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	15765	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.85 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4444e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.37	0/2683	0.59	0/3628
1	B	0.36	0/2683	0.59	0/3628
1	C	0.37	0/2683	0.59	0/3628
1	D	0.32	0/2683	0.54	0/3628
1	E	0.32	0/2690	0.53	0/3638
1	F	0.35	0/2683	0.55	0/3628
All	All	0.35	0/16105	0.56	0/21778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2627	0	2444	62	0
1	B	2627	0	2444	50	0
1	C	2627	0	2444	67	0
1	D	2627	0	2444	67	0
1	E	2630	0	2447	57	0
1	F	2627	0	2444	60	0
All	All	15765	0	14667	336	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 11.

All (336) 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:E:118:PHE:HD2	1:E:312:ASP:OD2	1.26	1.15
1:E:118:PHE:CD2	1:E:312:ASP:OD2	2.05	1.08
1:D:27:ASN:O	1:D:35:ASN:HB3	1.61	1.01
1:B:100:ARG:HG2	1:B:134:GLY:HA2	1.53	0.89
1:E:309:THR:HG22	1:E:336:ILE:HG12	1.57	0.87
1:A:99:GLY:HA2	1:C:39:THR:HG21	1.58	0.86
1:E:160:LYS:HG3	1:E:171:GLY:HA2	1.57	0.85
1:D:27:ASN:O	1:D:35:ASN:CB	2.25	0.85
1:D:27:ASN:C	1:D:35:ASN:HB3	1.98	0.84
1:D:25:LYS:HD2	1:D:329:ASP:CG	1.99	0.83
1:D:25:LYS:HD2	1:D:329:ASP:OD2	1.77	0.83
1:D:27:ASN:N	1:D:28:GLY:HA2	1.95	0.79
1:F:27:ASN:HB2	1:F:29:GLU:H	1.47	0.79
1:D:27:ASN:O	1:D:35:ASN:N	2.17	0.78
1:B:23:PHE:HB2	1:B:332:VAL:HB	1.66	0.76
1:D:27:ASN:O	1:D:35:ASN:CA	2.34	0.76
1:E:309:THR:CG2	1:E:336:ILE:HG12	2.17	0.74
1:B:69:ASN:ND2	1:B:77:THR:O	2.17	0.71
1:E:93:VAL:O	1:E:141:ASN:ND2	2.24	0.70
1:A:151:LEU:HD13	1:A:180:TYR:CE2	2.27	0.70
1:A:64:ASN:HB2	1:A:82:ARG:HD2	1.72	0.69
1:B:166:ALA:HB2	1:B:199:LEU:HG	1.75	0.68
1:B:141:ASN:ND2	1:B:153:PHE:CZ	2.53	0.68
1:C:29:GLU:C	1:C:31:SER:H	1.97	0.67
1:C:54:ASP:HB3	1:C:91:ALA:HB2	1.74	0.67
1:F:207:ASN:O	1:F:236:ASN:ND2	2.27	0.67
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.61	0.66
1:D:269:LEU:HD11	1:D:299:ALA:HB1	1.76	0.65
1:C:313:TYR:CD1	1:C:332:VAL:HG22	2.32	0.65
1:F:242:ASN:HB3	1:F:247:THR:HG22	1.78	0.65
1:E:272:SER:N	1:E:298:GLY:O	2.25	0.64
1:F:69:ASN:ND2	1:F:77:THR:O	2.21	0.64
1:A:64:ASN:ND2	1:A:66:GLN:OE1	2.30	0.64
1:D:141:ASN:HB3	1:D:153:PHE:CE1	2.34	0.63
1:C:83:LEU:HD11	1:C:102:TYR:HE1	1.63	0.63
1:A:269:LEU:HG	1:A:271:PRO:HD3	1.80	0.63
1:A:141:ASN:HB3	1:A:153:PHE:CE1	2.33	0.62
1:A:286:ILE:HG21	1:A:289:VAL:HG21	1.81	0.62
1:A:253:LYS:HE3	1:A:255:GLN:HE21	1.64	0.62
1:C:64:ASN:HB2	1:C:82:ARG:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:LEU:HD11	1:E:299:ALA:HB1	1.82	0.62
1:E:14:TYR:CE1	1:E:46:LYS:HG3	2.35	0.61
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.36	0.60
1:A:93:VAL:O	1:A:141:ASN:ND2	2.34	0.60
1:C:234:THR:OG1	1:C:254:THR:OG1	2.17	0.60
1:F:27:ASN:HB2	1:F:29:GLU:N	2.14	0.60
1:F:27:ASN:N	1:F:28:GLY:HA2	2.16	0.60
1:A:307:MET:HG2	1:B:88:LEU:HD21	1.84	0.60
1:C:31:SER:HA	1:C:329:ASP:HB2	1.83	0.59
1:B:1:ALA:HB1	1:C:4:TYR:CD1	2.37	0.59
1:C:28:GLY:O	1:C:31:SER:OG	2.16	0.59
1:D:24:SER:HB2	1:D:35:ASN:HB2	1.83	0.59
1:D:38:MET:HA	1:D:68:ASN:HD22	1.67	0.59
1:F:93:VAL:O	1:F:141:ASN:ND2	2.35	0.59
1:B:106:TYR:OH	1:B:113:ASP:OD2	2.18	0.59
1:E:300:THR:HG23	1:E:310:TYR:HB3	1.85	0.59
1:E:3:ILE:HG21	1:F:3:ILE:HD12	1.85	0.59
1:D:274:ALA:HB3	1:D:296:GLU:HB3	1.85	0.58
1:C:1:ALA:N	1:C:12:ASP:OD1	2.32	0.58
1:D:25:LYS:CD	1:D:329:ASP:OD2	2.49	0.58
1:C:19:GLY:HA2	1:C:39:THR:HG22	1.84	0.57
1:F:106:TYR:O	1:F:110:GLY:N	2.35	0.57
1:A:49:THR:HG21	1:C:307:MET:HB2	1.86	0.57
1:D:12:ASP:OD1	1:D:46:LYS:HB3	2.05	0.57
1:A:51:ILE:HD12	1:A:55:LEU:HG	1.86	0.57
1:E:274:ALA:HB3	1:E:296:GLU:HB3	1.86	0.57
1:E:214:TRP:NE1	1:E:233:GLU:HB2	2.20	0.57
1:E:277:LYS:HA	1:E:292:VAL:O	2.04	0.57
1:A:4:TYR:CE1	1:A:6:LYS:HB3	2.39	0.57
1:B:70:SER:OG	1:B:74:ASP:OD1	2.11	0.56
1:E:313:TYR:CD1	1:E:332:VAL:HG22	2.40	0.56
1:F:160:LYS:N	1:F:172:ASP:OD1	2.38	0.56
1:C:101:ASN:OD1	1:C:102:TYR:N	2.37	0.56
1:D:106:TYR:OH	1:D:113:ASP:OD2	2.17	0.56
1:F:27:ASN:H	1:F:28:GLY:HA2	1.69	0.56
1:F:313:TYR:CD1	1:F:332:VAL:HG22	2.39	0.56
1:C:29:GLU:C	1:C:31:SER:N	2.59	0.56
1:C:55:LEU:HD13	1:C:90:TYR:HD1	1.69	0.56
1:D:63:TYR:HD1	1:D:81:THR:HA	1.71	0.56
1:B:141:ASN:HD22	1:B:153:PHE:HZ	1.44	0.55
1:E:269:LEU:HG	1:E:271:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASN:C	1:D:35:ASN:CB	2.70	0.55
1:E:124:TYR:HE2	1:E:238:THR:HG23	1.72	0.55
1:F:300:THR:HG23	1:F:310:TYR:HB3	1.88	0.55
1:C:212:GLU:HB2	1:C:235:ARG:HB2	1.88	0.55
1:E:316:ASN:N	1:E:330:ASP:OD1	2.38	0.55
1:A:37:ASP:OD1	1:B:98:TYR:OH	2.23	0.55
1:C:28:GLY:O	1:C:31:SER:CB	2.54	0.55
1:B:1:ALA:HB1	1:C:4:TYR:CG	2.41	0.55
1:D:80:LYS:HD3	1:F:71:GLU:HB3	1.88	0.55
1:D:24:SER:N	1:D:35:ASN:OD1	2.25	0.54
1:D:340:PHE:CD2	1:E:11:VAL:HG21	2.42	0.54
1:E:114:MET:HG3	1:E:226:TYR:CE2	2.43	0.54
1:A:57:GLY:HA2	1:A:88:LEU:HD23	1.89	0.54
1:A:32:TYR:HB2	1:A:316:ASN:HD21	1.71	0.54
1:E:231:TYR:HD1	1:E:257:VAL:HG22	1.73	0.54
1:A:59:GLY:HA3	1:C:338:TYR:HB3	1.90	0.54
1:B:269:LEU:HD11	1:B:299:ALA:HB1	1.89	0.54
1:D:101:ASN:OD1	1:D:102:TYR:N	2.39	0.54
1:D:42:ARG:NE	1:D:64:ASN:OD1	2.38	0.54
1:F:274:ALA:HB3	1:F:296:GLU:HB3	1.89	0.54
1:C:207:ASN:O	1:C:236:ASN:ND2	2.40	0.53
1:D:253:LYS:HE3	1:D:255:GLN:HE21	1.73	0.53
1:C:12:ASP:HB3	1:C:46:LYS:HB2	1.89	0.53
1:B:57:GLY:HA2	1:B:88:LEU:HD23	1.91	0.53
1:B:63:TYR:HD2	1:B:65:PHE:CE2	2.27	0.53
1:F:83:LEU:HD11	1:F:102:TYR:HE1	1.73	0.53
1:C:214:TRP:NE1	1:C:233:GLU:HB2	2.23	0.53
1:E:106:TYR:OH	1:E:113:ASP:OD2	2.24	0.53
1:D:207:ASN:O	1:D:236:ASN:ND2	2.41	0.53
1:A:30:ASN:ND2	1:A:328:SER:OG	2.42	0.53
1:B:214:TRP:NE1	1:B:233:GLU:HB2	2.23	0.53
1:E:159:GLY:O	1:E:170:ASN:ND2	2.43	0.52
1:B:307:MET:HB2	1:C:49:THR:HG21	1.92	0.52
1:E:256:ASP:OD1	1:E:278:SER:OG	2.19	0.52
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.45	0.52
1:A:139:TYR:HD2	1:A:155:VAL:HG12	1.74	0.52
1:B:50:GLN:NE2	1:B:52:ASN:O	2.33	0.52
1:B:208:GLY:HA3	1:B:236:ASN:ND2	2.25	0.52
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.45	0.52
1:D:189:GLY:HA2	1:D:216:THR:HG22	1.91	0.51
1:F:114:MET:HG3	1:F:226:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:VAL:HG22	1:F:337:VAL:HG22	1.92	0.51
1:A:115:LEU:HD21	1:A:274:ALA:HB2	1.91	0.51
1:B:160:LYS:NZ	1:B:162:GLU:OE2	2.25	0.51
1:F:138:THR:OG1	1:F:156:GLN:NE2	2.40	0.51
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.46	0.51
1:E:303:PHE:HB2	1:E:307:MET:HB3	1.93	0.51
1:A:286:ILE:CG2	1:A:289:VAL:HG21	2.39	0.51
1:B:340:PHE:HE2	1:C:45:PHE:CD1	2.29	0.51
1:A:45:PHE:CD1	1:C:340:PHE:HE2	2.28	0.51
1:D:27:ASN:N	1:D:28:GLY:CA	2.73	0.51
1:E:311:VAL:HA	1:E:333:ALA:O	2.11	0.51
1:D:108:ALA:HA	1:D:188:VAL:HG11	1.93	0.50
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.93	0.50
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.93	0.50
1:A:83:LEU:HD11	1:A:102:TYR:HE1	1.77	0.50
1:C:115:LEU:HB2	1:C:118:PHE:O	2.11	0.50
1:D:211:ALA:HB1	1:D:237:ALA:HB2	1.94	0.50
1:F:101:ASN:OD1	1:F:102:TYR:N	2.40	0.50
1:A:286:ILE:CG2	1:A:289:VAL:CG2	2.89	0.50
1:A:61:TRP:HZ2	1:A:63:TYR:HD2	1.60	0.50
1:E:243:LYS:HD2	1:E:325:GLY:O	2.12	0.50
1:D:47:GLY:HA3	1:F:338:TYR:CE2	2.46	0.50
1:E:160:LYS:HE2	1:E:197:THR:HG22	1.93	0.50
1:A:253:LYS:HE3	1:A:255:GLN:NE2	2.25	0.49
1:A:30:ASN:O	1:A:328:SER:N	2.44	0.49
1:F:57:GLY:HA2	1:F:88:LEU:HD23	1.93	0.49
1:E:112:THR:HG21	1:E:258:LEU:HB2	1.94	0.49
1:E:235:ARG:HD3	1:E:253:LYS:HG2	1.94	0.49
1:E:273:ILE:HA	1:E:296:GLU:O	2.12	0.49
1:B:243:LYS:HD2	1:B:325:GLY:O	2.13	0.49
1:D:82:ARG:HA	1:F:71:GLU:OE2	2.12	0.49
1:A:38:MET:HA	1:A:68:ASN:HD22	1.77	0.49
1:C:20:LEU:H	1:C:39:THR:HG22	1.78	0.49
1:A:264:GLN:HE22	1:A:302:TYR:HD2	1.59	0.49
1:F:214:TRP:NE1	1:F:233:GLU:HB2	2.28	0.49
1:A:243:LYS:HD2	1:A:325:GLY:O	2.12	0.49
1:A:338:TYR:CE2	1:B:47:GLY:HA3	2.47	0.49
1:D:231:TYR:OH	1:D:233:GLU:OE2	2.29	0.49
1:A:235:ARG:HE	1:A:253:LYS:HG3	1.77	0.48
1:B:165:THR:O	1:B:169:SER:OG	2.20	0.48
1:E:46:LYS:HG2	1:E:60:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASN:HA	1:C:324:LEU:HD22	1.95	0.48
1:B:252:ASN:HB3	1:B:282:ASP:HB2	1.94	0.48
1:E:340:PHE:CD2	1:F:11:VAL:HG21	2.48	0.48
1:F:115:LEU:HB2	1:F:118:PHE:O	2.14	0.48
1:C:111:TYR:O	1:C:226:TYR:OH	2.23	0.48
1:D:289:VAL:HG21	1:D:324:LEU:HG	1.96	0.48
1:D:83:LEU:HD21	1:D:102:TYR:CD1	2.49	0.48
1:D:83:LEU:HD21	1:D:102:TYR:CE1	2.48	0.48
1:D:253:LYS:HE3	1:D:255:GLN:NE2	2.29	0.48
1:A:18:VAL:HG12	1:A:20:LEU:HB2	1.95	0.48
1:A:269:LEU:HD11	1:A:299:ALA:HB1	1.96	0.48
1:F:105:VAL:HA	1:F:190:ALA:HB1	1.95	0.47
1:B:51:ILE:HD12	1:B:55:LEU:HG	1.96	0.47
1:D:18:VAL:HG22	1:D:337:VAL:HG22	1.95	0.47
1:E:115:LEU:HB2	1:E:118:PHE:O	2.15	0.47
1:C:311:VAL:HA	1:C:333:ALA:O	2.14	0.47
1:A:51:ILE:HD13	1:C:303:PHE:HB3	1.96	0.47
1:E:143:ASN:HB2	1:E:146:GLY:HA2	1.96	0.47
1:F:313:TYR:OH	1:F:330:ASP:OD2	2.31	0.47
1:D:80:LYS:HB2	1:F:71:GLU:HG2	1.96	0.47
1:C:242:ASN:HB3	1:C:247:THR:HG22	1.97	0.47
1:D:191:TYR:HD1	1:D:214:TRP:HB3	1.78	0.47
1:F:166:ALA:HB1	1:F:200:GLN:HG2	1.97	0.47
1:A:22:TYR:CD1	1:A:38:MET:HG3	2.50	0.47
1:F:129:PHE:CD2	1:F:192:GLY:HA3	2.50	0.47
1:B:14:TYR:CE1	1:B:46:LYS:HG3	2.50	0.46
1:C:45:PHE:O	1:C:60:GLN:HG3	2.15	0.46
1:E:307:MET:SD	1:F:57:GLY:HA3	2.55	0.46
1:C:102:TYR:HA	1:C:132:ARG:HA	1.97	0.46
1:C:96:PHE:CZ	1:C:137:ALA:HB1	2.50	0.46
1:B:115:LEU:HB2	1:B:118:PHE:O	2.16	0.46
1:C:96:PHE:HA	1:C:138:THR:O	2.15	0.46
1:F:51:ILE:HD12	1:F:55:LEU:HG	1.97	0.46
1:C:82:ARG:O	1:C:132:ARG:HD2	2.15	0.46
1:C:208:GLY:HA3	1:C:236:ASN:ND2	2.30	0.46
1:B:303:PHE:HB2	1:B:307:MET:HB3	1.98	0.46
1:D:32:TYR:HE2	1:D:118:PHE:CD1	2.34	0.46
1:A:289:VAL:HG11	1:A:324:LEU:HG	1.98	0.46
1:B:235:ARG:HD3	1:B:253:LYS:HG2	1.98	0.46
1:B:61:TRP:HA	1:B:83:LEU:O	2.16	0.46
1:F:318:ILE:HD12	1:F:322:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:TYR:HE2	1:C:340:PHE:HD2	1.63	0.46
1:C:240:ILE:HD13	1:C:251:ALA:HB2	1.98	0.45
1:F:108:ALA:HA	1:F:188:VAL:HG11	1.97	0.45
1:A:243:LYS:HB2	1:A:325:GLY:HA3	1.98	0.45
1:B:63:TYR:HD1	1:B:81:THR:HA	1.82	0.45
1:C:51:ILE:HD12	1:C:55:LEU:HG	1.99	0.45
1:F:208:GLY:HA3	1:F:236:ASN:ND2	2.32	0.45
1:B:104:VAL:N	1:B:156:GLN:OE1	2.46	0.45
1:D:32:TYR:CE2	1:D:314:ILE:HG13	2.52	0.45
1:E:96:PHE:HA	1:E:138:THR:O	2.16	0.45
1:F:144:PHE:N	1:F:151:LEU:O	2.49	0.45
1:B:269:LEU:HG	1:B:271:PRO:HD3	1.98	0.45
1:D:242:ASN:HB3	1:D:247:THR:HG22	1.99	0.45
1:E:294:TYR:CE1	1:E:314:ILE:HD12	2.51	0.45
1:A:22:TYR:HE2	1:A:118:PHE:CE1	2.35	0.45
1:B:1:ALA:N	1:B:12:ASP:OD1	2.35	0.45
1:C:83:LEU:HD11	1:C:102:TYR:CE1	2.48	0.45
1:D:31:SER:HA	1:D:329:ASP:HB2	1.98	0.45
1:F:166:ALA:HB1	1:F:200:GLN:HA	1.99	0.45
1:B:127:ASP:O	1:B:130:VAL:HG22	2.17	0.44
1:D:181:GLU:HG2	1:D:186:GLY:HA2	1.99	0.44
1:A:92:ASP:O	1:A:145:PHE:HA	2.17	0.44
1:A:294:TYR:HA	1:A:317:GLN:HG2	1.98	0.44
1:D:107:ASP:CG	1:D:140:ARG:HH12	2.21	0.44
1:D:42:ARG:HD3	1:D:64:ASN:HA	1.98	0.44
1:F:30:ASN:O	1:F:328:SER:N	2.50	0.44
1:C:231:TYR:HD1	1:C:257:VAL:HG22	1.82	0.44
1:C:258:LEU:HG	1:C:276:THR:HG23	1.98	0.44
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.83	0.44
1:F:106:TYR:OH	1:F:113:ASP:OD2	2.35	0.44
1:F:265:PHE:HE2	1:F:271:PRO:HG3	1.81	0.44
1:F:231:TYR:HA	1:F:256:ASP:O	2.17	0.44
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.52	0.44
1:D:27:ASN:O	1:D:35:ASN:O	2.35	0.44
1:A:265:PHE:HE2	1:A:271:PRO:HG3	1.81	0.44
1:E:252:ASN:ND2	1:E:284:GLU:OE2	2.50	0.43
1:A:10:LYS:HB3	1:A:10:LYS:HE2	1.86	0.43
1:E:338:TYR:OH	1:F:47:GLY:HA3	2.18	0.43
1:E:258:LEU:HG	1:E:276:THR:HG23	2.00	0.43
1:E:276:THR:O	1:E:293:ASN:HA	2.18	0.43
1:F:262:GLN:HG2	1:F:272:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:O	1:A:132:ARG:HD2	2.19	0.43
1:B:160:LYS:HE2	1:B:162:GLU:HG3	2.01	0.43
1:C:42:ARG:HD3	1:C:64:ASN:HA	1.99	0.43
1:D:313:TYR:HD1	1:D:332:VAL:HG22	1.83	0.43
1:E:309:THR:HG22	1:E:336:ILE:CG1	2.40	0.43
1:D:217:GLY:HA2	1:D:229:ALA:O	2.19	0.43
1:D:313:TYR:CD1	1:D:332:VAL:HG22	2.53	0.43
1:D:71:GLU:HG3	1:E:100:ARG:NH2	2.33	0.43
1:F:82:ARG:O	1:F:132:ARG:HD2	2.19	0.43
1:A:307:MET:SD	1:A:338:TYR:HB2	2.58	0.43
1:D:18:VAL:HG22	1:D:337:VAL:HG13	2.00	0.43
1:E:50:GLN:NE2	1:E:52:ASN:O	2.37	0.43
1:A:4:TYR:HE1	1:A:6:LYS:HB3	1.84	0.43
1:F:105:VAL:HA	1:F:190:ALA:CB	2.49	0.43
1:B:62:GLU:O	1:B:82:ARG:N	2.47	0.43
1:D:141:ASN:HB3	1:D:153:PHE:HE1	1.79	0.43
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.53	0.42
1:C:191:TYR:HD1	1:C:214:TRP:HB3	1.84	0.42
1:C:20:LEU:HD21	1:C:22:TYR:HE1	1.84	0.42
1:F:180:TYR:CE2	1:F:182:TYR:HB2	2.54	0.42
1:A:286:ILE:HG22	1:A:289:VAL:CG2	2.49	0.42
1:A:54:ASP:HB3	1:A:91:ALA:HB2	2.01	0.42
1:D:184:GLY:O	1:D:220:TYR:HA	2.19	0.42
1:D:234:THR:OG1	1:D:254:THR:OG1	2.19	0.42
1:D:123:ALA:HA	1:D:130:VAL:O	2.20	0.42
1:C:138:THR:OG1	1:C:156:GLN:NE2	2.52	0.42
1:C:134:GLY:O	1:C:161:ASN:ND2	2.52	0.42
1:F:130:VAL:HG13	1:F:213:GLN:CD	2.39	0.42
1:B:71:GLU:HB2	1:C:168:ARG:HH12	1.84	0.42
1:E:324:LEU:HA	1:E:324:LEU:HD23	1.94	0.42
1:A:316:ASN:HD22	1:A:330:ASP:HA	1.84	0.42
1:D:55:LEU:HD13	1:D:90:TYR:HD1	1.85	0.42
1:E:304:ASN:ND2	1:F:51:ILE:HA	2.34	0.42
1:D:115:LEU:HB2	1:D:118:PHE:O	2.19	0.42
1:E:309:THR:HG22	1:E:336:ILE:HG23	2.02	0.42
1:B:122:THR:HG21	1:B:256:ASP:HB3	2.01	0.42
1:E:311:VAL:HG22	1:E:334:VAL:HG22	2.00	0.42
1:A:106:TYR:OH	1:A:113:ASP:OD2	2.33	0.42
1:B:311:VAL:HA	1:B:333:ALA:O	2.20	0.42
1:C:193:ALA:HA	1:C:211:ALA:O	2.20	0.42
1:D:124:TYR:HE2	1:D:238:THR:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD11	1:C:299:ALA:HB1	2.02	0.42
1:C:1:ALA:O	1:C:13:LEU:N	2.53	0.41
1:C:57:GLY:HA2	1:C:88:LEU:HD23	2.02	0.41
1:F:2:GLU:OE1	1:F:10:LYS:HD2	2.20	0.41
1:A:21:HIS:HD2	1:A:22:TYR:O	2.02	0.41
1:A:32:TYR:HE2	1:A:118:PHE:CD1	2.38	0.41
1:D:263:TYR:O	1:D:270:ARG:HA	2.20	0.41
1:D:19:GLY:HA2	1:D:39:THR:HG23	2.01	0.41
1:E:32:TYR:HE2	1:E:118:PHE:CD1	2.38	0.41
1:F:191:TYR:HD1	1:F:214:TRP:HB3	1.84	0.41
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.92	0.41
1:F:258:LEU:HG	1:F:276:THR:HG23	2.02	0.41
1:B:137:ALA:HB3	1:B:157:TYR:HB3	2.01	0.41
1:C:4:TYR:O	1:C:10:LYS:HA	2.20	0.41
1:C:166:ALA:HB1	1:C:200:GLN:HA	2.02	0.41
1:A:153:PHE:HB2	1:A:178:ILE:HG12	2.03	0.41
1:A:231:TYR:OH	1:A:233:GLU:OE2	2.39	0.41
1:E:80:LYS:HE2	1:E:80:LYS:HB3	1.93	0.41
1:F:14:TYR:CE1	1:F:46:LYS:HG3	2.55	0.41
1:A:18:VAL:HG22	1:A:337:VAL:HG22	2.02	0.41
1:B:229:ALA:HA	1:B:258:LEU:O	2.21	0.41
1:A:18:VAL:HG13	1:A:337:VAL:HG22	2.02	0.41
1:D:94:GLY:CA	1:D:141:ASN:HD22	2.34	0.41
1:D:63:TYR:CD1	1:D:81:THR:HA	2.54	0.41
1:E:294:TYR:CD1	1:E:314:ILE:HG23	2.55	0.41
1:A:96:PHE:HA	1:A:138:THR:O	2.21	0.41
1:B:136:VAL:HA	1:B:157:TYR:O	2.20	0.41
1:C:221:ASP:HA	1:C:225:ILE:O	2.21	0.41
1:F:173:GLY:HA3	1:F:194:ALA:HB2	2.02	0.41
1:B:71:GLU:HB3	1:C:80:LYS:HD2	2.02	0.41
1:C:229:ALA:HA	1:C:258:LEU:O	2.21	0.41
1:E:1:ALA:HB1	1:F:4:TYR:CD2	2.55	0.41
1:A:21:HIS:HD2	1:A:22:TYR:N	2.19	0.40
1:B:211:ALA:HB1	1:B:237:ALA:HB2	2.03	0.40
1:F:240:ILE:HD13	1:F:251:ALA:HB2	2.01	0.40
1:C:112:THR:O	1:C:260:VAL:HG21	2.22	0.40
1:A:45:PHE:CE1	1:C:340:PHE:HE2	2.39	0.40
1:D:153:PHE:HB2	1:D:178:ILE:HG12	2.03	0.40
1:E:30:ASN:OD1	1:E:327:GLY:HA2	2.21	0.40
1:F:203:GLN:HA	1:F:204:PRO:HD3	1.90	0.40
1:C:167:ARG:HA	1:C:250:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:TYR:C	1:C:338:TYR:CD2	2.92	0.40
1:D:23:PHE:HB2	1:D:332:VAL:HB	2.03	0.40
1:A:32:TYR:CB	1:A:316:ASN:HD21	2.32	0.40
1:A:32:TYR:HB2	1:A:316:ASN:ND2	2.34	0.40
1:B:10:LYS:HG2	1:B:48:GLU:O	2.21	0.40
1:B:240:ILE:HD13	1:B:251:ALA:HB2	2.03	0.40
1:C:136:VAL:HG23	1:C:136:VAL:O	2.21	0.40
1:F:276:THR:O	1:F:293:ASN:HA	2.22	0.40
1:E:20:LEU:HD13	1:E:310:TYR:OH	2.22	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	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	B	338/340 (99%)	319 (94%)	19 (6%)	0	100	100
1	C	338/340 (99%)	320 (95%)	18 (5%)	0	100	100
1	D	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	E	339/340 (100%)	323 (95%)	16 (5%)	0	100	100
1	F	338/340 (99%)	322 (95%)	16 (5%)	0	100	100
All	All	2029/2040 (100%)	1926 (95%)	103 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	263/263 (100%)	263 (100%)	0	100	100
1	B	263/263 (100%)	263 (100%)	0	100	100
1	C	263/263 (100%)	261 (99%)	2 (1%)	85	93
1	D	263/263 (100%)	261 (99%)	2 (1%)	85	93
1	E	264/263 (100%)	261 (99%)	3 (1%)	78	89
1	F	263/263 (100%)	262 (100%)	1 (0%)	93	97
All	All	1579/1578 (100%)	1571 (100%)	8 (0%)	91	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	247	THR
1	C	309	THR
1	D	247	THR
1	D	340	PHE
1	E	247	THR
1	E	297	VAL
1	E	340	PHE
1	F	12	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	316	ASN
1	C	76	GLN
1	D	68	ASN
1	D	264	GLN
1	F	21	HIS

5.3.3 RNA ⓘ

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 carbohydrates 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	340/340 (100%)	0.18	8 (2%) 59 49	25, 91, 154, 205	1 (0%)
1	B	340/340 (100%)	0.25	15 (4%) 35 27	18, 97, 153, 214	0
1	C	340/340 (100%)	0.30	18 (5%) 27 21	24, 83, 142, 188	1 (0%)
1	D	340/340 (100%)	0.63	42 (12%) 4 5	53, 136, 193, 246	0
1	E	340/340 (100%)	0.94	65 (19%) 1 2	59, 157, 214, 267	1 (0%)
1	F	340/340 (100%)	0.50	33 (9%) 8 7	51, 112, 175, 209	1 (0%)
All	All	2040/2040 (100%)	0.47	181 (8%) 10 8	18, 109, 190, 267	4 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	57	GLY	11.3
1	E	90	TYR	7.3
1	E	56[A]	THR	7.1
1	E	209	LYS	6.7
1	D	291	LEU	6.2
1	E	285	GLY	5.2
1	E	180	TYR	5.1
1	E	128	PHE	4.9
1	D	290	ASP	4.7
1	E	282	ASP	4.7
1	E	139	TYR	4.6
1	E	173	GLY	4.3
1	A	319	ASP	4.3
1	F	289	VAL	4.2
1	E	172	ASP	4.2
1	E	287	GLY	4.2
1	E	94	GLY	4.0
1	C	209	LYS	4.0
1	F	210	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	220	TYR	4.0
1	C	253	LYS	4.0
1	D	310	TYR	4.0
1	A	251	ALA	3.9
1	E	55	LEU	3.9
1	F	209	LYS	3.9
1	E	195	ASP	3.9
1	E	51	ILE	3.8
1	E	300	THR	3.8
1	D	317	GLN	3.7
1	E	196	ARG	3.6
1	D	182	TYR	3.6
1	E	207	ASN	3.6
1	E	210	LYS	3.6
1	E	281	LYS	3.6
1	D	318	ILE	3.6
1	E	206	GLY	3.5
1	E	171	GLY	3.4
1	F	280	ALA	3.4
1	C	210	LYS	3.4
1	C	264	GLN	3.4
1	D	309	THR	3.4
1	B	285	GLY	3.4
1	D	20	LEU	3.4
1	D	207	ASN	3.3
1	D	209	LYS	3.3
1	F	253	LYS	3.3
1	E	89	LYS	3.3
1	E	176	GLY	3.2
1	E	93	VAL	3.2
1	A	290	ASP	3.2
1	E	314	ILE	3.2
1	E	312	ASP	3.2
1	E	208	GLY	3.2
1	F	219	LYS	3.2
1	F	186	GLY	3.1
1	D	101	ASN	3.1
1	D	266	ASP	3.1
1	B	264	GLN	3.1
1	E	155	VAL	3.0
1	F	212	GLU	3.0
1	D	303	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	159	GLY	3.0
1	F	281	LYS	3.0
1	E	88	LEU	2.9
1	D	23	PHE	2.9
1	C	280	ALA	2.9
1	D	300	THR	2.9
1	E	181	GLU	2.9
1	C	255	GLN	2.9
1	F	287	GLY	2.9
1	D	313	TYR	2.9
1	D	36	GLY	2.8
1	F	290	ASP	2.8
1	C	285	GLY	2.8
1	E	255	GLN	2.8
1	B	90	TYR	2.8
1	E	49	THR	2.8
1	C	212	GLU	2.8
1	B	268	GLY	2.8
1	F	283	VAL	2.7
1	E	99	GLY	2.7
1	D	297	VAL	2.7
1	A	310	TYR	2.7
1	D	103	GLY	2.7
1	E	299	ALA	2.7
1	C	256	ASP	2.7
1	F	228	ALA	2.7
1	D	19	GLY	2.7
1	C	208	GLY	2.7
1	E	189	GLY	2.7
1	C	134	GLY	2.6
1	D	180	TYR	2.6
1	D	312	ASP	2.6
1	F	286	ILE	2.6
1	E	96	PHE	2.6
1	F	129	PHE	2.6
1	D	293	ASN	2.6
1	F	279	LYS	2.5
1	E	263	TYR	2.5
1	F	195	ASP	2.5
1	B	180	TYR	2.5
1	D	179	SER	2.5
1	E	162	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	263	TYR	2.5
1	F	300	THR	2.5
1	C	281	LYS	2.5
1	F	231	TYR	2.5
1	B	209	LYS	2.5
1	B	281	LYS	2.5
1	E	268	GLY	2.4
1	A	25	LYS	2.4
1	F	111	TYR	2.4
1	D	307	MET	2.4
1	D	253	LYS	2.4
1	E	160	LYS	2.4
1	F	158	LEU	2.4
1	E	101	ASN	2.4
1	D	21	HIS	2.4
1	E	264	GLN	2.4
1	E	154	ALA	2.4
1	F	316	ASN	2.4
1	E	191	TYR	2.3
1	D	292	VAL	2.3
1	E	107	ASP	2.3
1	E	151	LEU	2.3
1	E	194	ALA	2.3
1	F	288	ASP	2.3
1	B	208	GLY	2.3
1	E	290	ASP	2.3
1	E	87	GLY	2.3
1	F	225	ILE	2.3
1	D	172	ASP	2.3
1	D	221	ASP	2.3
1	C	289	VAL	2.3
1	D	183	GLU	2.3
1	F	171	GLY	2.3
1	E	92	ASP	2.3
1	E	262	GLN	2.2
1	F	184	GLY	2.2
1	B	30	ASN	2.2
1	C	286	ILE	2.2
1	F	263	TYR	2.2
1	B	175	GLY	2.2
1	D	283	VAL	2.2
1	E	134	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	251	ALA	2.2
1	F	211	ALA	2.2
1	C	128	PHE	2.2
1	D	267	PHE	2.2
1	E	279	LYS	2.2
1	B	300	THR	2.2
1	E	177	SER	2.2
1	A	207	ASN	2.2
1	D	268	GLY	2.2
1	D	333	ALA	2.2
1	D	262	GLN	2.2
1	E	190	ALA	2.2
1	D	195	ASP	2.2
1	E	188	VAL	2.2
1	E	310	TYR	2.2
1	E	91	ALA	2.1
1	A	111	TYR	2.1
1	D	295	PHE	2.1
1	F	257	VAL	2.1
1	F	226	TYR	2.1
1	A	253	LYS	2.1
1	B	286	ILE	2.1
1	F	221	ASP	2.1
1	B	172	ASP	2.1
1	C	195	ASP	2.1
1	E	335	GLY	2.1
1	C	207	ASN	2.1
1	D	27	ASN	2.1
1	C	129	PHE	2.1
1	B	57	GLY	2.1
1	B	56	THR	2.0
1	E	331	THR	2.0
1	E	286	ILE	2.0
1	D	271	PRO	2.0
1	E	284	GLU	2.0
1	F	181	GLU	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 carbohydrates 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.