



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:15 PM UTC

PDB ID : 2BHV / pdb_00002bhv
Title : Structure of ComB10 of the Com Type IV secretion system of *Helicobacter pylori*
Authors : Terradot, L.; Oomen, C.; Bayliss, R.; Leonard, G.; Waksman, G.
Deposited on : 2005-01-18
Resolution : 3.00 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:

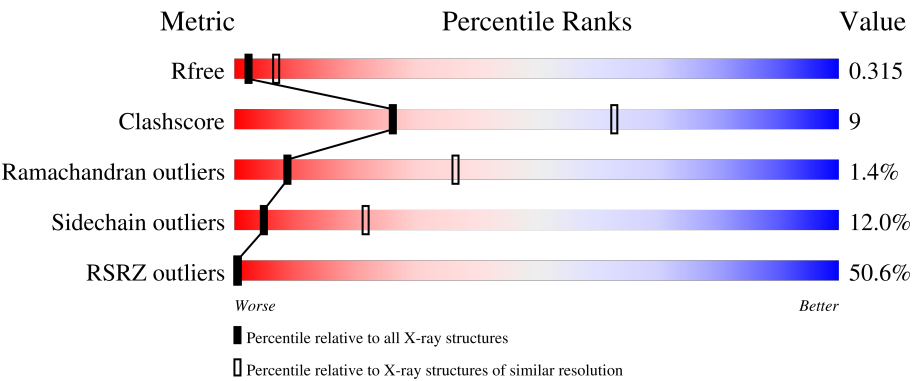
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	77% 55%17%••22%
1	B	246	72% 57%17%••22%
1	C	246	5% 59%14%•24%
1	D	246	4% 54%18%•23%
1	E	246	5% 53%21%••23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	246	71% 56% 19% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8759 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.

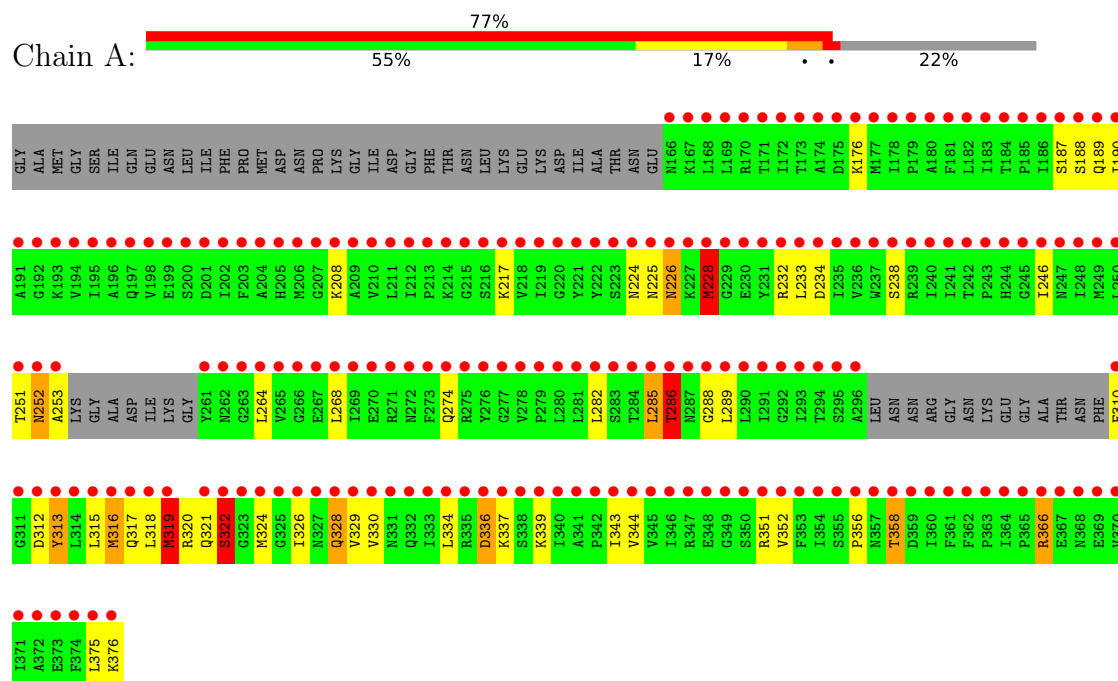
- Molecule 1 is a protein called COMB10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1468	945	253	263	7			
1	B	192	Total	C	N	O	S	0	0	0
			1466	944	254	261	7			
1	C	188	Total	C	N	O	S	0	0	0
			1457	941	250	259	7			
1	D	189	Total	C	N	O	S	0	0	0
			1464	944	251	262	7			
1	E	190	Total	C	N	O	S	0	0	0
			1447	931	251	258	7			
1	F	188	Total	C	N	O	S	0	0	0
			1457	939	250	261	7			

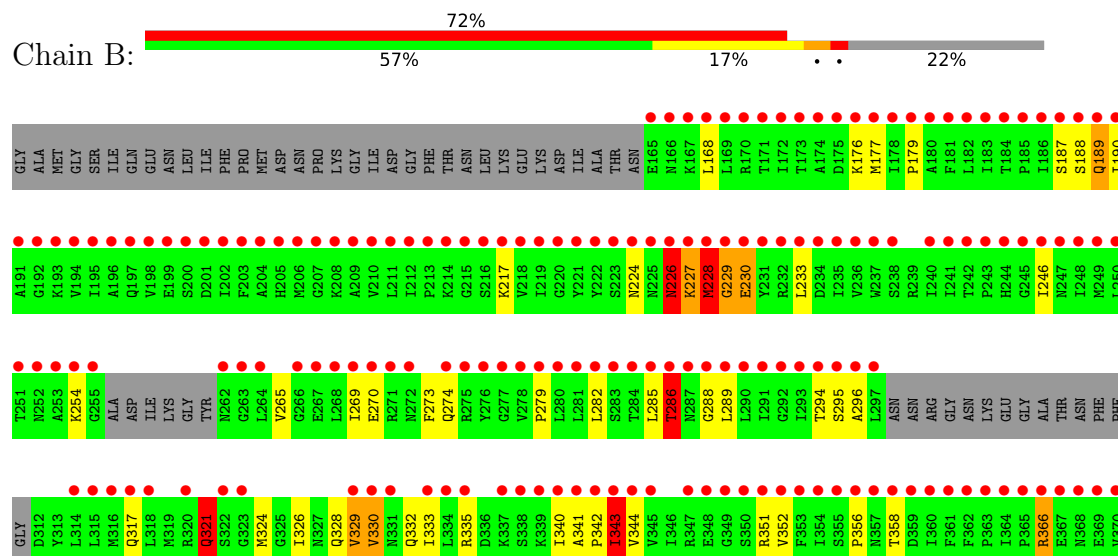
3 Residue-property plots

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

• Molecule 1: COMB10

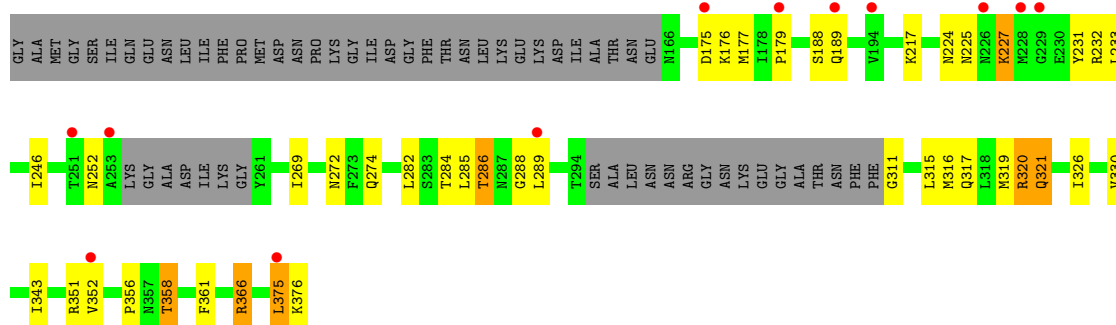


• Molecule 1: COMB10

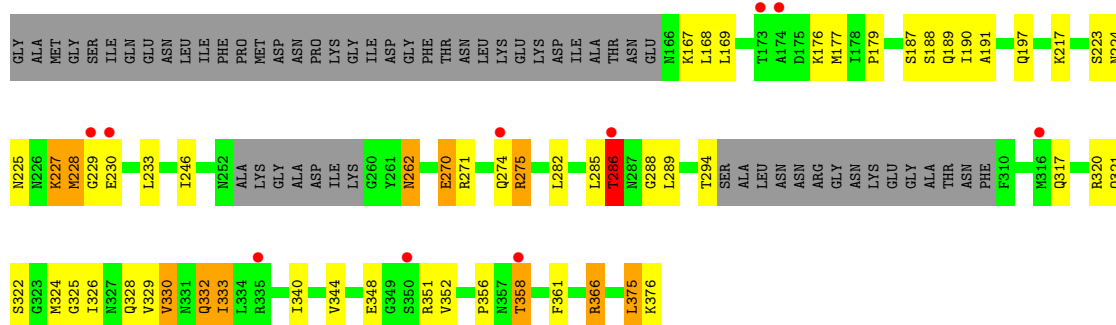




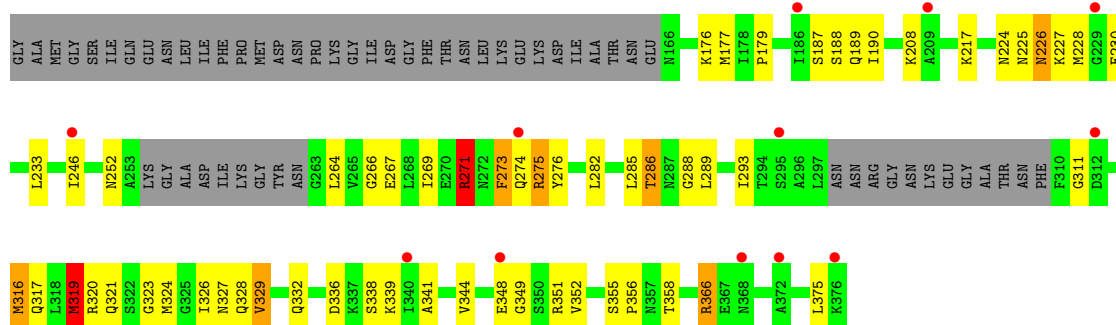
• Molecule 1: COMB10



• Molecule 1: COMB10



• Molecule 1: COMB10



• Molecule 1: COMB10





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.73Å 139.41Å 168.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.00) 97.9 (20.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.257 , 0.293 0.291 , 0.315	Depositor DCC
R_{free} test set	1674 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.86	5/1490 (0.3%)	0.87	2/2016 (0.1%)
1	B	0.76	1/1487 (0.1%)	0.92	4/2012 (0.2%)
1	C	0.77	1/1480 (0.1%)	0.85	1/2002 (0.0%)
1	D	0.68	0/1487	0.84	1/2011 (0.0%)
1	E	1.32	11/1468 (0.7%)	0.92	4/1986 (0.2%)
1	F	0.64	0/1480	0.84	1/2002 (0.0%)
All	All	0.87	18/8892 (0.2%)	0.88	13/12029 (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
1	A	0	1
1	B	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	319	MET	SD-CE	22.23	2.35	1.79
1	E	271	ARG	CZ-NH1	19.96	1.60	1.32
1	E	274	GLN	CD-OE1	19.22	1.60	1.23
1	E	274	GLN	CD-NE2	12.66	1.59	1.33
1	C	311	GLY	N-CA	12.31	1.65	1.45
1	E	271	ARG	CD-NE	12.02	1.63	1.46
1	A	318	LEU	C-N	11.56	1.48	1.33
1	A	316	MET	SD-CE	8.36	2.00	1.79
1	E	228	MET	SD-CE	7.87	1.99	1.79
1	E	316	MET	SD-CE	7.66	1.98	1.79
1	E	273	PHE	CG-CD2	6.30	1.52	1.38
1	E	271	ARG	CZ-NH2	6.23	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	PHE	CG-CD1	5.61	1.50	1.38
1	A	322	SER	CB-OG	5.58	1.53	1.42
1	A	310	PHE	CA-CB	5.39	1.64	1.53
1	A	319	MET	CG-SD	5.29	1.94	1.80
1	E	271	ARG	NE-CZ	5.09	1.38	1.33
1	B	343	ILE	CA-CB	5.02	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	271	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	B	321	GLN	N-CA-C	7.32	120.25	110.88
1	F	252	ASN	N-CA-C	6.16	117.83	110.19
1	C	252	ASN	N-CA-C	5.67	118.07	110.35
1	E	252	ASN	N-CA-C	5.65	118.24	109.60
1	B	333	ILE	N-CA-C	-5.61	106.99	111.81
1	E	271	ARG	CD-NE-CZ	-5.60	116.56	124.40
1	B	286	THR	CB-CA-C	-5.34	100.51	109.53
1	E	339	LYS	N-CA-C	-5.31	105.07	112.45
1	D	286	THR	CB-CA-C	-5.21	100.73	109.65
1	A	286	THR	CB-CA-C	-5.14	100.85	109.65
1	A	228	MET	N-CA-C	5.05	117.05	110.43
1	B	227	LYS	N-CA-C	-5.00	100.15	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	MET	Peptide
1	B	226	ASN	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	1468	0	1517	39	3
1	B	1466	0	1519	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1457	0	1513	26	2
1	D	1464	0	1515	35	0
1	E	1447	0	1493	34	0
1	F	1457	0	1506	29	1
All	All	8759	0	9063	167	3

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 9.

All (167) 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:C:175:ASP:OD2	1:E:208:LYS:HE3	1.30	1.26
1:A:226:ASN:HB3	1:A:228:MET:HG3	1.21	1.19
1:E:319:MET:SD	1:E:319:MET:CE	2.35	1.15
1:A:319:MET:HE3	1:A:319:MET:HA	1.45	0.94
1:A:319:MET:HE1	1:D:197:GLN:HE22	1.30	0.93
1:B:326:ILE:O	1:B:330:VAL:HG12	1.78	0.84
1:D:325:GLY:O	1:D:329:VAL:HG23	1.78	0.82
1:C:175:ASP:CG	1:E:208:LYS:HE3	2.06	0.80
1:C:286:THR:HG22	1:C:288:GLY:H	1.47	0.79
1:C:366:ARG:HB2	1:C:366:ARG:HH11	1.48	0.78
1:B:324:MET:HE3	1:B:328:GLN:HG2	1.65	0.78
1:B:366:ARG:HH11	1:B:366:ARG:HB2	1.49	0.78
1:B:286:THR:HG22	1:B:288:GLY:H	1.51	0.76
1:D:366:ARG:HB2	1:D:366:ARG:HH11	1.51	0.76
1:A:319:MET:HA	1:A:319:MET:CE	2.16	0.75
1:A:286:THR:HG22	1:A:288:GLY:H	1.53	0.73
1:F:286:THR:HG23	1:F:289:LEU:HG	1.72	0.72
1:F:286:THR:HG22	1:F:288:GLY:H	1.54	0.72
1:F:312:ASP:CG	1:F:313:TYR:H	1.98	0.71
1:A:226:ASN:HB3	1:A:228:MET:CG	2.13	0.71
1:D:286:THR:HG23	1:D:289:LEU:HG	1.74	0.70
1:D:225:ASN:ND2	1:D:227:LYS:HE2	2.06	0.69
1:E:286:THR:HG22	1:E:288:GLY:H	1.56	0.69
1:B:286:THR:HG23	1:B:289:LEU:HG	1.75	0.69
1:E:332:GLN:O	1:E:336:ASP:HB2	1.92	0.69
1:F:228:MET:O	1:F:230:GLU:N	2.22	0.69
1:D:286:THR:HG22	1:D:288:GLY:H	1.58	0.69
1:C:286:THR:HG23	1:C:289:LEU:HG	1.75	0.67
1:F:366:ARG:HH11	1:F:366:ARG:HB2	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ASN:O	1:F:227:LYS:HD2	1.94	0.67
1:B:265:VAL:O	1:B:269:ILE:HG12	1.95	0.66
1:E:286:THR:HG23	1:E:289:LEU:HG	1.76	0.66
1:E:366:ARG:HH11	1:E:366:ARG:HB2	1.60	0.66
1:A:366:ARG:HH11	1:A:366:ARG:HB2	1.61	0.65
1:B:286:THR:HG21	1:C:317:GLN:OE1	1.98	0.64
1:D:317:GLN:OE1	1:F:286:THR:HG21	1.98	0.64
1:C:175:ASP:OD2	1:E:208:LYS:CE	2.25	0.64
1:A:286:THR:HG23	1:A:289:LEU:HG	1.78	0.64
1:B:228:MET:O	1:B:229:GLY:C	2.41	0.63
1:C:225:ASN:HB3	1:C:232:ARG:HB3	1.80	0.62
1:F:228:MET:C	1:F:230:GLU:H	2.06	0.62
1:C:225:ASN:OD1	1:C:227:LYS:HB2	2.00	0.62
1:B:228:MET:O	1:B:230:GLU:N	2.33	0.61
1:A:286:THR:HG21	1:E:317:GLN:OE1	2.00	0.60
1:B:226:ASN:C	1:B:228:MET:N	2.60	0.59
1:B:188:SER:HA	1:B:224:ASN:OD1	2.02	0.59
1:A:188:SER:HA	1:A:224:ASN:OD1	2.02	0.58
1:B:326:ILE:HG12	1:C:284:THR:O	2.02	0.58
1:E:227:LYS:HG2	1:E:230:GLU:HB3	1.86	0.58
1:B:286:THR:CG2	1:C:317:GLN:OE1	2.52	0.57
1:E:317:GLN:HA	1:E:321:GLN:HG2	1.87	0.57
1:A:319:MET:HE1	1:D:197:GLN:NE2	2.11	0.57
1:A:286:THR:CG2	1:E:317:GLN:OE1	2.53	0.56
1:E:225:ASN:O	1:E:226:ASN:HB3	2.06	0.56
1:B:294:THR:C	1:B:296:ALA:H	2.13	0.56
1:D:227:LYS:O	1:D:229:GLY:O	2.22	0.56
1:C:188:SER:HA	1:C:224:ASN:OD1	2.05	0.56
1:D:326:ILE:O	1:D:330:VAL:HG12	2.04	0.56
1:B:227:LYS:O	1:B:229:GLY:N	2.39	0.56
1:F:223:SER:HB2	1:F:262:ASN:HD22	1.70	0.55
1:E:316:MET:SD	1:E:320:ARG:HG3	2.47	0.55
1:D:329:VAL:O	1:D:333:ILE:HD12	2.06	0.55
1:D:317:GLN:OE1	1:F:286:THR:CG2	2.55	0.54
1:A:264:LEU:O	1:A:268:LEU:HG	2.08	0.54
1:A:343:ILE:HD12	1:A:343:ILE:H	1.72	0.54
1:B:317:GLN:HA	1:B:321:GLN:HG3	1.89	0.53
1:A:336:ASP:O	1:A:339:LYS:HB2	2.09	0.53
1:F:188:SER:HA	1:F:224:ASN:OD1	2.09	0.53
1:D:230:GLU:HB3	1:F:331:ASN:OD1	2.08	0.53
1:C:315:LEU:O	1:C:319:MET:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLN:HA	1:A:321:GLN:HB2	1.91	0.52
1:D:188:SER:HA	1:D:224:ASN:OD1	2.09	0.52
1:B:177:MET:O	1:B:179:PRO:HD3	2.10	0.52
1:E:266:GLY:HA2	1:E:269:ILE:HD12	1.92	0.52
1:C:282:LEU:HD13	1:C:356:PRO:HA	1.92	0.52
1:A:324:MET:HE3	1:A:328:GLN:HB3	1.92	0.51
1:F:231:TYR:CD1	1:F:231:TYR:C	2.88	0.51
1:B:282:LEU:HD13	1:B:356:PRO:HA	1.91	0.51
1:E:275:ARG:HD3	1:E:276:TYR:CE2	2.46	0.50
1:D:167:LYS:C	1:D:169:LEU:H	2.19	0.50
1:F:282:LEU:HD13	1:F:356:PRO:HA	1.94	0.50
1:A:334:LEU:O	1:A:337:LYS:HB2	2.11	0.50
1:A:315:LEU:HD22	1:D:348:GLU:HG3	1.94	0.49
1:C:225:ASN:O	1:C:227:LYS:HD2	2.12	0.49
1:B:168:LEU:HD21	1:D:320:ARG:NH2	2.27	0.49
1:D:187:SER:OG	1:D:190:ILE:HB	2.12	0.49
1:E:188:SER:HA	1:E:224:ASN:OD1	2.12	0.49
1:E:267:GLU:O	1:E:271:ARG:HG2	2.12	0.49
1:D:289:LEU:HD11	1:F:326:ILE:HG12	1.95	0.49
1:A:326:ILE:HA	1:A:329:VAL:HG22	1.96	0.48
1:B:329:VAL:HG11	1:C:286:THR:OG1	2.13	0.48
1:D:282:LEU:HD13	1:D:356:PRO:HA	1.94	0.48
1:D:328:GLN:O	1:D:332:GLN:HB2	2.13	0.48
1:E:282:LEU:HD13	1:E:356:PRO:HA	1.95	0.48
1:F:312:ASP:CG	1:F:313:TYR:N	2.68	0.48
1:A:317:GLN:OE1	1:E:289:LEU:N	2.40	0.48
1:A:282:LEU:HD13	1:A:356:PRO:HA	1.96	0.47
1:D:177:MET:O	1:D:179:PRO:HD3	2.14	0.47
1:C:317:GLN:HA	1:C:321:GLN:HG3	1.96	0.47
1:E:324:MET:HE2	1:E:329:VAL:N	2.31	0.46
1:B:189:GLN:HG3	1:B:343:ILE:HD13	1.98	0.46
1:E:225:ASN:O	1:E:226:ASN:CB	2.64	0.46
1:F:228:MET:C	1:F:230:GLU:N	2.69	0.46
1:A:315:LEU:O	1:A:319:MET:HG2	2.16	0.46
1:F:177:MET:O	1:F:179:PRO:HD3	2.15	0.46
1:B:188:SER:HB3	1:B:344:VAL:O	2.17	0.45
1:C:326:ILE:H	1:D:228:MET:HE3	1.80	0.45
1:A:321:GLN:O	1:A:322:SER:C	2.59	0.45
1:A:225:ASN:C	1:A:225:ASN:HD22	2.25	0.45
1:D:275:ARG:HD2	1:D:275:ARG:H	1.81	0.45
1:A:319:MET:CE	1:A:319:MET:CA	2.91	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:O	1:A:330:VAL:HG23	2.17	0.45
1:D:191:ALA:CB	1:D:262:ASN:HB3	2.47	0.45
1:E:177:MET:O	1:E:179:PRO:HD3	2.17	0.45
1:C:269:ILE:HA	1:C:272:ASN:HD22	1.82	0.44
1:A:232:ARG:HA	1:E:327:ASN:OD1	2.18	0.44
1:A:285:LEU:HG	1:E:323:GLY:O	2.18	0.44
1:E:226:ASN:HD21	1:E:341:ALA:HB2	1.82	0.44
1:D:167:LYS:C	1:D:169:LEU:N	2.75	0.44
1:C:177:MET:O	1:C:179:PRO:HD3	2.18	0.44
1:B:317:GLN:HA	1:B:321:GLN:CG	2.48	0.44
1:F:315:LEU:O	1:F:319:MET:HG3	2.18	0.44
1:E:293:ILE:O	1:E:293:ILE:HG23	2.17	0.43
1:C:316:MET:O	1:C:320:ARG:HG2	2.18	0.43
1:F:188:SER:HB3	1:F:344:VAL:O	2.19	0.43
1:E:188:SER:HB3	1:E:344:VAL:O	2.18	0.43
1:B:330:VAL:HG11	1:C:231:TYR:CE2	2.54	0.43
1:D:321:GLN:HG2	1:D:324:MET:SD	2.58	0.43
1:F:192:GLY:HA2	1:F:261:TYR:CD1	2.53	0.43
1:E:348:GLU:HG3	1:F:315:LEU:HD22	2.01	0.43
1:B:321:GLN:NE2	1:B:324:MET:HE1	2.34	0.42
1:A:252:ASN:HB3	1:A:253:ALA:H	1.48	0.42
1:B:294:THR:C	1:B:296:ALA:N	2.76	0.42
1:D:361:PHE:HB2	1:D:375:LEU:HD21	2.01	0.42
1:F:276:TYR:CE2	1:F:374:PHE:CD1	3.07	0.42
1:A:316:MET:SD	1:A:320:ARG:NH2	2.93	0.42
1:D:270:GLU:O	1:D:271:ARG:C	2.63	0.42
1:B:187:SER:OG	1:B:190:ILE:HB	2.20	0.42
1:E:326:ILE:O	1:E:327:ASN:C	2.62	0.42
1:F:361:PHE:HB2	1:F:375:LEU:HD21	2.01	0.42
1:A:225:ASN:C	1:A:225:ASN:ND2	2.78	0.42
1:D:223:SER:HB2	1:D:262:ASN:HB2	2.01	0.42
1:E:349:GLY:HA3	1:F:314:LEU:HD23	2.01	0.42
1:C:361:PHE:HB2	1:C:375:LEU:HD21	2.01	0.42
1:E:187:SER:OG	1:E:190:ILE:HB	2.20	0.42
1:A:188:SER:HB3	1:A:344:VAL:O	2.19	0.41
1:C:343:ILE:N	1:C:343:ILE:HD12	2.35	0.41
1:A:238:SER:HB2	1:A:251:THR:O	2.20	0.41
1:D:228:MET:O	1:D:228:MET:HE2	2.20	0.41
1:A:187:SER:OG	1:A:190:ILE:HB	2.21	0.41
1:F:355:SER:HA	1:F:356:PRO:HD3	1.97	0.41
1:B:279:PRO:HB2	1:D:227:LYS:NZ	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:ASP:C	1:E:338:SER:H	2.28	0.41
1:F:275:ARG:HG2	1:F:276:TYR:CE2	2.55	0.41
1:C:358:THR:HG21	1:C:376:LYS:HA	2.03	0.41
1:B:341:ALA:HA	1:B:342:PRO:HD3	1.97	0.41
1:D:223:SER:CB	1:D:262:ASN:HB2	2.50	0.41
1:A:324:MET:HE2	1:A:329:VAL:CG1	2.52	0.40
1:A:358:THR:HG21	1:A:376:LYS:HA	2.03	0.40
1:D:188:SER:HB3	1:D:344:VAL:O	2.21	0.40
1:F:223:SER:HB2	1:F:262:ASN:ND2	2.35	0.40
1:A:336:ASP:OD1	1:A:339:LYS:HE2	2.22	0.40
1:C:343:ILE:HD12	1:C:343:ILE:H	1.86	0.40
1:A:312:ASP:CG	1:A:313:TYR:H	2.29	0.40
1:D:358:THR:HG21	1:D:376:LYS:HA	2.03	0.40
1:E:355:SER:HA	1:E:356:PRO:HD3	1.98	0.40
1:F:213:PRO:O	1:F:216:SER:OG	2.34	0.40

All (3) 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)
1:A:208:LYS:CE	1:F:175:ASP:OD2[3_555]	1.95	0.25
1:A:232:ARG:NH1	1:C:366:ARG:CD[4_455]	2.06	0.14
1:A:234:ASP:OD1	1:C:366:ARG:NE[4_455]	2.09	0.11

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	185/246 (75%)	166 (90%)	15 (8%)	4 (2%)	5	26
1	B	186/246 (76%)	172 (92%)	8 (4%)	6 (3%)	3	18
1	C	182/246 (74%)	172 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	183/246 (74%)	171 (93%)	10 (6%)	2 (1%)	11	43
1	E	184/246 (75%)	166 (90%)	16 (9%)	2 (1%)	11	43
1	F	182/246 (74%)	171 (94%)	10 (6%)	1 (0%)	24	60
All	All	1102/1476 (75%)	1018 (92%)	69 (6%)	15 (1%)	9	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	MET
1	B	254	LYS
1	A	313	TYR
1	B	229	GLY
1	B	274	GLN
1	F	229	GLY
1	A	252	ASN
1	A	322	SER
1	B	295	SER
1	D	168	LEU
1	D	340	ILE
1	E	226	ASN
1	E	311	GLY
1	A	226	ASN
1	B	273	PHE

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	159/209 (76%)	143 (90%)	16 (10%)	7	29
1	B	158/209 (76%)	135 (85%)	23 (15%)	3	15
1	C	159/209 (76%)	142 (89%)	17 (11%)	6	26
1	D	160/209 (77%)	137 (86%)	23 (14%)	3	15
1	E	155/209 (74%)	136 (88%)	19 (12%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	159/209 (76%)	143 (90%)	16 (10%)	7	29
All	All	950/1254 (76%)	836 (88%)	114 (12%)	5	22

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	189	GLN
1	A	217	LYS
1	A	233	LEU
1	A	246	ILE
1	A	274	GLN
1	A	285	LEU
1	A	286	THR
1	A	319	MET
1	A	328	GLN
1	A	336	ASP
1	A	351	ARG
1	A	352	VAL
1	A	358	THR
1	A	366	ARG
1	A	375	LEU
1	B	176	LYS
1	B	189	GLN
1	B	217	LYS
1	B	226	ASN
1	B	228	MET
1	B	230	GLU
1	B	233	LEU
1	B	246	ILE
1	B	270	GLU
1	B	285	LEU
1	B	286	THR
1	B	321	GLN
1	B	329	VAL
1	B	330	VAL
1	B	332	GLN
1	B	335	ARG
1	B	340	ILE
1	B	343	ILE
1	B	351	ARG
1	B	352	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	THR
1	B	366	ARG
1	B	375	LEU
1	C	176	LYS
1	C	189	GLN
1	C	217	LYS
1	C	227	LYS
1	C	233	LEU
1	C	246	ILE
1	C	274	GLN
1	C	285	LEU
1	C	286	THR
1	C	320	ARG
1	C	321	GLN
1	C	330	VAL
1	C	351	ARG
1	C	352	VAL
1	C	358	THR
1	C	366	ARG
1	C	375	LEU
1	D	176	LYS
1	D	189	GLN
1	D	217	LYS
1	D	227	LYS
1	D	228	MET
1	D	233	LEU
1	D	246	ILE
1	D	262	ASN
1	D	270	GLU
1	D	274	GLN
1	D	275	ARG
1	D	285	LEU
1	D	286	THR
1	D	294	THR
1	D	322	SER
1	D	330	VAL
1	D	332	GLN
1	D	333	ILE
1	D	351	ARG
1	D	352	VAL
1	D	358	THR
1	D	366	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	375	LEU
1	E	176	LYS
1	E	189	GLN
1	E	217	LYS
1	E	233	LEU
1	E	246	ILE
1	E	264	LEU
1	E	271	ARG
1	E	273	PHE
1	E	275	ARG
1	E	285	LEU
1	E	286	THR
1	E	319	MET
1	E	328	GLN
1	E	329	VAL
1	E	351	ARG
1	E	352	VAL
1	E	358	THR
1	E	366	ARG
1	E	375	LEU
1	F	176	LYS
1	F	189	GLN
1	F	217	LYS
1	F	231	TYR
1	F	233	LEU
1	F	246	ILE
1	F	274	GLN
1	F	285	LEU
1	F	286	THR
1	F	328	GLN
1	F	330	VAL
1	F	351	ARG
1	F	352	VAL
1	F	358	THR
1	F	366	ARG
1	F	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	225	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	ASN
1	A	274	GLN
1	A	328	GLN
1	B	321	GLN
1	C	189	GLN
1	C	272	ASN
1	D	189	GLN
1	D	197	GLN
1	E	189	GLN
1	E	226	ASN
1	F	189	GLN
1	F	262	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/246 (77%)	6.13	190 (99%) 0 0	33, 47, 56, 68	0
1	B	192/246 (78%)	4.20	177 (92%) 0 0	28, 47, 57, 68	0
1	C	188/246 (76%)	0.77	12 (6%) 25 13	32, 47, 54, 67	0
1	D	189/246 (76%)	0.74	10 (5%) 32 16	34, 47, 57, 62	0
1	E	190/246 (77%)	0.82	12 (6%) 26 13	25, 47, 56, 63	0
1	F	188/246 (76%)	4.35	175 (93%) 0 0	35, 47, 54, 67	0
All	All	1138/1476 (77%)	2.84	576 (50%) 0 0	25, 47, 56, 68	0

All (576) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	230	GLU	15.3
1	A	235	ILE	15.0
1	A	276	TYR	13.9
1	A	288	GLY	13.7
1	F	376	LYS	12.3
1	B	376	LYS	12.1
1	A	208	LYS	11.7
1	A	286	THR	11.4
1	A	296	ALA	11.3
1	F	372	ALA	10.9
1	A	375	LEU	10.9
1	F	175	ASP	10.9
1	A	234	ASP	10.9
1	A	250	LEU	10.7
1	A	179	PRO	10.5
1	A	225	ASN	10.1
1	B	231	TYR	9.8
1	F	286	THR	9.7
1	A	369	GLU	9.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	190	ILE	9.6
1	F	166	ASN	9.5
1	A	230	GLU	9.4
1	A	198	VAL	9.3
1	F	247	ASN	9.3
1	A	290	LEU	9.2
1	A	267	GLU	9.1
1	A	289	LEU	9.1
1	A	233	LEU	9.0
1	A	215	GLY	9.0
1	A	190	ILE	9.0
1	A	376	LYS	9.0
1	A	231	TYR	8.9
1	A	244	HIS	8.7
1	A	178	ILE	8.6
1	A	271	ARG	8.5
1	A	210	VAL	8.5
1	A	224	ASN	8.5
1	A	367	GLU	8.3
1	A	293	ILE	8.3
1	F	189	GLN	8.3
1	F	262	ASN	8.3
1	B	366	ARG	8.3
1	F	228	MET	8.3
1	A	280	LEU	8.3
1	F	223	SER	8.2
1	B	374	PHE	8.1
1	B	180	ALA	8.1
1	A	341	ALA	8.0
1	A	321	GLN	8.0
1	F	289	LEU	8.0
1	A	343	ILE	8.0
1	A	171	THR	7.9
1	A	261	TYR	7.9
1	A	371	ILE	7.8
1	A	370	VAL	7.8
1	A	285	LEU	7.8
1	A	253	ALA	7.6
1	F	362	PHE	7.6
1	A	207	GLY	7.6
1	A	177	MET	7.5
1	F	265	VAL	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	358	THR	7.4
1	A	236	VAL	7.4
1	B	200	SER	7.4
1	A	314	LEU	7.4
1	A	197	GLN	7.4
1	A	333	ILE	7.3
1	A	181	PHE	7.3
1	A	275	ARG	7.3
1	A	183	ILE	7.3
1	A	264	LEU	7.3
1	B	209	ALA	7.3
1	A	350	SER	7.2
1	B	277	GLY	7.2
1	B	173	THR	7.2
1	A	287	ASN	7.2
1	A	189	GLN	7.2
1	A	240	ILE	7.1
1	A	229	GLY	7.1
1	A	173	THR	7.1
1	F	173	THR	7.0
1	A	318	LEU	7.0
1	A	362	PHE	7.0
1	B	181	PHE	7.0
1	F	231	TYR	7.0
1	A	364	ILE	7.0
1	A	342	PRO	6.9
1	B	190	ILE	6.9
1	A	205	HIS	6.9
1	A	291	ILE	6.9
1	A	221	TYR	6.8
1	F	253	ALA	6.8
1	A	317	GLN	6.8
1	B	230	GLU	6.7
1	A	311	GLY	6.7
1	A	223	SER	6.7
1	B	262	ASN	6.7
1	A	360	ILE	6.7
1	B	290	LEU	6.7
1	A	344	VAL	6.7
1	A	212	ILE	6.6
1	A	184	THR	6.6
1	A	246	ILE	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	183	ILE	6.6
1	A	185	PRO	6.6
1	A	237	TRP	6.5
1	B	297	LEU	6.5
1	A	353	PHE	6.5
1	B	364	ILE	6.5
1	A	294	THR	6.5
1	F	367	GLU	6.4
1	F	243	PRO	6.4
1	B	205	HIS	6.4
1	F	270	GLU	6.4
1	A	239	ARG	6.4
1	A	282	LEU	6.4
1	F	201	ASP	6.4
1	A	355	SER	6.4
1	B	375	LEU	6.4
1	A	312	ASP	6.3
1	F	234	ASP	6.3
1	A	200	SER	6.3
1	B	255	GLY	6.3
1	B	369	GLU	6.3
1	A	279	PRO	6.3
1	B	222	TYR	6.3
1	A	248	ILE	6.3
1	B	188	SER	6.3
1	F	241	ILE	6.3
1	A	361	PHE	6.3
1	A	172	ILE	6.2
1	B	219	ILE	6.2
1	F	209	ALA	6.1
1	F	250	LEU	6.1
1	B	357	ASN	6.1
1	F	187	SER	6.1
1	B	276	TYR	6.1
1	F	351	ARG	6.1
1	A	363	PRO	6.1
1	F	375	LEU	6.0
1	A	219	ILE	6.0
1	A	328	GLN	6.0
1	A	368	ASN	6.0
1	A	269	ILE	6.0
1	A	243	PRO	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	358	THR	5.9
1	A	283	SER	5.9
1	B	288	GLY	5.9
1	F	239	ARG	5.9
1	A	195	ILE	5.9
1	A	247	ASN	5.9
1	F	287	ASN	5.9
1	F	368	ASN	5.9
1	B	362	PHE	5.9
1	B	208	LYS	5.9
1	A	366	ARG	5.9
1	B	179	PRO	5.9
1	A	357	ASN	5.8
1	A	346	ILE	5.8
1	B	252	ASN	5.8
1	A	325	GLY	5.8
1	A	209	ALA	5.8
1	B	165	GLU	5.7
1	A	295	SER	5.7
1	F	238	SER	5.7
1	A	249	MET	5.7
1	A	201	ASP	5.7
1	F	264	LEU	5.7
1	B	240	ILE	5.7
1	F	288	GLY	5.7
1	B	340	ILE	5.7
1	F	246	ILE	5.7
1	B	250	LEU	5.7
1	B	221	TYR	5.6
1	A	187	SER	5.6
1	A	338	SER	5.6
1	B	251	THR	5.6
1	A	337	LYS	5.6
1	F	178	ILE	5.6
1	B	166	ASN	5.6
1	A	206	MET	5.6
1	F	374	PHE	5.6
1	F	227	LYS	5.6
1	B	187	SER	5.6
1	A	348	GLU	5.5
1	B	287	ASN	5.5
1	B	373	GLU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	363	PRO	5.5
1	B	235	ILE	5.5
1	B	246	ILE	5.5
1	B	347	ARG	5.5
1	A	203	PHE	5.5
1	A	251	THR	5.5
1	F	294	THR	5.5
1	F	229	GLY	5.5
1	F	279	PRO	5.5
1	A	186	ILE	5.5
1	B	245	GLY	5.4
1	A	217	LYS	5.4
1	F	236	VAL	5.4
1	A	277	GLY	5.4
1	F	313	TYR	5.4
1	A	352	VAL	5.4
1	B	234	ASP	5.4
1	B	220	GLY	5.3
1	F	251	THR	5.3
1	F	226	ASN	5.3
1	A	327	ASN	5.3
1	A	191	ALA	5.3
1	F	291	ILE	5.3
1	A	292	GLY	5.3
1	A	196	ALA	5.3
1	B	203	PHE	5.2
1	B	291	ILE	5.3
1	B	210	VAL	5.2
1	F	176	LYS	5.2
1	A	329	VAL	5.2
1	B	314	LEU	5.2
1	B	223	SER	5.2
1	B	211	LEU	5.2
1	B	349	GLY	5.2
1	F	205	HIS	5.2
1	B	341	ALA	5.2
1	B	207	GLY	5.2
1	F	268	LEU	5.1
1	C	229	GLY	5.1
1	F	237	TRP	5.1
1	A	373	GLU	5.1
1	A	310	PHE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	284	THR	5.1
1	F	242	THR	5.1
1	A	351	ARG	5.1
1	F	202	ILE	5.1
1	B	348	GLU	5.1
1	A	354	ILE	5.1
1	F	350	SER	5.1
1	F	221	TYR	5.1
1	A	202	ILE	5.0
1	B	271	ARG	5.0
1	B	264	LEU	5.0
1	F	282	LEU	5.0
1	B	224	ASN	5.0
1	B	225	ASN	5.0
1	B	353	PHE	5.0
1	A	347	ARG	5.0
1	B	248	ILE	5.0
1	A	374	PHE	5.0
1	A	332	GLN	5.0
1	A	228	MET	5.0
1	A	180	ALA	5.0
1	B	198	VAL	5.0
1	A	238	SER	4.9
1	B	370	VAL	4.9
1	B	171	THR	4.9
1	A	340	ILE	4.9
1	A	365	PRO	4.9
1	A	281	LEU	4.9
1	F	203	PHE	4.9
1	A	345	VAL	4.9
1	F	174	ALA	4.9
1	F	276	TYR	4.9
1	B	268	LEU	4.9
1	A	245	GLY	4.8
1	A	313	TYR	4.8
1	A	214	LYS	4.8
1	B	172	ILE	4.8
1	F	235	ILE	4.8
1	F	192	GLY	4.8
1	B	344	VAL	4.8
1	B	238	SER	4.8
1	F	177	MET	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	204	ALA	4.7
1	B	178	ILE	4.7
1	F	224	ASN	4.7
1	A	211	LEU	4.7
1	B	169	LEU	4.7
1	F	315	LEU	4.7
1	B	197	GLN	4.7
1	B	358	THR	4.7
1	B	371	ILE	4.7
1	F	244	HIS	4.7
1	A	349	GLY	4.7
1	A	174	ALA	4.7
1	B	199	GLU	4.7
1	A	216	SER	4.7
1	F	215	GLY	4.7
1	F	284	THR	4.6
1	F	222	TYR	4.6
1	A	372	ALA	4.6
1	A	315	LEU	4.6
1	B	215	GLY	4.6
1	F	260	GLY	4.6
1	A	273	PHE	4.6
1	F	283	SER	4.6
1	F	211	LEU	4.6
1	B	175	ASP	4.6
1	B	233	LEU	4.6
1	B	229	GLY	4.6
1	A	199	GLU	4.6
1	A	232	ARG	4.6
1	F	266	GLY	4.6
1	A	278	VAL	4.6
1	A	227	LYS	4.5
1	F	200	SER	4.5
1	A	220	GLY	4.5
1	B	216	SER	4.5
1	F	191	ALA	4.5
1	F	366	ARG	4.5
1	B	338	SER	4.5
1	F	274	GLN	4.5
1	A	194	VAL	4.5
1	A	324	MET	4.5
1	F	184	THR	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	219	ILE	4.5
1	F	167	LYS	4.5
1	B	284	THR	4.5
1	B	342	PRO	4.5
1	B	350	SER	4.4
1	A	213	PRO	4.4
1	A	167	LYS	4.4
1	A	222	TYR	4.4
1	B	194	VAL	4.4
1	B	202	ILE	4.4
1	F	240	ILE	4.4
1	F	252	ASN	4.4
1	B	372	ALA	4.4
1	F	169	LEU	4.4
1	B	237	TRP	4.4
1	A	242	THR	4.4
1	B	185	PRO	4.4
1	F	352	VAL	4.4
1	B	293	ILE	4.4
1	B	204	ALA	4.3
1	A	169	LEU	4.3
1	F	210	VAL	4.3
1	A	359	ASP	4.3
1	E	368	ASN	4.3
1	F	364	ILE	4.3
1	B	286	THR	4.3
1	F	208	LYS	4.3
1	A	175	ASP	4.3
1	F	249	MET	4.3
1	F	183	ILE	4.3
1	B	201	ASP	4.3
1	A	330	VAL	4.3
1	A	263	GLY	4.2
1	A	182	LEU	4.2
1	F	275	ARG	4.2
1	B	318	LEU	4.2
1	F	290	LEU	4.2
1	B	351	ARG	4.2
1	A	319	MET	4.2
1	A	170	ARG	4.2
1	A	218	VAL	4.2
1	A	274	GLN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	354	ILE	4.1
1	B	269	ILE	4.1
1	F	245	GLY	4.1
1	F	360	ILE	4.1
1	F	217	LYS	4.0
1	F	172	ILE	4.0
1	B	278	VAL	4.0
1	B	365	PRO	4.0
1	F	233	LEU	4.0
1	A	335	ARG	4.0
1	A	270	GLU	4.0
1	B	275	ARG	4.0
1	A	241	ILE	4.0
1	F	371	ILE	4.0
1	A	193	LYS	4.0
1	B	274	GLN	3.9
1	B	177	MET	3.9
1	B	244	HIS	3.9
1	B	247	ASN	3.9
1	F	278	VAL	3.9
1	F	197	GLN	3.9
1	A	266	GLY	3.9
1	A	166	ASN	3.9
1	F	185	PRO	3.9
1	A	188	SER	3.9
1	F	337	LYS	3.8
1	B	168	LEU	3.8
1	B	182	LEU	3.8
1	F	285	LEU	3.8
1	B	184	THR	3.8
1	A	336	ASP	3.7
1	B	333	ILE	3.7
1	B	322	SER	3.7
1	B	254	LYS	3.7
1	A	326	ILE	3.7
1	B	368	ASN	3.7
1	E	229	GLY	3.7
1	B	212	ILE	3.7
1	A	268	LEU	3.6
1	F	194	VAL	3.6
1	F	186	ILE	3.6
1	F	248	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	192	GLY	3.6
1	F	357	ASN	3.6
1	F	232	ARG	3.6
1	B	195	ILE	3.6
1	F	212	ILE	3.6
1	F	353	PHE	3.5
1	B	292	GLY	3.5
1	B	213	PRO	3.5
1	F	218	VAL	3.5
1	B	289	LEU	3.5
1	A	252	ASN	3.5
1	F	343	ILE	3.5
1	A	322	SER	3.5
1	F	193	LYS	3.5
1	F	182	LEU	3.5
1	B	317	GLN	3.5
1	B	228	MET	3.5
1	B	355	SER	3.5
1	F	359	ASP	3.5
1	B	279	PRO	3.5
1	F	267	GLU	3.5
1	F	356	PRO	3.5
1	B	359	ASP	3.5
1	A	323	GLY	3.4
1	B	316	MET	3.4
1	A	356	PRO	3.4
1	B	281	LEU	3.4
1	B	189	GLN	3.4
1	B	218	VAL	3.4
1	B	241	ILE	3.4
1	F	195	ILE	3.4
1	B	331	ASN	3.4
1	F	355	SER	3.4
1	F	331	ASN	3.3
1	B	236	VAL	3.3
1	B	296	ALA	3.3
1	F	339	LYS	3.3
1	F	281	LEU	3.3
1	A	176	LYS	3.3
1	B	192	GLY	3.3
1	B	206	MET	3.3
1	B	243	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	285	LEU	3.2
1	B	337	LYS	3.2
1	B	361	PHE	3.2
1	F	220	GLY	3.2
1	F	277	GLY	3.2
1	B	334	LEU	3.2
1	B	191	ALA	3.2
1	A	262	ASN	3.2
1	D	316	MET	3.2
1	F	293	ILE	3.2
1	F	216	SER	3.1
1	B	249	MET	3.1
1	A	339	LYS	3.1
1	C	289	LEU	3.1
1	B	330	VAL	3.1
1	B	294	THR	3.1
1	F	365	PRO	3.1
1	B	335	ARG	3.1
1	A	168	LEU	3.0
1	B	253	ALA	3.0
1	F	314	LEU	3.0
1	F	348	GLU	3.0
1	B	356	PRO	3.0
1	F	341	ALA	3.0
1	A	226	ASN	3.0
1	B	214	LYS	3.0
1	F	317	GLN	3.0
1	B	360	ILE	3.0
1	F	214	LYS	3.0
1	D	174	ALA	3.0
1	F	332	GLN	3.0
1	F	271	ARG	2.9
1	B	329	VAL	2.9
1	F	199	GLU	2.9
1	F	346	ILE	2.9
1	B	354	ILE	2.9
1	C	375	LEU	2.9
1	B	242	THR	2.9
1	F	207	GLY	2.9
1	B	232	ARG	2.9
1	F	347	ARG	2.9
1	B	167	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	376	LYS	2.9
1	F	320	ARG	2.8
1	B	174	ALA	2.8
1	C	189	GLN	2.8
1	A	272	ASN	2.8
1	F	327	ASN	2.8
1	F	344	VAL	2.8
1	B	352	VAL	2.7
1	B	226	ASN	2.7
1	F	225	ASN	2.7
1	F	261	TYR	2.7
1	F	263	GLY	2.7
1	F	370	VAL	2.7
1	F	342	PRO	2.7
1	F	369	GLU	2.7
1	F	273	PHE	2.7
1	B	193	LYS	2.7
1	D	286	THR	2.7
1	B	186	ILE	2.6
1	B	176	LYS	2.6
1	B	339	LYS	2.6
1	F	326	ILE	2.6
1	F	179	PRO	2.6
1	F	361	PHE	2.6
1	A	204	ALA	2.6
1	F	322	SER	2.6
1	B	282	LEU	2.6
1	B	263	GLY	2.5
1	B	345	VAL	2.5
1	F	329	VAL	2.5
1	B	343	ILE	2.5
1	E	340	ILE	2.5
1	F	316	MET	2.5
1	F	181	PHE	2.5
1	B	227	LYS	2.5
1	F	335	ARG	2.5
1	F	321	GLN	2.5
1	B	363	PRO	2.5
1	B	217	LYS	2.5
1	B	266	GLY	2.5
1	C	253	ALA	2.5
1	F	349	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	372	ALA	2.4
1	E	295	SER	2.4
1	B	270	GLU	2.4
1	F	312	ASP	2.4
1	F	280	LEU	2.4
1	F	198	VAL	2.4
1	E	186	ILE	2.4
1	A	334	LEU	2.4
1	D	274	GLN	2.4
1	F	171	THR	2.3
1	E	348	GLU	2.3
1	C	194	VAL	2.3
1	D	229	GLY	2.3
1	C	228	MET	2.3
1	B	323	GLY	2.3
1	A	316	MET	2.3
1	F	269	ILE	2.3
1	F	188	SER	2.3
1	B	280	LEU	2.3
1	B	283	SER	2.3
1	B	170	ARG	2.3
1	B	320	ARG	2.3
1	B	295	SER	2.2
1	E	274	GLN	2.2
1	E	312	ASP	2.2
1	F	168	LEU	2.2
1	E	246	ILE	2.2
1	A	331	ASN	2.2
1	F	213	PRO	2.2
1	F	345	VAL	2.2
1	B	272	ASN	2.2
1	F	336	ASP	2.2
1	D	350	SER	2.1
1	D	335	ARG	2.1
1	F	373	GLU	2.1
1	B	315	LEU	2.1
1	C	175	ASP	2.1
1	C	352	VAL	2.1
1	F	333	ILE	2.1
1	D	173	THR	2.1
1	B	267	GLU	2.1
1	F	330	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	292	GLY	2.1
1	D	230	GLU	2.1
1	C	226	ASN	2.0
1	B	196	ALA	2.0
1	E	209	ALA	2.0
1	C	179	PRO	2.0
1	A	265	VAL	2.0
1	F	340	ILE	2.0
1	C	251	THR	2.0
1	D	358	THR	2.0
1	B	367	GLU	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.